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SUPPORTING INFORMATION FOR

The regioselectivity of the sulfonylation of tetrazoles: a theoretical view

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Part 1: Computational details

The theoretical calculations were performed with the Gaussian 09[1] program. The stationary structures were optimized at the M06-2X[2]/6-31+G (d, p) level. The solvent effect was considered by the SMD model[3] with the solvent chloroform (eps=4.81). All the optimized stationary points had been identified as minima (zero imaginary frequencies) and transition states (one imaginary frequency), via the vibrational analysis at same level with the temperature T = 243.15 K. The CYLView[4] software was applied to render the picture of the optimized structures. Independent gradient model (IGM)[5] analysis was performed using Multiwfn[6] and VMD.[7]

Part 2: The relative Gibbs free energy profiles for the release of dinitrogen from 2,5-disubstituted tetrazole.

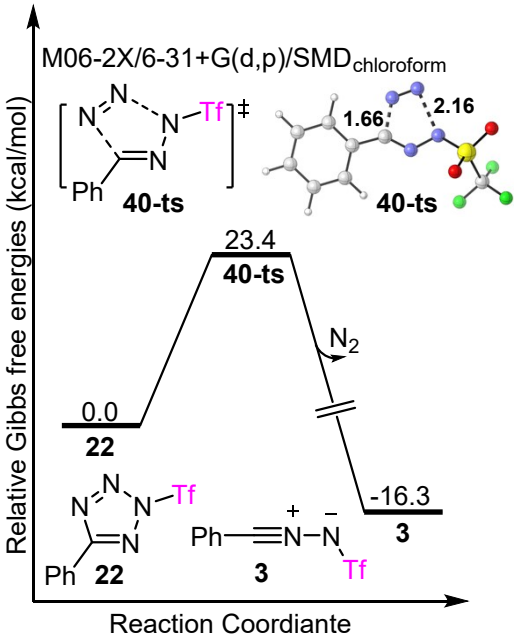
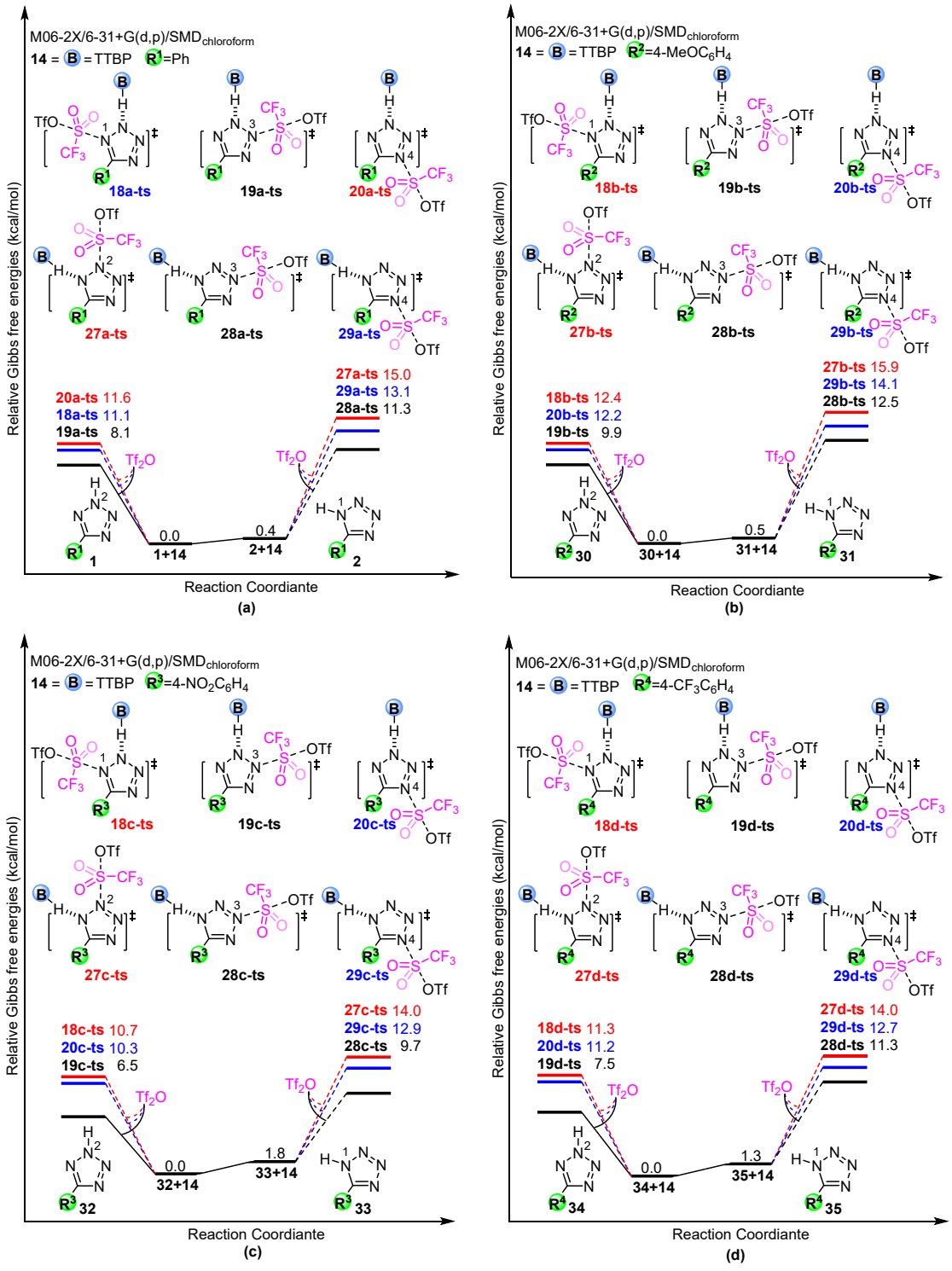


Figure S1. The relative Gibbs free energy profiles for the release of dinitrogen from 2,5-disubstituted tetrazole.

When the stable 2,5-disubstituted tetrazole is formed, it can be further denitrogenated to form the dipolar nitrile imine. Therefore, we further calculated the free energy distribution of the release of gaseous dinitrogen from 2,5-disubstituted tetrazoles **22**. The relative free energy of 2,5-disubstituted tetrazoles **22** was set to zero. As shown in Figure S1, synergistic nitrogen release process of 2,5-disubstituted tetrazoles **22** could occur via transition state **40-ts** with an energy barrier of 23.4 kcal/mol to yield the 1,3-dipolar nitrile imine product **3**. This process was calculated to be exothermic, by 16.3 kcal/mol. It suggests that the release of gaseous dinitrogen could easily occur under the reaction conditions.

Part 3: The possible structures and the related corresponding free energy in the reaction.



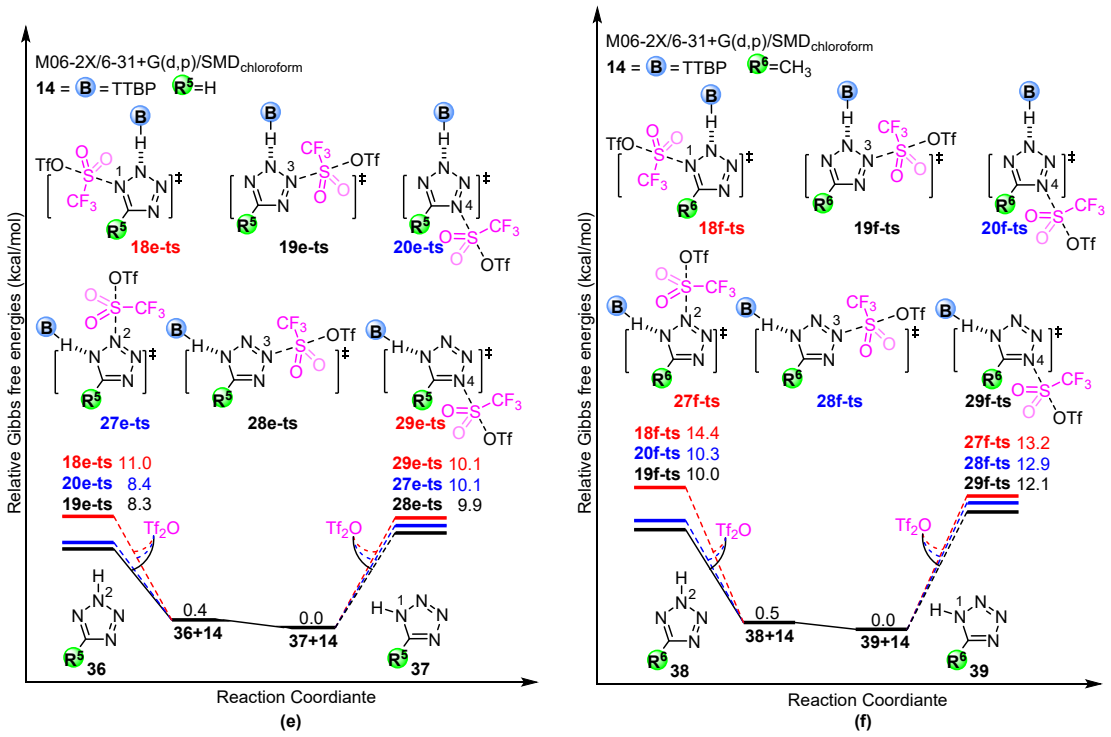


Figure S2. The possible structures and the related corresponding free energy in the reaction. (a) : R^1=Ph; (b) : R^2=4-$MeOC_6H_4$; (c) : R^3=4-$NO_2C_6H_4$; (d) : R^4=4-$CF_3C_6H_4$; (e) : R^5=H; (f) : R^6=CH_3.

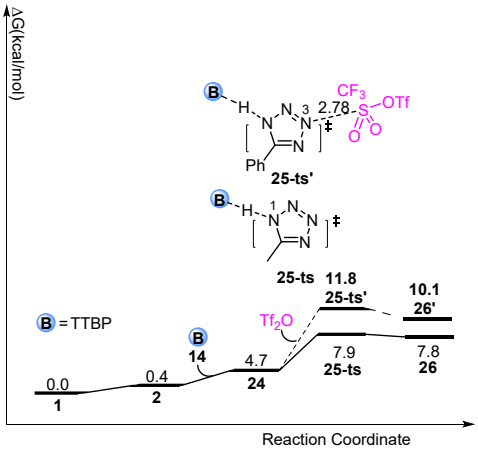


Fig. S3 Free-energy profiles for the sulfonylation of 1*H*-tetrazole at M06-2X/6-31+G(d, p)/SMDchloroform (unit of length: Å)

Part 4: List of the Cartesian coordinates for all the optimized compounds and transition states

1

Zero-point correction= 0.130330
Thermal correction to Energy= 0.135729
Thermal correction to Enthalpy= 0.136499
Thermal correction to Gibbs Free Energy= 0.104289
Sum of electronic and zero-point Energies= -489.032115
Sum of electronic and thermal Energies= -489.026716
Sum of electronic and thermal Enthalpies= -489.025946
Sum of electronic and thermal Free Energies= -489.058156

Cartesian coordinates

C	-1.036515	-0.000939	0.000610
N	-1.795220	-1.123487	0.073070
N	-3.036575	-0.731644	0.046550
N	-3.000012	0.573806	-0.036898
N	-1.791250	1.089540	-0.071567
C	0.433007	0.003930	0.000955
C	1.131855	1.215178	0.036061
C	1.132884	-1.206188	-0.034112
C	2.523732	1.212999	0.034946
H	0.583606	2.151899	0.068285
C	2.525424	-1.201417	-0.036522
H	0.584631	-2.142641	-0.063984
C	3.222936	0.005968	-0.001776
H	3.063197	2.154700	0.065105
H	3.066038	-2.142412	-0.067303
H	4.308804	0.006837	-0.003092
H	-3.844819	1.136909	-0.078069

Vibrational frequencies

58.1972	112.3920	158.0236
301.2429	353.0470	411.1766
457.9669	512.1765	625.3558
664.8549	704.7763	712.3135
742.8114	760.4265	818.4365
874.7988	963.1378	1010.8137
1012.4658	1029.2823	1031.4399
1062.1873	1073.0692	1112.6984
1155.2436	1171.6357	1194.6715

1212.9465	1257.7381	1320.2865
1345.8701	1362.6281	1404.0626
1494.6430	1498.3021	1555.8645
1597.4529	1675.8399	1698.1640
3203.0443	3211.5927	3217.6577
3224.3830	3228.7217	3614.5613

2

Zero-point correction= 0.130226
Thermal correction to Energy= 0.135614
Thermal correction to Enthalpy= 0.136384
Thermal correction to Gibbs Free Energy= 0.104198
Sum of electronic and zero-point Energies= -489.031536
Sum of electronic and thermal Energies= -489.026148
Sum of electronic and thermal Enthalpies= -489.025378
Sum of electronic and thermal Free Energies= -489.057564

Cartesian coordinates

C	-1.041528	-0.044861	-0.002448
N	-1.801499	-1.126395	-0.062244
H	-1.672686	2.004599	0.117343
N	-3.076265	-0.699503	-0.038468
N	-3.134511	0.581781	0.031593
N	-1.870740	1.012147	0.055753
C	0.425008	-0.007177	-0.000086
C	1.121364	1.205813	-0.032070
C	1.127925	-1.216882	0.031617
C	2.513420	1.206418	-0.031783
H	0.590349	2.153220	-0.063028
C	2.519030	-1.208687	0.031916
H	0.578550	-2.152491	0.058503
C	3.213734	0.000901	-0.000039
H	3.050152	2.149398	-0.059425
H	3.061569	-2.148435	0.058152
H	4.299456	0.004355	-0.000632

Vibrational frequencies

53.2080	119.8479	175.6692
302.0271	357.4048	407.7902
451.6417	504.3073	625.6443
649.7027	703.5004	706.8964
734.8916	754.4730	799.9675
867.7991	956.9137	1010.0918
1013.1778	1034.0561	1035.1820

1056.6704	1070.6801	1119.3334
1135.9045	1166.1670	1175.2684
1214.9902	1220.2680	1336.7170
1347.1940	1375.2838	1433.9151
1450.1435	1518.2422	1539.5831
1635.2239	1676.3610	1700.8004
3206.0338	3212.3558	3219.7078
3226.9499	3232.2148	3628.3493

3

Zero-point correction= 0.131409
Thermal correction to Energy= 0.141327
Thermal correction to Enthalpy= 0.142097
Thermal correction to Gibbs Free Energy= 0.098009
Sum of electronic and zero-point Energies= -1264.928667
Sum of electronic and thermal Energies= -1264.918749
Sum of electronic and thermal Enthalpies= -1264.917979
Sum of electronic and thermal Free Energies= -1264.962067

Cartesian coordinates

C	1.237876	-0.356378	-0.544828
N	0.129858	-0.590301	-0.765918
N	-1.077377	-0.897776	-1.147050
C	2.609551	-0.104447	-0.247017
C	3.108933	1.206270	-0.311486
C	3.433807	-1.184459	0.104713
C	4.448911	1.429662	-0.019512
H	2.451074	2.026778	-0.584021
C	4.770622	-0.943552	0.393225
H	3.023257	-2.189646	0.149501
C	5.275791	0.360475	0.331579
H	4.848266	2.438953	-0.062650
H	5.421411	-1.768923	0.666571
H	6.319845	0.542113	0.560123
S	-2.140166	-0.859991	0.103289
O	-3.314063	-1.607519	-0.304436
O	-1.511894	-1.053051	1.401017
C	-2.683599	0.914200	0.117918
F	-3.527301	1.127663	1.120130
F	-3.280408	1.227869	-1.027910
F	-1.613654	1.697918	0.273161

Vibrational frequencies

22.5651	40.6089	44.0875

62.1211	78.0425	132.7862
187.5445	200.7557	278.1690
289.8077	310.1161	329.7547
372.5543	404.8688	409.7264
424.5028	478.8772	531.4579
543.5264	554.1141	557.0723
576.8581	624.6595	627.3296
693.8495	745.1807	774.3764
779.2726	821.3033	877.2110
973.3724	1013.6436	1020.0711
1042.4542	1052.6020	1098.0081
1115.2713	1142.2310	1176.1633
1197.8242	1229.4937	1249.8623
1265.4642	1330.3750	1334.6941
1359.1643	1372.7152	1488.6576
1534.1199	1650.3737	1677.6968
2470.2661	3208.6092	3212.3483
3221.8729	3224.2184	3247.0597

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Zero-point correction= 0.426580
Thermal correction to Energy= 0.441051
Thermal correction to Enthalpy= 0.441821
Thermal correction to Gibbs Free Energy= 0.389136
Sum of electronic and zero-point Energies= -719.350275
Sum of electronic and thermal Energies= -719.335804
Sum of electronic and thermal Enthalpies= -719.335034
Sum of electronic and thermal Free Energies= -719.387719

Cartesian coordinates

C	-0.727955	-1.123423	-0.007692
C	-0.563314	1.184580	0.000664
C	0.829792	1.120283	0.001966
C	1.474919	-0.122388	-0.002925
C	0.666022	-1.259520	-0.008783
H	1.413123	2.033729	0.006606
H	1.107270	-2.247176	-0.013599
N	-1.316792	0.075310	-0.002477
C	-1.680431	-2.321790	-0.001330
C	-0.940335	-3.661081	-0.051440
C	-2.520246	-2.264786	1.284530
C	-2.612070	-2.220925	-1.218948
H	-0.333436	-3.758400	-0.958531
H	-0.288591	-3.800834	0.818031

H	-1.671030	-4.476716	-0.051357
H	-3.078994	-1.326409	1.340244
H	-3.233574	-3.096713	1.304090
H	-1.883306	-2.339432	2.173138
H	-3.321674	-3.055876	-1.216982
H	-3.176887	-1.285140	-1.199358
H	-2.042370	-2.259066	-2.154413
C	-1.339458	2.503185	-0.000171
C	-2.219072	2.553481	-1.259678
C	-2.237668	2.546703	1.246384
C	-0.415147	3.724009	0.009710
H	-1.607398	2.520601	-2.168606
H	-2.912740	1.708316	-1.282591
H	-2.801596	3.481605	-1.273532
H	-1.639531	2.502902	2.163846
H	-2.815634	3.477750	1.259630
H	-2.935949	1.705149	1.251368
H	-1.020489	4.636502	0.008494
H	0.219125	3.748380	0.902938
H	0.230324	3.753844	-0.875266
C	3.003664	-0.187586	-0.000348
C	3.542853	0.537405	-1.245294
C	3.535086	0.508355	1.264455
C	3.522679	-1.628659	-0.015902
H	3.163162	0.075160	-2.163003
H	3.258244	1.594088	-1.254029
H	4.637286	0.484698	-1.262481
H	3.152839	0.022523	2.168793
H	4.629630	0.459201	1.285288
H	3.245936	1.563397	1.297139
H	4.617556	-1.618367	-0.015192
H	3.194792	-2.188978	0.866325
H	3.195533	-2.168974	-0.910853

Vibrational frequencies

7.5332	20.8765	29.3601
73.7964	122.8945	132.5703
134.6403	144.1266	198.6606
207.3794	211.2265	246.9764
251.8579	255.5797	260.9353
274.9008	292.4492	293.3765
312.4582	319.0269	335.9065
340.3665	342.1146	349.5362
360.1315	371.9825	375.2309

388.2165	391.6672	423.7376
456.1975	459.5571	538.8686
550.1980	569.5455	580.7068
685.8519	704.2654	782.6072
797.7757	798.7361	848.2169
899.7416	922.3564	930.6162
935.6601	947.0324	947.6078
950.5823	951.9426	954.1961
956.2868	957.1985	961.8042
965.8416	1022.5201	1041.1073
1042.4305	1045.6567	1046.7954
1048.7759	1051.2307	1167.7776
1181.3311	1207.3864	1240.3942
1241.8530	1243.6397	1243.7381
1255.5623	1270.4502	1283.9988
1293.6370	1306.4780	1372.2976
1386.9310	1390.7272	1392.8981
1395.8664	1397.9084	1398.1889
1416.8514	1421.8708	1423.4383
1463.2054	1468.7953	1474.5772
1475.3795	1475.8985	1477.0415
1478.1699	1480.4688	1482.7153
1483.4781	1487.4450	1491.6190
1495.0294	1496.1478	1498.8980
1500.3612	1500.7600	1510.7243
1512.2898	1515.0965	1644.6563
1675.1222	3047.3444	3048.8490
3050.3800	3052.2495	3052.9155
3053.0774	3053.7690	3058.6925
3058.9502	3123.4676	3124.5006
3125.7372	3127.3565	3127.5936
3127.9652	3128.6347	3129.7796
3133.3481	3134.7922	3136.6454
3137.0180	3143.4515	3144.7677
3145.0206	3146.4855	3147.8209
3148.7060	3246.9752	3248.0763

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Zero-point correction= 0.559853
Thermal correction to Energy= 0.580547
Thermal correction to Enthalpy= 0.581317
Thermal correction to Gibbs Free Energy= 0.514300
Sum of electronic and zero-point Energies= -1208.391904
Sum of electronic and thermal Energies= -1208.371209

Sum of electronic and thermal Enthalpies= -1208.370439
Sum of electronic and thermal Free Energies= -1208.437456

Cartesian coordinates

C	-3.691684	-0.005446	-0.437104
N	-3.502371	-0.037882	-1.777511
N	-2.210446	-0.014159	-1.963256
N	-1.665741	0.034416	-0.775270
N	-2.533441	0.042745	0.213207
C	-5.010502	-0.013669	0.212357
C	-5.109417	-0.015902	1.607575
C	-6.170725	-0.017184	-0.569258
C	-6.362120	-0.020355	2.214751
H	-4.206098	-0.014624	2.210173
C	-7.420875	-0.021682	0.043951
H	-6.086285	-0.014831	-1.651698
C	-7.519954	-0.023027	1.435374
H	-6.434670	-0.022045	3.298075
H	-8.319021	-0.023403	-0.566053
H	-8.496059	-0.026211	1.911310
C	1.884469	1.185853	-0.155155
C	1.875699	-1.139567	-0.161851
C	3.230400	-1.170047	0.160251
C	3.948124	0.015743	0.336253
C	3.246251	1.205913	0.166008
H	3.733917	-2.121573	0.273864
H	3.750332	2.154571	0.280619
N	1.214375	0.029334	-0.306531
C	1.097236	2.485717	-0.352357
C	0.487644	2.500353	-1.764677
C	0.006072	2.585941	0.727565
C	1.985482	3.729723	-0.225941
H	-0.159264	1.644523	-1.963649
H	-0.108584	3.409231	-1.900304
H	1.280444	2.496900	-2.521238
H	0.461007	2.679061	1.720113
H	-0.609997	3.474368	0.550309
H	-0.654514	1.717850	0.749404
H	1.370548	4.620250	-0.392409
H	2.430762	3.819066	0.770406
H	2.788547	3.737185	-0.970727
C	1.076825	-2.428903	-0.373628
C	-0.021121	-2.528369	0.699420
C	0.477541	-2.423799	-1.790245

C	1.952530	-3.682170	-0.253188
H	0.428045	-2.642805	1.692368
H	-0.667653	-1.650320	0.731738
H	-0.650275	-3.404220	0.506362
H	1.276560	-2.432337	-2.540263
H	-0.136511	-3.319162	-1.936315
H	-0.148890	-1.553166	-1.989226
H	1.330185	-4.565386	-0.430817
H	2.759292	-3.690517	-0.994011
H	2.391636	-3.783960	0.744752
C	5.434866	-0.035927	0.686554
C	5.611436	-0.787980	2.017077
C	6.183923	-0.789399	-0.426487
C	6.043765	1.361921	0.828926
H	5.077734	-0.281612	2.828558
H	5.238799	-1.815013	1.952745
H	6.674079	-0.829653	2.280661
H	6.057393	-0.289065	-1.392596
H	7.254422	-0.823959	-0.196097
H	5.827624	-1.819424	-0.526664
H	7.104951	1.269971	1.081717
H	5.971369	1.932506	-0.103139
H	5.560062	1.935852	1.626663
H	-0.621718	0.044341	-0.626151

Vibrational frequencies

14.7867	19.2752	34.8264
35.5655	42.9745	53.6931
67.0144	76.8602	87.5930
101.9197	114.1998	134.6153
137.0586	140.5806	148.5591
160.0724	191.3735	196.4662
204.1778	242.7377	250.2984
254.8238	259.1695	272.0333
290.0565	298.9759	311.7331
312.7839	320.1783	329.9357
349.9140	353.0923	357.6367
369.2928	370.9134	376.2303
384.2050	391.3981	397.2652
409.9767	417.3134	432.1942
463.2539	465.4688	467.7572
521.4422	547.1204	555.5135
571.0989	581.4797	626.9192
682.7539	703.0346	704.2497

714.0323	722.2663	759.1875
785.6184	795.4473	803.8171
823.0209	847.7120	881.6525
916.2606	926.7716	927.1948
932.9383	948.6710	949.6618
950.6226	951.3760	953.9213
956.9252	958.3530	958.8974
962.5704	965.2371	1010.1089
1017.9768	1026.0500	1028.5721
1032.3938	1041.6988	1042.6362
1044.1567	1045.0279	1048.4943
1050.5778	1057.2319	1067.8766
1111.1572	1114.0572	1162.4912
1172.8824	1177.6810	1195.3365
1197.9158	1219.0122	1231.6233
1240.4790	1241.5683	1242.8881
1243.6537	1252.2512	1265.8288
1275.9297	1290.1084	1294.5917
1305.3971	1315.8177	1335.5936
1364.2496	1370.1619	1395.3145
1397.8296	1398.5952	1399.2469
1399.9676	1401.1928	1419.8763
1425.3296	1427.0517	1428.8893
1469.0222	1472.5810	1473.6621
1478.2464	1479.1765	1481.1667
1483.3808	1485.2844	1487.0432
1487.2402	1489.8704	1496.9992
1498.1606	1500.1781	1500.4604
1501.1638	1502.3332	1503.9034
1512.7999	1513.9991	1518.1745
1520.1206	1588.7654	1617.7020
1638.0542	1673.9159	1683.1800
1701.6334	2894.6279	3054.3114
3055.4913	3055.9220	3057.3030
3061.6039	3061.8768	3062.9144
3067.4455	3069.6071	3129.4760
3130.3780	3133.0695	3133.5911
3134.2973	3135.7684	3136.5155
3136.7464	3137.5598	3139.9447
3140.0099	3140.8164	3141.0618
3145.4788	3181.1876	3186.4279
3191.0217	3195.9295	3201.3564
3217.3012	3220.3281	3235.7963
3238.1925	3257.7472	3284.7844

16-ts

Zero-point correction= 0.555723
Thermal correction to Energy= 0.576110
Thermal correction to Enthalpy= 0.576880
Thermal correction to Gibbs Free Energy= 0.510957
Sum of electronic and zero-point Energies= -1208.391442
Sum of electronic and thermal Energies= -1208.371055
Sum of electronic and thermal Enthalpies= -1208.370285
Sum of electronic and thermal Free Energies= -1208.436208

Cartesian coordinates

C	3.517344	-0.003029	-0.430185
N	3.335056	-0.004686	-1.765536
H	0.180672	0.018811	-0.572524
N	2.032378	0.006943	-1.944071
N	1.462585	0.015764	-0.765730
N	2.350793	0.010498	0.213803
C	4.833408	-0.011669	0.227261
C	4.928164	-0.024410	1.623146
C	6.000470	-0.007055	-0.545153
C	6.177612	-0.031598	2.237872
H	4.021350	-0.028689	2.220418
C	7.247662	-0.014286	0.074282
H	5.921461	0.002934	-1.627995
C	7.340570	-0.026582	1.466255
H	6.243522	-0.041537	3.321800
H	8.148917	-0.010314	-0.531467
H	8.314076	-0.032329	1.947628
C	-1.771717	-1.159499	-0.179878
C	-1.764924	1.196222	-0.172181
C	-3.116517	1.210200	0.173010
C	-3.820657	0.024394	0.359596
C	-3.116810	-1.166508	0.166777
H	-3.615296	2.159777	0.293584
H	-3.626471	-2.112768	0.287047
N	-1.113131	0.020116	-0.328440
C	-1.005826	-2.463037	-0.417047
C	-0.436761	-2.464788	-1.846976
C	0.101364	-2.614133	0.641451
C	-1.920186	-3.689640	-0.293466
H	0.224834	-1.623132	-2.052176
H	0.135680	-3.384427	-2.007934
H	-1.252240	-2.439977	-2.578558

H	-0.340573	-2.701729	1.640280
H	0.671141	-3.527813	0.440696
H	0.802556	-1.780404	0.655745
H	-1.324334	-4.585251	-0.494816
H	-2.340194	-3.793669	0.712233
H	-2.740149	-3.667529	-1.019008
C	-0.994149	2.500272	-0.393523
C	0.109336	2.635432	0.671088
C	-0.418897	2.515467	-1.820951
C	-1.903607	3.729651	-0.260371
H	-0.335854	2.708848	1.669649
H	0.810456	1.801477	0.675465
H	0.679453	3.552092	0.485509
H	-1.231125	2.498108	-2.556336
H	0.154299	3.436621	-1.970030
H	0.243340	1.675617	-2.031295
H	-1.302628	4.624312	-0.450428
H	-2.721367	3.719176	-0.988599
H	-2.326518	3.825676	0.744884
C	-5.298684	-0.015283	0.739483
C	-5.893362	1.387393	0.891623
C	-6.072774	-0.766240	-0.358311
C	-5.450108	-0.764564	2.074789
H	-5.389219	1.959177	1.678177
H	-5.838087	1.955561	-0.043038
H	-6.949100	1.302531	1.167552
H	-5.731211	-1.801189	-0.457943
H	-7.139099	-0.786005	-0.108988
H	-5.956841	-0.272246	-1.328912
H	-6.507639	-0.800364	2.357961
H	-5.084202	-1.793507	2.005010
H	-4.899077	-0.258540	2.874661

Vibrational frequencies

-921.3557	15.5121	17.7526
32.2398	40.3572	49.5931
55.9691	73.5296	94.9362
116.0728	121.8490	128.9925
134.0485	147.6997	153.1165
158.3546	168.4974	180.0427
185.0716	208.0702	236.8417
242.7301	254.2969	257.3208
265.9702	291.1609	302.2693
313.6089	314.5513	323.0744

335.8675	350.8927	361.5080
366.5731	373.7463	376.2530
385.1328	392.8648	397.6033
399.1194	414.6607	418.2451
432.6553	465.2789	468.2484
482.7226	525.0661	557.4109
566.6312	578.8496	580.7926
627.4386	686.0566	700.6601
705.7094	714.5767	751.1742
758.0618	793.2090	795.1117
803.0535	819.2019	849.5732
881.3849	921.2443	926.2972
932.6425	939.3603	950.6379
952.2640	952.8364	958.1742
958.6976	959.2742	960.0659
963.2546	964.3881	968.7429
1012.2813	1016.8096	1029.7460
1033.8410	1042.4476	1045.6853
1048.7565	1049.5418	1052.6350
1053.4789	1066.0650	1066.7234
1109.0159	1118.4144	1171.5760
1175.5103	1185.0878	1197.3847
1202.2664	1211.1852	1239.8154
1241.9076	1242.6703	1243.2113
1252.4558	1253.8106	1261.6154
1263.5268	1283.4945	1294.1292
1310.7108	1326.1462	1339.3828
1363.1665	1370.9688	1397.0201
1398.6014	1399.3390	1399.7554
1407.2623	1407.9234	1426.0635
1430.2340	1432.2221	1436.1686
1462.1503	1476.3415	1478.2912
1478.6156	1480.0219	1481.4842
1483.9671	1485.7561	1486.3870
1487.6025	1493.5721	1497.3233
1498.1042	1498.6009	1499.5556
1502.0496	1504.4540	1508.9298
1512.8255	1514.6005	1516.3421
1520.4459	1572.9841	1581.5753
1593.8552	1666.5821	1671.1332
1692.1306	1701.0209	3056.2254
3057.7956	3057.9628	3060.4133
3062.6760	3063.0063	3064.9256
3067.3419	3068.8168	3131.4554

3131.6987	3134.0685	3135.3835
3136.6568	3138.6422	3139.3706
3139.6761	3141.4672	3142.0769
3142.8622	3143.1025	3144.9084
3146.1950	3193.1494	3194.2390
3199.1583	3200.5525	3201.6258
3214.5771	3218.7701	3233.1433
3236.0100	3270.6451	3301.9458

17

Zero-point correction= 0.560554
Thermal correction to Energy= 0.581082
Thermal correction to Enthalpy= 0.581852
Thermal correction to Gibbs Free Energy= 0.515844
Sum of electronic and zero-point Energies= -1208.391854
Sum of electronic and thermal Energies= -1208.371326
Sum of electronic and thermal Enthalpies= -1208.370556
Sum of electronic and thermal Free Energies= -1208.436565

Cartesian coordinates

C	-3.681286	0.003752	-0.461756
N	-3.499656	-0.030555	-1.790654
H	0.215456	0.050691	-0.494741
N	-2.185237	0.012246	-1.959981
N	-1.602592	0.072327	-0.787937
N	-2.511085	0.070709	0.182078
C	-4.996801	-0.015317	0.198006
C	-5.092511	-0.018047	1.594539
C	-6.168184	-0.026880	-0.569080
C	-6.340661	-0.030764	2.212590
H	-4.184126	-0.009917	2.189313
C	-7.414448	-0.039559	0.052350
H	-6.090996	-0.023789	-1.652137
C	-7.506048	-0.041287	1.444687
H	-6.403667	-0.032604	3.296969
H	-8.316682	-0.047046	-0.552283
H	-8.478578	-0.050867	1.928135
C	1.891202	1.221285	-0.134850
C	1.866133	-1.169190	-0.150213
C	3.214368	-1.184431	0.162685
C	3.933860	0.003763	0.337705
C	3.245614	1.206546	0.177279
H	3.714121	-2.137652	0.270201
H	3.757774	2.149926	0.293118

N	1.250882	0.036418	-0.277482
C	1.090450	2.501725	-0.335663
C	0.494480	2.503308	-1.755639
C	-0.015120	2.581464	0.732822
C	1.982633	3.739381	-0.193026
H	-0.177033	1.661234	-1.934826
H	-0.083604	3.422094	-1.896858
H	1.291889	2.482533	-2.506537
H	0.422950	2.621965	1.736148
H	-0.593084	3.498038	0.576081
H	-0.709742	1.740383	0.688443
H	1.366476	4.628217	-0.357754
H	2.418861	3.820444	0.807949
H	2.789244	3.752168	-0.933625
C	1.037720	-2.427524	-0.374109
C	-0.075227	-2.501206	0.686758
C	0.451549	-2.392914	-1.797409
C	1.902253	-3.686262	-0.247141
H	0.356540	-2.575788	1.690844
H	-0.746329	-1.640667	0.659013
H	-0.677631	-3.397472	0.506514
H	1.254683	-2.385761	-2.542500
H	-0.153062	-3.291728	-1.955523
H	-0.193320	-1.529133	-1.970724
H	1.268149	-4.558859	-0.429587
H	2.711920	-3.703922	-0.984349
H	2.331829	-3.792450	0.754462
C	5.419701	-0.058701	0.677853
C	5.594246	-0.825684	2.000980
C	6.151032	-0.809107	-0.450152
C	6.037490	1.333906	0.828617
H	5.067173	-0.324847	2.819798
H	5.220457	-1.851421	1.928575
H	6.658013	-0.871242	2.256826
H	6.021179	-0.299740	-1.410779
H	7.222060	-0.849784	-0.226122
H	5.789753	-1.836736	-0.554660
H	7.098299	1.229949	1.075729
H	5.967407	1.912300	-0.098620
H	5.562775	1.903938	1.634331

Vibrational frequencies

18.7718	24.3487	35.4290
41.1513	44.9500	59.7327

73.9493	81.0046	97.2639
110.6176	121.8078	133.3028
138.8853	145.4718	153.8225
162.1929	180.8227	188.1607
201.5396	251.0356	254.7387
260.9594	269.4849	279.7592
293.6406	305.2799	309.6735
311.9701	320.5751	334.8050
353.3600	357.4407	361.3864
365.8610	369.0058	378.0571
385.0482	389.8111	393.9558
403.7860	419.2854	423.6342
461.3455	466.0411	468.4007
526.4103	540.8173	554.4404
570.6310	571.8404	627.8444
686.4367	694.9786	704.6430
715.3246	757.6370	767.6734
783.8416	791.5143	794.4674
822.5535	848.1465	881.3391
918.0904	925.0072	928.4157
940.9062	951.3134	952.4426
953.6695	956.9178	960.2573
960.9697	962.0137	967.4718
968.1910	969.6786	1013.3282
1015.7279	1018.1310	1027.0540
1036.9466	1046.4070	1047.4906
1050.9806	1051.2832	1054.1246
1055.4030	1066.8594	1086.8301
1110.6611	1118.2665	1170.3596
1170.9865	1181.2722	1196.2467
1196.4510	1210.8295	1225.6746
1238.3571	1239.4515	1241.8838
1243.2572	1249.3220	1257.1169
1266.2204	1292.4607	1296.4575
1305.0037	1319.7074	1324.3524
1362.1470	1370.1036	1395.8183
1399.4351	1400.4651	1402.4228
1405.7312	1407.7774	1426.6633
1430.1778	1434.4586	1440.5465
1456.8223	1474.9309	1478.9340
1479.9742	1480.8544	1481.6914
1482.1538	1485.4517	1486.2570
1488.9788	1496.4966	1498.2954
1499.5990	1500.8695	1502.6300

1505.0861	1506.3466	1511.8164
1513.9184	1515.0345	1516.4930
1520.6603	1575.7906	1589.6654
1668.9112	1699.2638	1700.4334
1713.6318	2823.9471	3057.4251
3059.4949	3060.3968	3060.7060
3062.4226	3063.4717	3065.5039
3066.9108	3068.3198	3137.0720
3137.3542	3138.1181	3139.0630
3140.5822	3141.0736	3141.8733
3142.0368	3142.3236	3142.7754
3145.5847	3146.9636	3148.2842
3150.6507	3175.9820	3179.8956
3181.0433	3185.5366	3196.7055
3211.4803	3216.9890	3230.6008
3234.2640	3275.2499	3295.5422

18a-ts

Zero-point correction= 0.616536
Thermal correction to Energy= 0.647979
Thermal correction to Enthalpy= 0.648749
Thermal correction to Gibbs Free Energy= 0.557252
Sum of electronic and zero-point Energies= -3055.543179
Sum of electronic and thermal Energies= -3055.511736
Sum of electronic and thermal Enthalpies= -3055.510966
Sum of electronic and thermal Free Energies= -3055.602462

Cartesian coordinates

C	2.373363	-2.636013	-0.429293
N	1.450425	-1.715933	-0.083944
H	-1.675952	-1.818406	-0.202491
N	0.290036	-2.371628	-0.029967
N	0.493061	-3.620226	-0.315986
N	1.782198	-3.825640	-0.567981
C	3.825653	-2.460621	-0.620150
C	4.671429	-3.520108	-0.268800
C	4.372153	-1.296153	-1.169123
C	6.047017	-3.410397	-0.454497
H	4.243279	-4.424553	0.152291
C	5.749202	-1.189971	-1.350747
H	3.721532	-0.476678	-1.452189
C	6.589895	-2.244178	-0.994078
H	6.694441	-4.235875	-0.174333
H	6.163955	-0.280646	-1.775083

C	-2.981053	-0.757360	-1.385660
C	-3.297877	-1.266680	0.934537
C	-4.430615	-0.472494	0.952411
C	-4.845228	0.229139	-0.186902
C	-4.115715	0.044507	-1.362282
H	-5.002860	-0.406708	1.868095
H	-4.427838	0.519938	-2.280100
N	-2.590210	-1.332596	-0.223907
C	-2.196031	-1.067035	-2.657752
C	-2.036222	-2.593258	-2.784604
C	-2.945033	-0.552520	-3.892525
C	-0.812215	-0.400151	-2.612702
H	-3.011136	-3.091684	-2.813295
H	-1.509156	-2.818854	-3.716739
H	-1.447646	-3.023382	-1.968566
H	-3.019771	0.539673	-3.904615
H	-2.385906	-0.852864	-4.783150
H	-3.951684	-0.976611	-3.969551
H	-0.314656	-0.553334	-3.575926
H	-0.892349	0.677047	-2.433773
H	-0.183804	-0.842036	-1.840161
C	-2.833161	-2.108170	2.118273
C	-3.891790	-2.115355	3.226000
C	-2.609297	-3.555984	1.643433
C	-1.527035	-1.534129	2.688525
H	-4.034058	-1.122330	3.664383
H	-4.857770	-2.489459	2.870915
H	-3.548702	-2.779170	4.024745
H	-1.799011	-3.640224	0.913186
H	-2.331349	-4.172215	2.504014
H	-3.522812	-3.972623	1.205156
H	-1.228984	-2.128819	3.558595
H	-0.726451	-1.578835	1.951715
H	-1.657777	-0.494488	3.006998
C	-6.081004	1.121316	-0.116696
C	-7.293446	0.262417	0.286344
C	-5.843108	2.207493	0.948308
C	-6.380981	1.799943	-1.456158
H	-7.471678	-0.533619	-0.444300
H	-7.160208	-0.197208	1.270130
H	-8.187341	0.893216	0.329806
H	-4.971423	2.820833	0.698279
H	-6.719196	2.862267	1.000490
H	-5.686108	1.776396	1.941574

H	-7.266209	2.433268	-1.345179
H	-5.553549	2.438853	-1.782863
H	-6.592686	1.069924	-2.244772
O	1.096164	2.258870	0.846912
S	2.252996	3.320403	0.767285
S	1.206329	0.513811	0.263020
C	1.710644	4.254700	-0.735751
C	2.232042	0.038437	1.814300
F	1.696207	3.462959	-1.796415
F	2.562506	5.253413	-0.939852
F	0.494468	4.748222	-0.537968
F	2.416794	1.075783	2.607393
F	3.393465	-0.418839	1.408599
F	1.552160	-0.879927	2.467897
O	3.524288	2.702412	0.458566
O	2.112327	4.241823	1.870828
O	1.915975	0.753764	-0.967099
O	-0.201982	0.282221	0.448019
H	7.662998	-2.157516	-1.136846

Vibrational frequencies

-101.3789	4.3185	17.3610
23.6125	30.3148	35.4525
41.4804	44.9337	49.9622
54.4462	55.7215	61.2783
63.8029	68.1220	73.1218
79.8108	82.6802	90.1692
98.7021	111.9582	125.0338
129.2490	134.9013	136.6547
156.5015	162.6740	170.5294
182.0490	189.3853	194.9301
206.8829	218.4822	222.6098
232.6912	240.3812	248.3077
253.9490	254.6426	269.5016
285.4278	292.7856	294.1823
303.2045	305.2621	311.0807
316.4770	323.0349	323.6944
325.5757	342.2784	343.7148
350.9330	354.4156	361.1602
369.6638	372.1892	376.5699
379.5862	389.4958	389.9262
391.3650	395.1336	400.3156
417.9638	420.1432	422.7367
462.8266	467.7872	477.7381

516.6120	541.9832	546.1797
546.5322	554.2259	554.3777
563.9140	568.1535	569.4626
575.2986	579.9303	617.5551
618.9852	628.1654	681.4117
690.0686	705.3846	714.0652
761.1303	767.7332	776.2537
776.8348	785.7503	788.1045
793.6267	817.6708	849.3387
880.8956	884.4979	900.7892
924.3344	925.7276	929.9826
947.7346	951.0068	955.6657
960.4309	961.7620	962.4321
964.6433	965.9004	972.4267
972.8323	974.5422	1014.1515
1018.7684	1031.4820	1032.7936
1042.5391	1047.7822	1051.1855
1053.1857	1055.2054	1055.5382
1059.6821	1069.2774	1076.4494
1088.0880	1114.8240	1149.3615
1170.5317	1172.6090	1180.0595
1184.0268	1201.1435	1202.0717
1207.6939	1210.4160	1238.7621
1243.7037	1244.0727	1245.2719
1249.0215	1258.1570	1261.6802
1262.7107	1265.3232	1279.9173
1284.3242	1285.6104	1297.1380
1311.5398	1319.8414	1327.1627
1355.0240	1360.4294	1364.7346
1389.8013	1393.3970	1400.7320
1402.0543	1403.7083	1405.1316
1406.5436	1420.6003	1422.1873
1425.7669	1430.9364	1434.2340
1437.8184	1468.5732	1471.3648
1478.0383	1478.5229	1483.0819
1483.4400	1485.2391	1486.5176
1487.9194	1496.7345	1500.1032
1500.4147	1500.7449	1504.5533
1505.7133	1506.3502	1506.7153
1511.7197	1515.6993	1517.7386
1520.4238	1554.8351	1588.0803
1668.4203	1685.5587	1697.8399
1698.3891	3057.6532	3059.6792
3063.3859	3064.6536	3064.9138

3066.9780	3069.1234	3069.6709
3072.2179	3138.9481	3139.5346
3140.0692	3140.8021	3142.1225
3144.2589	3144.7227	3145.6383
3146.8403	3148.1569	3148.9102
3150.3095	3153.6729	3155.3507
3156.1413	3156.9684	3203.3124
3205.6072	3206.0098	3215.9263
3224.6510	3230.0785	3249.5976
3266.8180	3278.2114	3280.4294

19a-ts

Zero-point correction= 0.616607
Thermal correction to Energy= 0.647737
Thermal correction to Enthalpy= 0.648507
Thermal correction to Gibbs Free Energy= 0.559099
Sum of electronic and zero-point Energies= -3055.549678
Sum of electronic and thermal Energies= -3055.518548
Sum of electronic and thermal Enthalpies= -3055.517778
Sum of electronic and thermal Free Energies= -3055.607187

Cartesian coordinates

C	4.151409	-0.423847	0.040518
N	3.601754	0.781573	-0.145551
H	0.373607	-1.674984	0.328215
N	2.314042	0.586688	0.066812
N	2.077135	-0.669619	0.355881
N	3.217573	-1.336063	0.353892
C	5.588090	-0.715012	-0.091842
C	6.073238	-1.998152	0.184979
C	6.478184	0.284861	-0.499883
C	7.431801	-2.275989	0.056259
H	5.380865	-2.772115	0.502336
C	7.836022	0.002280	-0.628043
H	6.099166	1.279237	-0.716266
C	8.317416	-1.277610	-0.350767
H	7.799442	-3.274339	0.274947
H	8.519416	0.783793	-0.946949
H	9.376611	-1.495519	-0.450760
C	-1.086035	-2.357276	-0.956086
C	-1.361916	-1.976612	1.392661
C	-2.717348	-2.229587	1.273652
C	-3.295074	-2.527140	0.033023
C	-2.447281	-2.612582	-1.072578

H	-3.332363	-2.205884	2.163393
H	-2.837042	-2.889685	-2.040715
N	-0.610642	-2.004587	0.261003
C	-0.102714	-2.507066	-2.114670
C	0.422386	-1.130192	-2.555487
C	1.069108	-3.399320	-1.664747
C	-0.783207	-3.172259	-3.317501
H	1.038295	-0.668026	-1.784095
H	1.044536	-1.259009	-3.447170
H	-0.401145	-0.452822	-2.804910
H	0.714969	-4.390272	-1.360219
H	1.761271	-3.525715	-2.502975
H	1.639478	-2.961357	-0.840725
H	-0.030889	-3.327489	-4.096054
H	-1.207543	-4.148843	-3.061286
H	-1.571625	-2.543567	-3.743598
C	-0.657404	-1.727051	2.722197
C	0.553723	-2.672552	2.826315
C	-0.191563	-0.265126	2.808738
C	-1.599539	-2.013637	3.896682
H	0.243094	-3.720112	2.745814
H	1.310230	-2.470013	2.061620
H	1.032641	-2.531034	3.800146
H	-1.027309	0.428739	2.674256
H	0.249753	-0.092865	3.796317
H	0.565028	-0.049668	2.055368
H	-1.035969	-1.895873	4.826725
H	-2.438367	-1.310795	3.932274
H	-1.992299	-3.035767	3.869141
C	-4.797943	-2.774624	-0.058898
C	-5.172123	-3.938669	0.876003
C	-5.531656	-1.498364	0.390962
C	-5.242305	-3.123331	-1.482009
H	-4.639693	-4.854273	0.597364
H	-4.943005	-3.712495	1.921592
H	-6.247398	-4.132459	0.803748
H	-5.281288	-0.651577	-0.256200
H	-6.613080	-1.662062	0.338323
H	-5.281574	-1.227528	1.421215
H	-6.325021	-3.280532	-1.489544
H	-5.019000	-2.316576	-2.188370
H	-4.771598	-4.044569	-1.841968
O	-1.884056	2.779764	1.347523
S	-2.088127	3.389620	0.054292

S	0.452630	1.956268	-0.589759
C	-3.351081	2.375751	-0.849177
C	1.265213	3.006019	0.788947
F	-4.505692	2.493892	-0.204317
F	-2.992430	1.102708	-0.883118
F	-3.484122	2.832605	-2.085393
F	0.615575	4.148318	0.942451
F	2.496385	3.259432	0.415578
F	1.224568	2.327608	1.913377
O	-0.831323	3.158854	-0.891017
O	-2.502461	4.762279	-0.091775
O	1.113941	2.117452	-1.854363
O	-0.329632	0.837570	-0.135428

Vibrational frequencies

-66.7646	17.1217	18.3828
25.8265	30.3598	36.3061
40.9966	43.6879	48.2422
53.3359	57.3735	65.8681
73.5627	77.4956	82.0581
83.6672	85.2473	96.0887
99.8879	112.2563	119.9064
133.1787	141.1957	148.2486
152.9157	172.7621	178.2601
188.4432	193.9113	211.2668
221.9864	235.6354	239.8234
242.1532	244.6193	255.2580
256.7747	270.5599	276.2600
285.7421	289.7077	296.0705
306.2448	309.5717	312.8173
318.0470	319.5165	322.8046
326.3654	330.0361	345.4009
352.0094	358.2122	361.8214
362.6067	366.6459	369.1593
376.4595	381.9430	388.7522
390.3052	393.4590	400.5324
413.4985	420.7314	440.5399
463.8959	467.1584	480.2788
519.8711	526.4058	544.4228
548.2939	553.9895	554.4032
563.6517	564.3627	570.2641
573.1823	581.1492	613.2262
626.4005	636.8630	685.8689
691.9142	703.8941	711.9052

756.8381	765.9958	782.1071
783.9986	784.8893	786.8248
793.4563	824.0472	847.9702
857.0565	874.1236	914.0622
924.8027	926.2571	944.6682
950.5405	951.1045	956.4349
956.7393	958.2518	961.5750
964.8810	966.4334	969.9244
977.5241	997.3873	1009.5926
1012.5756	1024.5812	1034.9830
1043.0897	1044.4110	1049.1982
1050.9870	1052.2254	1054.3637
1062.5871	1063.5996	1085.0041
1098.0491	1109.3085	1149.7736
1169.7259	1172.9958	1181.4598
1182.1854	1191.8165	1202.9454
1218.8200	1239.8803	1242.1529
1243.5589	1248.7234	1249.3773
1255.4909	1257.1120	1261.6852
1264.7317	1269.9202	1285.0158
1285.6271	1288.2412	1288.7173
1312.2317	1312.6021	1322.1211
1326.8611	1358.5318	1365.8676
1392.6788	1397.0687	1400.7131
1402.2171	1404.0161	1405.3285
1407.7771	1420.9839	1428.8106
1431.0980	1439.1769	1440.0048
1441.6434	1471.5368	1472.4500
1475.2408	1478.7398	1480.6659
1482.6029	1484.1414	1485.3453
1489.1345	1492.7249	1496.7841
1497.5838	1500.8477	1503.2634
1504.7447	1509.4658	1510.9932
1513.2485	1513.8286	1516.8311
1521.6505	1557.7144	1583.6810
1669.8665	1691.0446	1697.3664
1700.8705	3054.6574	3054.7328
3057.5628	3059.6911	3061.8281
3062.0635	3064.9644	3065.9834
3070.0247	3134.2664	3134.4722
3135.1404	3136.6889	3137.5943
3137.9904	3139.6010	3141.0405
3141.8697	3143.4857	3144.3904
3152.0566	3153.5060	3153.9817

3156.3754	3156.4315	3186.0054
3197.6735	3200.8700	3205.5751
3209.2147	3214.0871	3219.9313
3223.9899	3282.0499	3283.5997

20a-ts

Zero-point correction= 0.616298
Thermal correction to Energy= 0.647877
Thermal correction to Enthalpy= 0.648647
Thermal correction to Gibbs Free Energy= 0.556778
Sum of electronic and zero-point Energies= -3055.542180
Sum of electronic and thermal Energies= -3055.510600
Sum of electronic and thermal Enthalpies= -3055.509830
Sum of electronic and thermal Free Energies= -3055.601700

Cartesian coordinates

C	0.790668	1.995675	0.078644
N	0.985473	0.710291	-0.278756
H	-2.965124	0.572668	0.100137
N	-0.217599	0.150973	-0.310677
N	-1.098459	1.048050	0.004553
N	-0.512021	2.218010	0.257456
C	1.813787	3.041330	0.253252
C	1.585615	4.068090	1.177685
C	2.987722	3.050087	-0.506260
C	2.525066	5.082493	1.345447
H	0.673179	4.061263	1.766081
C	3.925017	4.065760	-0.336660
H	3.167628	2.263818	-1.229447
C	3.698039	5.083188	0.590021
H	2.343280	5.870211	2.070430
H	4.833610	4.061087	-0.930935
H	4.432191	5.872199	0.722705
C	-4.424366	-0.246672	1.308675
C	-4.675637	0.254154	-1.019316
C	-5.962466	-0.252838	-0.988337
C	-6.509766	-0.776607	0.190032
C	-5.717758	-0.752561	1.339374
H	-6.545736	-0.245894	-1.899005
H	-6.099590	-1.134184	2.274499
N	-3.951538	0.226225	0.130772
C	-3.502346	-0.208971	2.520932
C	-2.321585	-1.166425	2.272880
C	-3.011440	1.232291	2.750535

C	-4.235266	-0.668651	3.785731
H	-1.729424	-0.891856	1.397494
H	-1.656704	-1.146095	3.142500
H	-2.681267	-2.192556	2.141185
H	-3.854121	1.895826	2.972449
H	-2.334384	1.242202	3.610440
H	-2.462289	1.639091	1.898538
H	-3.542290	-0.597587	4.628947
H	-5.101262	-0.037462	4.011840
H	-4.564094	-1.710514	3.716651
C	-4.020044	0.834661	-2.265394
C	-3.533498	2.265061	-1.968007
C	-2.849743	-0.074635	-2.682615
C	-5.015706	0.901709	-3.428910
H	-4.373992	2.906289	-1.681609
H	-2.779420	2.302872	-1.178987
H	-3.080953	2.680598	-2.873784
H	-3.215861	-1.071914	-2.948903
H	-2.359295	0.356537	-3.561600
H	-2.095836	-0.179918	-1.899780
H	-4.509736	1.348046	-4.289914
H	-5.365052	-0.091243	-3.730436
H	-5.883302	1.526338	-3.190713
C	-7.920559	-1.357581	0.172006
C	-8.906347	-0.282352	-0.319636
C	-7.936024	-2.552103	-0.799727
C	-8.366106	-1.840195	1.555157
H	-8.900067	0.592165	0.339298
H	-8.675933	0.051290	-1.335860
H	-9.919991	-0.696206	-0.326670
H	-7.235067	-3.329151	-0.477421
H	-8.940421	-2.987059	-0.828121
H	-7.670096	-2.250827	-1.817582
H	-9.381109	-2.242508	1.483287
H	-7.720270	-2.638003	1.936806
H	-8.382732	-1.024019	2.285633
O	4.070662	-2.022637	0.081648
S	5.537416	-1.779396	-0.452859
S	2.748154	-0.778680	0.087421
C	6.428450	-1.539578	1.152720
C	2.546088	-0.894622	-1.817553
F	5.976389	-0.465880	1.777228
F	7.721123	-1.389789	0.886277
F	6.256312	-2.607322	1.918984

F	3.365784	-1.798930	-2.326787
F	2.818464	0.281341	-2.340584
F	1.310205	-1.259797	-2.068350
O	5.628071	-0.537531	-1.188779
O	6.034767	-3.020344	-0.996339
O	3.483979	0.350635	0.588302
O	1.805040	-1.610370	0.782725

Vibrational frequencies

-108.6799	10.8881	16.4537
20.0284	27.0002	30.8212
32.7045	36.7581	42.2351
50.0041	50.9706	56.5474
61.4492	72.6683	78.5017
87.7166	97.0560	102.4906
112.7249	114.5300	121.0330
136.5465	137.2846	148.9563
154.3806	158.1332	161.7936
184.9478	194.0903	195.4278
197.3941	200.6812	224.5071
225.8848	233.9085	241.4779
244.7399	253.2873	254.7725
262.6127	277.8562	292.5084
299.3770	305.2056	309.5958
311.5246	316.2915	322.5700
326.7027	330.4289	345.1092
349.1142	356.5928	357.1769
363.9620	365.8021	369.0929
374.0019	384.5605	388.1552
391.9530	394.9453	404.6684
417.5971	424.7960	435.2780
460.0903	465.0758	470.9821
516.2557	541.3641	542.2199
548.3172	553.7139	556.1976
566.7502	568.2622	569.2174
573.7180	578.5457	617.0567
624.3536	631.9484	692.0422
694.2922	707.9701	713.1073
757.8276	765.7566	780.4120
784.5331	787.5007	790.6595
793.6154	819.3706	846.9310
867.1683	878.5754	925.0976
927.9732	931.3448	949.5464
950.8519	953.6061	954.9824

955.8559	958.5867	960.2434
963.0564	963.6843	965.6687
966.8976	1012.8308	1015.4963
1019.8817	1030.5291	1040.9922
1044.5572	1045.8483	1048.2512
1050.1440	1052.5043	1053.5566
1058.3721	1075.6405	1083.8020
1090.7901	1121.1283	1149.2840
1177.7993	1181.1127	1182.9361
1183.7748	1206.6978	1208.4781
1216.6915	1228.1419	1237.7536
1241.8629	1242.8335	1247.7014
1249.5531	1254.1256	1263.6801
1264.9779	1270.1620	1286.2924
1288.1514	1289.7636	1290.8615
1314.1550	1318.8117	1333.4913
1353.7353	1367.2395	1367.9520
1394.4972	1395.6857	1400.4860
1400.5694	1402.6967	1403.6277
1406.5866	1426.0729	1427.2162
1432.6543	1433.2266	1440.9318
1446.2934	1472.9876	1474.0509
1476.1091	1477.0912	1478.1707
1481.0336	1483.0920	1484.1303
1485.9890	1492.8881	1497.9727
1499.5732	1501.2918	1502.9481
1504.0018	1505.8823	1508.1960
1513.1839	1514.7559	1515.5158
1519.6385	1565.9213	1593.5661
1671.4414	1699.3693	1702.1235
1705.8572	3054.7673	3056.9887
3058.1919	3061.6510	3061.9665
3062.1847	3064.1910	3065.7080
3068.6145	3069.3932	3134.7750
3136.0909	3138.0381	3138.3675
3138.7334	3139.7335	3141.8608
3142.0513	3142.9140	3143.1766
3144.5840	3147.5016	3148.0142
3148.2686	3173.8161	3174.8016
3185.7976	3188.4502	3211.3182
3221.5516	3230.8881	3235.9698
3263.7362	3278.5976	3311.6082

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Zero-point correction= 0.471012
Thermal correction to Energy= 0.491492
Thermal correction to Enthalpy= 0.492262
Thermal correction to Gibbs Free Energy= 0.427050
Sum of electronic and zero-point Energies= -1681.169053
Sum of electronic and thermal Energies= -1681.148572
Sum of electronic and thermal Enthalpies= -1681.147802
Sum of electronic and thermal Free Energies= -1681.213015

Cartesian coordinates

O	4.463207	0.084287	-1.611075
S	3.530307	-0.415328	-0.601795
C	4.069417	0.430280	0.950091
F	5.310284	0.070193	1.285952
F	3.255847	0.113476	1.966427
F	4.045524	1.759367	0.805325
O	3.626525	-1.836845	-0.263703
O	2.143922	0.086409	-0.749398
H	0.289032	-0.015829	-0.409204
C	-1.348726	-1.213082	-0.128094
C	-1.372623	1.182617	-0.225773
C	-2.741179	1.174393	-0.025762
C	-3.447100	-0.027271	0.123067
C	-2.723511	-1.220286	0.067604
H	-3.267477	2.118684	0.015822
H	-3.221921	-2.171806	0.180059
N	-0.733876	-0.015482	-0.267298
C	-0.480700	-2.461827	-0.181231
C	0.240546	-2.520971	-1.540233
C	0.535051	-2.398871	0.974514
C	-1.326958	-3.728019	-0.022610
H	-0.483291	-2.599376	-2.358507
H	0.877505	-1.650187	-1.712712
H	0.883509	-3.406198	-1.563009
H	0.018802	-2.341582	1.938951
H	1.148670	-3.304420	0.962824
H	1.214646	-1.548135	0.884283
H	-0.663997	-4.596111	-0.077184
H	-1.839287	-3.762199	0.944548
H	-2.070187	-3.827134	-0.820775
C	-0.534292	2.439257	-0.409847
C	0.524545	2.507172	0.706147
C	0.133727	2.394439	-1.797053
C	-1.406601	3.695494	-0.331668

H	0.046506	2.572283	1.689378
H	1.196208	1.645780	0.693930
H	1.135966	3.403630	0.561811
H	-0.623088	2.354203	-2.587725
H	0.724333	3.305647	-1.934828
H	0.811557	1.544960	-1.907960
H	-0.764990	4.571063	-0.466713
H	-2.165639	3.715098	-1.120653
H	-1.901138	3.791930	0.640470
C	-4.956522	0.010206	0.341370
C	-5.249195	0.809508	1.624146
C	-5.614865	0.710272	-0.861881
C	-5.555160	-1.391605	0.485560
H	-4.773124	0.345797	2.494436
H	-4.896496	1.842552	1.548936
H	-6.329922	0.833635	1.797971
H	-5.401849	0.176628	-1.794026
H	-6.700195	0.730065	-0.719328
H	-5.272154	1.743798	-0.971014
H	-6.635277	-1.305089	0.637124
H	-5.392706	-1.998309	-0.411593
H	-5.141037	-1.924140	1.348497

Vibrational frequencies

18.8053	26.4410	40.1632
48.0273	55.3772	68.7408
78.0919	83.5334	94.0257
112.4675	115.0247	138.3672
140.4007	143.5281	153.5639
197.0041	199.0632	204.5651
224.3252	241.1588	243.7982
252.5734	264.8316	276.7350
288.6820	300.9212	303.6538
311.9928	313.8349	320.7484
333.3569	340.3360	342.9705
346.5981	350.4614	354.8934
363.5348	376.0162	384.7292
390.5098	398.1948	420.2032
461.9719	462.6366	507.9458
508.4770	543.6885	552.6998
564.4942	571.4124	572.2080
573.9859	622.1214	683.9609
693.8402	776.9840	780.2702
785.1598	793.9428	846.8018

906.3288	924.0950	926.4992
927.5640	936.0830	949.5252
951.7445	953.1963	961.1979
963.1613	964.0906	968.4480
969.7152	971.4255	1027.9779
1035.5272	1045.4931	1047.2582
1048.6256	1050.6333	1055.3473
1057.7563	1180.9711	1186.4013
1202.0290	1215.8450	1221.4709
1239.1544	1241.6761	1242.6429
1244.9489	1248.0506	1257.4966
1264.4526	1267.8974	1289.9421
1292.5875	1299.0400	1318.7222
1368.6941	1392.3658	1396.9647
1400.9560	1402.1695	1403.4832
1407.5357	1422.2958	1426.8471
1434.1067	1440.8516	1471.7761
1474.2181	1476.3535	1478.4768
1479.9160	1480.5525	1481.7762
1483.5634	1484.6743	1495.3586
1499.2159	1500.1053	1501.1955
1503.7019	1504.3495	1508.4960
1511.7671	1513.5064	1516.7571
1555.5960	1687.6813	1702.7713
3055.7841	3058.0099	3060.4837
3060.5454	3061.6651	3062.8898
3066.8886	3067.1119	3069.9291
3136.7771	3138.7060	3139.7496
3139.8694	3140.8325	3142.3176
3143.1000	3143.6702	3144.1111
3145.3697	3147.1419	3147.2019
3147.6128	3149.8209	3164.8229
3170.1319	3171.4823	3172.2290
3267.4285	3293.0394	3313.7738

22

Zero-point correction= 0.144485
Thermal correction to Energy= 0.154825
Thermal correction to Enthalpy= 0.155595
Thermal correction to Gibbs Free Energy= 0.111099
Sum of electronic and zero-point Energies= -1374.398197
Sum of electronic and thermal Energies= -1374.387857
Sum of electronic and thermal Enthalpies= -1374.387087
Sum of electronic and thermal Free Energies= -1374.431583

Cartesian coordinates

C	1.289500	0.530405	-0.092395
N	0.306313	-0.200676	-0.577320
N	-0.724321	0.628870	-0.451564
N	-0.420518	1.804345	0.105553
N	0.841113	1.761848	0.325879
C	2.691414	0.107045	-0.016201
C	3.654879	0.991283	0.479430
C	3.060866	-1.170269	-0.451326
C	4.987759	0.593513	0.539576
H	3.359235	1.981755	0.810959
C	4.394709	-1.559480	-0.387468
H	2.306783	-1.849450	-0.837806
C	5.359133	-0.679142	0.106367
H	5.735908	1.279861	0.923374
H	4.683211	-2.549840	-0.725211
H	6.399801	-0.985538	0.151851
S	-2.345809	0.165717	-0.800907
O	-3.101211	1.381864	-0.917237
O	-2.280165	-0.869887	-1.793885
C	-2.781064	-0.625976	0.831631
F	-4.032888	-1.038282	0.754726
F	-2.648514	0.271994	1.790325
F	-1.969961	-1.645831	1.044371

Vibrational frequencies

32.4385	48.1038	54.2845
78.6568	88.6261	111.0041
184.3726	192.3972	204.9533
242.7133	277.3056	313.2889
321.2292	339.5465	403.3530
413.1335	414.8142	504.5100
512.0235	536.4717	564.0701
578.0681	614.0324	625.6583
676.3181	710.4936	715.1159
760.2067	795.2087	824.5376
882.0738	970.3116	1002.8273
1014.5818	1019.5062	1038.6433
1040.1147	1068.5882	1116.7863
1117.7793	1173.2528	1176.3915
1177.0908	1202.2336	1251.7011
1288.3397	1297.9146	1302.9225
1329.0470	1364.2902	1375.5243

1450.9559	1464.4329	1497.6570
1545.8660	1611.5778	1674.6912
1696.2318	3212.9174	3220.7231
3227.0743	3232.3028	3240.4980

23

Zero-point correction= 0.144484
Thermal correction to Energy= 0.154773
Thermal correction to Enthalpy= 0.155543
Thermal correction to Gibbs Free Energy= 0.111305
Sum of electronic and zero-point Energies= -1374.393732
Sum of electronic and thermal Energies= -1374.383443
Sum of electronic and thermal Enthalpies= -1374.382673
Sum of electronic and thermal Free Energies= -1374.426911

Cartesian coordinates

C	-0.664843	1.285346	-0.101430
N	-0.632583	2.543856	0.265566
N	0.631731	2.990971	0.061120
N	1.381501	2.086264	-0.413813
N	0.598791	0.975650	-0.551166
C	-1.850885	0.421651	-0.043221
C	-2.249516	-0.350546	-1.139557
C	-2.624839	0.454199	1.122823
C	-3.415452	-1.104690	-1.056591
H	-1.662832	-0.351323	-2.051957
C	-3.785016	-0.310112	1.198563
H	-2.310662	1.070551	1.959789
C	-4.178809	-1.090280	0.111243
H	-3.728893	-1.700977	-1.907305
H	-4.380898	-0.295003	2.105340
H	-5.086157	-1.683552	0.170711
S	1.410680	-0.508903	-0.845560
O	0.415216	-1.493408	-1.172093
O	2.558104	-0.210035	-1.655021
C	2.001093	-0.872967	0.887263
F	2.620035	-2.039140	0.856004
F	0.951731	-0.932116	1.689763
F	2.824401	0.077647	1.283430

Vibrational frequencies

27.1810	41.7076	67.6341
77.2960	95.1073	129.5468
185.8911	190.1714	201.9862

257.3902	280.2249	302.1564
329.8681	355.7674	361.9399
414.2485	419.0136	474.8283
524.7781	556.4120	569.8002
579.5549	614.7771	624.3064
703.8983	717.6193	726.2226
754.4830	794.4235	800.7806
892.8796	980.1456	1010.9603
1018.6141	1027.3575	1039.3186
1042.2127	1071.7071	1105.3638
1118.4964	1132.3401	1162.3473
1177.7465	1207.7989	1246.2529
1249.3941	1292.7437	1303.2943
1334.3964	1363.6522	1370.5886
1451.2397	1475.1973	1493.0447
1533.6963	1610.7410	1666.0104
1692.8881	3219.5528	3227.9523
3234.7005	3242.1228	3247.3977

24

Zero-point correction= 0.558444
Thermal correction to Energy= 0.579214
Thermal correction to Enthalpy= 0.579984
Thermal correction to Gibbs Free Energy= 0.513879
Sum of electronic and zero-point Energies= -1208.393845
Sum of electronic and thermal Energies= -1208.373075
Sum of electronic and thermal Enthalpies= -1208.372305
Sum of electronic and thermal Free Energies= -1208.438410

Cartesian coordinates

C	3.084058	0.186255	-0.525381
N	4.377827	-0.059194	-0.663544
H	1.544774	-1.100152	0.320152
N	4.575417	-1.304844	-0.199963
N	3.472043	-1.824328	0.211674
N	2.522019	-0.908243	0.017503
C	2.389376	1.431828	-0.871346
C	1.014679	1.444388	-1.129624
C	3.121586	2.623650	-0.915514
C	0.376926	2.647933	-1.418088
H	0.439199	0.521148	-1.119845
C	2.477181	3.822140	-1.207720
H	4.187272	2.602970	-0.709074
C	1.103809	3.837504	-1.454437

H	-0.689794	2.652272	-1.617672
H	3.046884	4.745720	-1.235739
H	0.601393	4.774041	-1.677015
C	-0.678846	-0.229258	1.493069
C	-0.990091	-1.622220	-0.342729
C	-2.120122	-0.905343	-0.730155
C	-2.538245	0.212100	0.002666
C	-1.795794	0.536256	1.136732
H	-2.684249	-1.225205	-1.599376
H	-2.082248	1.375420	1.758305
N	-0.268489	-1.257627	0.735975
C	0.101489	0.085296	2.774704
C	0.959767	-1.108971	3.210260
C	1.003731	1.308574	2.542120
C	-0.880776	0.404211	3.916225
H	1.749742	-1.344130	2.492708
H	1.441593	-0.875357	4.165427
H	0.349728	-2.008638	3.342937
H	0.427979	2.170148	2.185298
H	1.496349	1.590240	3.479823
H	1.785200	1.094833	1.806661
H	-0.323279	0.521484	4.851367
H	-1.429701	1.335070	3.746517
H	-1.607295	-0.404168	4.053301
C	-0.514773	-2.845295	-1.135537
C	0.300955	-2.370778	-2.351580
C	0.349490	-3.763882	-0.262228
C	-1.718508	-3.659416	-1.639257
H	-0.291259	-1.703980	-2.988368
H	1.208579	-1.839922	-2.046321
H	0.608833	-3.233177	-2.953545
H	-0.195419	-4.085996	0.631670
H	0.622897	-4.654401	-0.837850
H	1.275837	-3.286784	0.065849
H	-1.359260	-4.579320	-2.111986
H	-2.383837	-3.939496	-0.815310
H	-2.304417	-3.118270	-2.388018
C	-3.799625	0.970646	-0.413219
C	-3.687822	1.415645	-1.880580
C	-5.003755	0.023740	-0.265463
C	-4.039493	2.209530	0.454927
H	-4.603842	1.937506	-2.178037
H	-2.847732	2.103230	-2.022871
H	-3.552943	0.568141	-2.559184

H	-5.107813	-0.319691	0.769340
H	-5.924445	0.545939	-0.548294
H	-4.902788	-0.856652	-0.908097
H	-4.932206	2.733414	0.098516
H	-4.208500	1.945910	1.504398
H	-3.198130	2.910302	0.405736

Vibrational frequencies

18.0054	27.1511	34.0965
47.5239	52.3566	57.8944
71.7213	76.9321	94.3487
101.8407	116.7834	127.4992
131.5956	134.7861	152.3672
155.8304	170.8362	210.6022
231.2441	243.0368	256.3477
259.0579	270.4421	273.1605
291.7837	294.8102	296.7022
303.4823	313.0820	318.1585
321.0025	324.8364	337.8674
346.8795	353.2238	369.3954
378.6539	390.5232	398.6219
405.3630	418.4435	428.3997
446.1344	465.7368	466.6123
523.0799	544.0542	549.2375
569.6669	580.4437	628.6532
675.8531	703.2416	705.8744
708.7465	734.8218	758.0132
784.8649	794.8003	798.0625
807.5015	848.1350	873.8548
912.0266	921.7191	928.5516
929.3513	946.4473	947.6515
949.2254	952.2438	952.4246
956.3245	958.8927	959.7220
964.0070	964.0653	982.3431
1009.8190	1015.6407	1026.7229
1031.7662	1035.1328	1039.7373
1041.0808	1044.7746	1045.8394
1048.7470	1052.1595	1058.7416
1069.2754	1115.3095	1142.4057
1161.8428	1173.7839	1179.3850
1184.3395	1202.8394	1204.6558
1215.3195	1238.4193	1240.8011
1241.5328	1242.5283	1247.3802
1257.7885	1280.3755	1284.8199

1307.7534	1331.2749	1353.5409
1366.2467	1369.0143	1390.2105
1393.1575	1395.0940	1402.0131
1403.0741	1405.9828	1424.9468
1426.8503	1427.8461	1440.3512
1459.3312	1462.5715	1468.6442
1472.5913	1473.7472	1474.3788
1476.7935	1478.5255	1479.6326
1481.5442	1484.8560	1490.0317
1492.0090	1497.7672	1500.8990
1502.0924	1505.3664	1507.2972
1507.6242	1511.4618	1512.3988
1517.2254	1539.5875	1637.4819
1642.1310	1671.1725	1674.5068
1701.3636	3049.6867	3052.0465
3052.9721	3055.5682	3056.6488
3059.7094	3060.8671	3062.7864
3070.0369	3096.4707	3125.1488
3130.1531	3130.1728	3130.4831
3133.4249	3134.7812	3135.2516
3135.5845	3136.3425	3137.2077
3139.7620	3140.0019	3143.0769
3143.8310	3144.0204	3150.2145
3157.5624	3163.8899	3205.0309
3210.5775	3220.8169	3231.8128
3240.8704	3242.3896	3256.7806

25-ts

Zero-point correction= 0.555461
Thermal correction to Energy= 0.575607
Thermal correction to Enthalpy= 0.576377
Thermal correction to Gibbs Free Energy= 0.512332
Sum of electronic and zero-point Energies= -1208.390172
Sum of electronic and thermal Energies= -1208.370027
Sum of electronic and thermal Enthalpies= -1208.369257
Sum of electronic and thermal Free Energies= -1208.433302

Cartesian coordinates

C	3.175737	-0.366167	-0.016900
N	4.314945	-1.054338	-0.025245
H	0.813728	-1.109046	0.006679
N	3.958533	-2.342342	-0.019650
N	2.666571	-2.450619	-0.008692
N	2.139906	-1.224500	-0.006765

C	3.088253	1.102917	-0.020089
C	1.852859	1.761576	-0.017372
C	4.267211	1.859563	-0.025906
C	1.797147	3.153231	-0.020838
H	0.928296	1.191245	-0.012452
C	4.207601	3.250045	-0.028941
H	5.224987	1.348857	-0.027966
C	2.973790	3.901727	-0.026508
H	0.832269	3.651746	-0.018984
H	5.127783	3.826367	-0.033227
H	2.929761	4.986704	-0.029036
C	-1.050856	-0.631881	1.201646
C	-1.076255	-0.646731	-1.159717
C	-2.321517	-0.032454	-1.157588
C	-2.950874	0.326743	0.037248
C	-2.300014	-0.012347	1.220534
H	-2.816479	0.158545	-2.100186
H	-2.766694	0.191889	2.172528
N	-0.441690	-0.885835	0.018879
C	-0.364271	-1.068933	2.500316
C	0.110850	-2.525058	2.360711
C	0.813617	-0.135323	2.828253
C	-1.339681	-1.014502	3.686094
H	0.840908	-2.664118	1.562170
H	0.582575	-2.840452	3.297067
H	-0.739058	-3.189099	2.167239
H	0.477040	0.903545	2.915593
H	1.250115	-0.434407	3.787173
H	1.601333	-0.183635	2.077176
H	-0.835541	-1.424176	4.566569
H	-1.640447	0.009295	3.930178
H	-2.238393	-1.613511	3.504892
C	-0.413249	-1.100942	-2.464336
C	0.761039	-0.174893	-2.824962
C	0.059375	-2.556910	-2.316041
C	-1.409753	-1.056607	-3.632750
H	0.424830	0.863507	-2.919110
H	1.563235	-0.215254	-2.088667
H	1.179092	-0.486926	-3.787964
H	-0.790179	-3.216191	-2.105505
H	0.518581	-2.883163	-3.254932
H	0.798808	-2.690376	-1.525126
H	-0.922958	-1.476058	-4.518413
H	-2.306193	-1.651976	-3.429157

H	-1.712855	-0.034464	-3.881196
C	-4.311359	1.017918	0.004454
C	-4.200189	2.306663	-0.828277
C	-5.328973	0.069129	-0.652831
C	-4.810285	1.379592	1.406442
H	-3.465997	2.994614	-0.395236
H	-3.908014	2.100073	-1.862389
H	-5.170741	2.813367	-0.850750
H	-5.418892	-0.862783	-0.084505
H	-6.312994	0.549022	-0.683250
H	-5.044669	-0.182477	-1.679249
H	-5.776133	1.887735	1.324201
H	-4.956478	0.490411	2.029086
H	-4.119688	2.056476	1.921201

Vibrational frequencies

-984.9545	19.3014	23.7961
46.6647	56.6531	60.3823
71.3228	83.3080	95.0195
108.7695	130.9567	137.7028
145.3342	150.5495	163.5463
178.7490	180.4016	192.4767
200.6592	215.4305	242.0834
244.3975	252.1688	253.0321
268.5547	288.6753	298.4420
303.1572	319.3821	326.4535
339.2543	350.3757	353.5154
358.8539	360.8081	373.3473
378.2203	386.2787	394.7299
396.5576	406.7128	410.8146
426.4839	458.1776	467.1892
487.9821	521.1402	556.6269
567.3337	578.5379	582.4768
626.9433	686.4907	698.4988
705.7230	706.5223	749.2480
762.6307	791.3758	794.1580
803.0446	812.3985	848.9538
869.7307	916.3980	924.4323
932.3052	939.0911	947.4451
950.9947	951.8917	952.4983
953.1832	953.3443	957.9811
958.4158	961.8872	964.9905
1005.2013	1015.3483	1029.2619
1041.8289	1043.8390	1045.7929

1048.1614	1050.2852	1051.0271
1053.1205	1065.4321	1071.4426
1096.4811	1115.7490	1171.9337
1177.2765	1191.0833	1199.9218
1202.7360	1210.6510	1213.1766
1233.6124	1240.3569	1242.5120
1243.6451	1244.4159	1253.1769
1260.2556	1284.2504	1287.9505
1310.3331	1328.1612	1337.4467
1362.2266	1366.3560	1393.1834
1394.3791	1397.7546	1399.0904
1400.2688	1401.1275	1423.7151
1426.3667	1429.1407	1445.4334
1460.4832	1472.6316	1474.2527
1477.9093	1478.8244	1479.4557
1479.7175	1481.5157	1483.6646
1487.1215	1490.6048	1494.6023
1497.1438	1498.4529	1501.2735
1503.4251	1506.0599	1510.2366
1514.0459	1514.3361	1518.6886
1521.3784	1551.0240	1581.3852
1616.0968	1670.8940	1676.1385
1694.3438	1697.6316	3054.5536
3056.7476	3059.3731	3059.4051
3061.4307	3063.9083	3064.6741
3067.1519	3068.0343	3133.5827
3133.8893	3134.2657	3134.4977
3135.2620	3135.6089	3136.0467
3140.9510	3141.6877	3141.9363
3143.1847	3143.2678	3147.0451
3148.2916	3188.6350	3189.6982
3199.9301	3209.0216	3212.0343
3212.4385	3218.8363	3228.2036
3231.1913	3268.2779	3284.5671

26

Zero-point correction= 0.560212
Thermal correction to Energy= 0.580584
Thermal correction to Enthalpy= 0.581354
Thermal correction to Gibbs Free Energy= 0.516395
Sum of electronic and zero-point Energies= -1208.389596
Sum of electronic and thermal Energies= -1208.369224
Sum of electronic and thermal Enthalpies= -1208.368454
Sum of electronic and thermal Free Energies= -1208.433414

Cartesian coordinates

C	-3.348633	-0.006896	-0.552884
N	-4.416049	-0.008543	-1.357130
H	-0.387528	0.021835	-1.031212
N	-3.921077	0.012279	-2.593569
N	-2.616164	0.025864	-2.548773
N	-2.217574	0.012932	-1.275737
C	-3.421330	-0.026618	0.917461
C	-2.262696	-0.033839	1.705019
C	-4.670837	-0.036845	1.551196
C	-2.351128	-0.051521	3.095243
H	-1.286118	-0.025200	1.229013
C	-4.757082	-0.054473	2.940422
H	-5.570197	-0.031058	0.943354
C	-3.598408	-0.061695	3.718823
H	-1.443057	-0.057136	3.691329
H	-5.732872	-0.062031	3.417289
H	-3.667626	-0.075072	4.802455
C	1.217924	1.221145	-0.489073
C	1.239530	-1.172415	-0.526379
C	2.508706	-1.166554	0.026583
C	3.153368	0.030462	0.360111
C	2.490786	1.223063	0.069480
H	3.009845	-2.110657	0.191152
H	2.966514	2.172199	0.265800
N	0.623305	0.024998	-0.723435
C	0.481398	2.498020	-0.885297
C	0.027200	2.378987	-2.351556
C	-0.728615	2.718037	0.038868
C	1.403322	3.717789	-0.766474
H	-0.684152	1.565042	-2.510776
H	-0.470577	3.308465	-2.645163
H	0.887459	2.228401	-3.013082
H	-0.418927	2.770024	1.088330
H	-1.206339	3.667631	-0.223540
H	-1.473627	1.929720	-0.073357
H	0.857258	4.596358	-1.121580
H	1.699833	3.912224	0.269377
H	2.304608	3.613088	-1.379618
C	0.521024	-2.446882	-0.960846
C	-0.692466	-2.707017	-0.051896
C	0.074876	-2.295544	-2.426328
C	1.458681	-3.656777	-0.866819

H	-0.388970	-2.786044	0.997718
H	-1.446175	-1.924544	-0.146399
H	-1.157587	-3.653826	-0.345192
H	0.937558	-2.120758	-3.078690
H	-0.412713	-3.221834	-2.746138
H	-0.643082	-1.484403	-2.569875
H	0.926275	-4.534406	-1.244317
H	2.360940	-3.525216	-1.473382
H	1.753368	-3.870552	0.165863
C	4.544628	-0.008453	0.985048
C	4.483739	-0.834515	2.282376
C	5.512360	-0.677619	-0.007215
C	5.069452	1.391309	1.315810
H	3.783766	-0.392147	2.999008
H	4.176310	-1.867780	2.095314
H	5.476023	-0.858976	2.744418
H	5.564248	-0.114300	-0.944919
H	6.516461	-0.709147	0.428453
H	5.213967	-1.704434	-0.239383
H	6.058813	1.301863	1.774469
H	5.175696	2.009726	0.418115
H	4.418724	1.913338	2.025633

Vibrational frequencies

19.6266	21.4527	37.3251
46.9124	62.1357	76.1924
83.3257	88.9233	99.1480
113.4981	129.3043	130.2840
149.9495	151.6452	161.5727
164.7774	178.4251	219.7171
229.7460	235.0615	252.8260
261.8738	269.4878	273.0156
288.7859	300.8210	305.7778
316.2624	322.9476	329.7873
341.0937	350.4254	355.5147
359.9874	364.3269	369.8434
382.0041	388.4303	390.6771
402.5049	420.9808	421.5026
459.6790	465.3407	467.6561
523.1542	541.4937	554.0456
570.1035	572.8924	627.7730
688.7981	694.2821	704.4617
715.6476	751.1620	767.6500
784.0291	789.7866	793.5563

809.0332	847.7803	880.4578
923.4041	926.1958	926.3504
946.5419	951.5062	952.4068
956.6860	957.7392	959.2713
960.4781	962.9368	964.5988
966.4494	975.3892	1004.6100
1013.8352	1015.3924	1027.1485
1042.3385	1045.4162	1047.9098
1049.8205	1050.5286	1054.2297
1056.2000	1065.6732	1081.3658
1085.1056	1113.0889	1161.6057
1169.9668	1180.5246	1192.7323
1196.1373	1208.4298	1217.4803
1219.0093	1238.7133	1241.8665
1242.5413	1248.4701	1255.8245
1262.7210	1286.1854	1287.7389
1308.3275	1317.5468	1322.2817
1358.5576	1365.0990	1394.2275
1396.9472	1398.6446	1400.9684
1402.3882	1403.6380	1423.7292
1428.4662	1431.9480	1441.2363
1448.2329	1471.7844	1473.3557
1475.0224	1477.5778	1478.9049
1481.8561	1485.0883	1486.0445
1487.2326	1495.2023	1496.4897
1497.6276	1502.3067	1502.9739
1505.4516	1506.3678	1510.3150
1512.7020	1514.7390	1515.3790
1520.7818	1570.7515	1585.0749
1667.4954	1696.1842	1697.1059
1703.8789	2842.7078	3056.4813
3058.0560	3059.4848	3059.6536
3062.0071	3062.1010	3063.3055
3066.2005	3066.5014	3135.7895
3136.2092	3136.4894	3136.7064
3137.5544	3138.5754	3138.8390
3140.8008	3141.6811	3145.7320
3146.8067	3147.6291	3148.2018
3149.3236	3171.4222	3172.9494
3198.4980	3199.2728	3200.5610
3208.0186	3215.2597	3228.4297
3240.6360	3275.0530	3288.6825

27a-ts

Zero-point correction= 0.618522
Thermal correction to Energy= 0.648896
Thermal correction to Enthalpy= 0.649666
Thermal correction to Gibbs Free Energy= 0.563527
Sum of electronic and zero-point Energies= -3055.541250
Sum of electronic and thermal Energies= -3055.510876
Sum of electronic and thermal Enthalpies= -3055.510106
Sum of electronic and thermal Free Energies= -3055.596245

Cartesian coordinates

C	3.765919	-0.754827	-0.205200
N	4.114749	-1.995023	-0.587124
H	1.083708	0.918644	0.069015
N	2.987361	-2.672083	-0.666812
N	1.998628	-1.887732	-0.339423
N	2.437776	-0.660584	-0.049685
C	4.767124	0.310291	0.001009
C	4.413900	1.633667	0.289021
C	6.126729	-0.018697	-0.097214
C	5.395055	2.605280	0.477823
H	3.369892	1.916457	0.363520
C	7.105169	0.953166	0.090381
H	6.408453	-1.042312	-0.321364
C	6.744137	2.269595	0.379420
H	5.101643	3.626934	0.701277
H	8.153327	0.680206	0.012028
H	7.508121	3.027095	0.525808
C	-0.283034	1.837295	1.308564
C	-0.178087	2.090130	-1.077332
C	-1.323656	2.866150	-1.035506
C	-1.979871	3.144607	0.167941
C	-1.423672	2.631203	1.337225
H	-1.713027	3.268721	-1.959981
H	-1.886592	2.833907	2.290573
N	0.287212	1.584331	0.101451
C	0.334214	1.257271	2.581006
C	0.145244	-0.267697	2.594794
C	1.837133	1.568101	2.631076
C	-0.329710	1.849889	3.830204
H	0.719884	-0.733401	1.794060
H	0.511025	-0.659424	3.550130
H	-0.906086	-0.550857	2.480633
H	2.041504	2.636737	2.500478
H	2.229871	1.261117	3.605257

H	2.377272	0.997131	1.874430
H	0.174061	1.439386	4.709700
H	-0.236729	2.940556	3.869591
H	-1.387796	1.580165	3.904613
C	0.585610	1.834120	-2.378689
C	2.059939	2.222218	-2.192182
C	0.504423	0.353693	-2.783516
C	0.001408	2.676875	-3.519884
H	2.169604	3.240738	-1.803533
H	2.568710	1.525399	-1.524709
H	2.569381	2.166380	-3.159244
H	-0.533078	0.012855	-2.854063
H	0.974175	0.231733	-3.764894
H	1.040315	-0.282532	-2.078805
H	0.605375	2.503863	-4.414671
H	-1.027874	2.391315	-3.760386
H	0.029019	3.749180	-3.298315
C	-3.248116	3.990775	0.157803
C	-2.916697	5.372302	-0.434250
C	-4.298459	3.289522	-0.722436
C	-3.827177	4.181497	1.562286
H	-2.159099	5.885808	0.167243
H	-2.546543	5.299909	-1.461598
H	-3.820654	5.989905	-0.445913
H	-4.549381	2.301153	-0.323272
H	-5.213786	3.890027	-0.745623
H	-3.950536	3.166062	-1.752578
H	-4.737878	4.784187	1.495783
H	-4.095935	3.225856	2.025524
H	-3.128938	4.706223	2.223442
O	-2.525468	-2.374934	1.533385
S	-3.068545	-2.523328	0.202280
S	-0.256856	-2.427290	-0.724316
C	-3.466459	-0.796957	-0.420806
C	0.194180	-3.734898	0.606409
F	-2.887491	0.112288	0.345754
F	-4.783238	-0.642110	-0.357815
F	-3.065986	-0.650162	-1.675045
F	1.157146	-4.472484	0.108876
F	-0.845042	-4.503847	0.871699
F	0.573554	-3.112754	1.700553
O	-4.239662	-3.321741	-0.062927
O	-1.951018	-2.997441	-0.819906
O	-0.516610	-1.085566	-0.255079

O	0.121879	-2.853743	-2.043508

Vibrational frequencies

-72.5422	23.0876	24.9573
28.8304	38.3156	40.7352
45.8962	52.9338	60.8530
63.1802	73.0597	73.9334
74.3972	78.9721	86.0213
96.0485	102.6123	107.1430
108.7515	130.5750	133.7367
136.1064	151.5653	160.1836
165.2192	179.3776	187.1478
204.2063	213.8975	221.5556
230.7440	231.3010	249.2593
255.2620	259.1599	269.8056
273.7780	279.3630	286.6525
294.8975	299.7501	305.1357
312.4662	315.5149	321.4107
322.6305	324.6258	329.8650
331.4782	335.2332	337.1932
340.0772	356.6664	359.6642
362.7508	377.7876	383.3112
384.9858	388.3744	391.5827
395.0558	397.5393	412.3672
423.9164	435.0188	458.4811
463.3772	474.8243	477.0407
521.7699	530.0334	540.2654
547.9523	555.1079	559.3211
564.2662	569.8865	573.1055
577.4563	583.2733	602.2412
627.4311	653.0265	686.2511
693.6357	702.1930	728.0028
753.4942	759.0631	781.4023
783.6015	784.1401	786.5345
796.4814	826.5412	851.5019
858.1861	887.1907	921.7373
923.0275	926.2861	947.4230
949.5505	954.2810	956.7940
959.2305	959.9242	962.8073
967.4542	969.4359	975.8899
982.2436	990.6965	1013.4308
1025.4318	1025.8305	1037.3582
1038.9002	1043.1324	1045.6120
1052.3789	1057.1207	1059.6341

1066.0079	1069.7207	1078.2760
1088.0133	1117.4013	1139.3164
1167.9079	1172.8107	1179.9357
1187.0691	1201.8355	1202.5797
1210.3022	1223.8674	1237.7751
1244.0968	1245.6361	1249.6908
1250.0740	1253.4120	1260.9113
1264.6330	1270.0269	1280.5803
1281.9783	1284.5655	1300.3866
1310.0112	1324.1120	1325.0308
1326.2817	1359.7415	1361.5069
1392.6162	1397.1155	1398.4212
1399.1943	1400.4672	1403.9938
1409.1305	1422.6399	1423.1155
1425.2199	1433.2978	1437.4063
1441.7850	1473.0264	1475.8062
1476.2472	1477.2466	1477.5438
1481.8619	1486.4082	1490.8415
1491.4407	1493.4597	1494.2342
1497.4569	1500.0886	1504.3851
1505.5611	1506.8342	1510.2146
1512.0435	1512.7071	1521.3514
1526.9768	1565.4577	1579.1590
1667.8402	1689.4447	1693.5665
1697.3084	3054.7363	3058.6465
3059.9325	3061.8224	3062.3558
3064.4786	3065.4029	3073.0502
3075.9496	3134.3339	3138.6180
3140.3649	3141.2055	3141.5052
3142.0825	3142.5310	3143.7517
3144.1888	3145.9255	3146.7934
3147.7042	3149.0883	3151.8009
3179.1697	3184.6062	3200.4576
3202.8576	3210.3344	3215.8583
3235.9436	3238.5477	3243.3454
3244.3054	3294.2360	3294.8619

28a-ts

Zero-point correction= 0.616395
Thermal correction to Energy= 0.647673
Thermal correction to Enthalpy= 0.648443
Thermal correction to Gibbs Free Energy= 0.557430
Sum of electronic and zero-point Energies= -3055.543201
Sum of electronic and thermal Energies= -3055.511924

Sum of electronic and thermal Enthalpies= -3055.511154
Sum of electronic and thermal Free Energies= -3055.602166

Cartesian coordinates

C	0.409131	2.456253	-0.276940
N	-0.920149	2.581564	-0.251121
H	2.296261	-0.027137	0.031815
N	-1.359675	1.357996	0.008946
N	-0.369904	0.521511	0.136018
N	0.768730	1.181857	-0.038046
C	1.341825	3.565676	-0.535028
C	2.727762	3.364671	-0.527155
C	0.840538	4.846953	-0.797783
C	3.595728	4.426388	-0.773747
H	3.129260	2.374205	-0.330663
C	1.710224	5.905346	-1.044932
H	-0.233745	5.003013	-0.807428
C	3.090621	5.700111	-1.033335
H	4.668412	4.256548	-0.764440
H	1.308288	6.893652	-1.247644
H	3.767734	6.526689	-1.226796
C	3.642874	-1.095381	-1.116983
C	3.811983	-0.745643	1.247426
C	5.030951	-1.400314	1.253357
C	5.594746	-1.904021	0.074710
C	4.865811	-1.755161	-1.105173
H	5.546647	-1.529360	2.195179
H	5.242739	-2.159431	-2.032393
N	3.179755	-0.586714	0.052054
C	2.789309	-0.944315	-2.371529
C	1.398071	-1.547685	-2.103106
C	2.669368	0.543235	-2.743808
C	3.418257	-1.687866	-3.555127
H	0.868209	-1.050448	-1.286861
H	0.784865	-1.439419	-3.003268
H	1.476346	-2.614978	-1.869403
H	3.656394	0.993710	-2.894972
H	2.105464	0.630372	-3.678076
H	2.133222	1.107782	-1.980587
H	2.750335	-1.590336	-4.415526
H	4.387341	-1.264804	-3.839847
H	3.543755	-2.756086	-3.350427
C	3.129467	-0.228788	2.509565
C	3.034198	1.305579	2.461522

C	1.724694	-0.850940	2.608087
C	3.922986	-0.625611	3.759659
H	4.024799	1.760258	2.352044
H	2.393578	1.643291	1.645612
H	2.595285	1.664248	3.398111
H	1.785845	-1.942811	2.668406
H	1.237907	-0.485051	3.517716
H	1.083263	-0.584115	1.764776
H	3.378796	-0.271643	4.639855
H	4.031444	-1.711640	3.849773
H	4.917207	-0.167078	3.779319
C	6.952948	-2.595940	0.123608
C	7.990975	-1.594991	0.663918
C	6.862689	-3.806876	1.069964
C	7.406255	-3.082446	-1.255842
H	8.061460	-0.713740	0.017565
H	7.743916	-1.259950	1.675948
H	8.974866	-2.074023	0.698807
H	6.119798	-4.528629	0.714726
H	7.834740	-4.309151	1.110483
H	6.595572	-3.512034	2.089140
H	8.384219	-3.563785	-1.160322
H	6.713236	-3.819392	-1.675408
H	7.510709	-2.255882	-1.966890
O	-4.961032	-1.890948	1.270089
S	-5.978924	-1.256714	0.467986
S	-3.722829	0.531636	-0.298717
C	-6.222952	-2.281426	-1.058297
C	-3.598552	0.998893	1.548706
F	-6.721549	-3.453038	-0.687658
F	-5.069157	-2.461610	-1.675865
F	-7.074562	-1.668815	-1.865242
F	-4.770205	0.802823	2.139373
F	-3.289617	2.271756	1.638982
F	-2.695612	0.231859	2.115532
O	-5.417530	0.078500	-0.214583
O	-7.293322	-0.959650	0.976245
O	-3.877295	1.686247	-1.135703
O	-3.067639	-0.703656	-0.620813

Vibrational frequencies

-37.0151	11.5686	17.2217
20.4348	23.5262	24.2913
35.8779	43.2369	46.3131

51.3221	55.8588	62.7606
64.6897	79.6383	82.5809
84.9048	95.9999	103.6120
109.0859	116.1170	118.1183
133.7217	143.8217	149.0490
156.4398	161.7577	165.6390
185.8669	193.1730	197.7674
222.3569	227.9377	238.9611
242.0511	248.4826	253.5783
258.5973	260.2543	273.2796
280.8945	285.3577	289.6481
295.1857	303.9861	311.1072
314.6983	321.7082	323.6995
324.7424	335.4323	346.7715
357.3532	357.8656	361.5375
362.0598	364.0909	366.9487
373.3571	382.7170	389.8552
390.6261	392.9844	402.4098
422.3914	423.4885	438.3251
457.3424	471.2592	471.9271
520.7362	524.5951	540.5618
550.4026	554.4913	554.9292
565.6458	566.0164	570.9446
571.7426	581.3724	613.3769
626.1946	644.9727	685.9915
696.1205	703.8811	718.1543
754.7534	765.0130	783.1748
784.9270	785.9067	790.1291
793.9452	817.4888	835.3717
846.9228	880.1454	923.5736
925.5310	929.3488	948.6853
951.8838	952.6536	953.8992
956.5632	959.7208	960.5949
961.2338	965.4398	969.2349
980.2233	1002.9887	1012.5252
1013.9590	1027.1900	1035.0966
1041.8975	1046.7255	1048.5145
1048.7568	1050.8322	1052.9638
1054.8713	1066.4731	1088.6301
1095.4773	1110.5164	1145.3673
1167.4722	1174.2666	1180.3594
1188.7118	1196.9083	1204.6654
1224.5709	1237.2348	1238.6316
1242.2147	1243.3175	1248.9017

1250.0478	1257.2283	1263.1964
1264.4753	1279.0599	1279.4378
1285.6435	1288.1253	1293.1521
1317.3506	1320.4866	1325.5521
1327.2550	1357.2117	1366.8440
1391.9886	1398.0399	1399.8731
1401.4813	1403.2594	1407.1721
1414.0844	1423.5030	1429.4113
1431.7941	1436.5440	1443.4191
1448.5336	1472.8879	1475.5156
1476.3077	1476.9261	1480.4614
1481.8620	1484.8337	1486.2132
1486.6015	1494.5372	1494.9342
1499.8318	1500.6438	1501.9581
1504.3135	1506.4835	1510.7520
1511.8441	1515.5909	1517.0957
1520.3372	1560.6226	1583.8012
1666.9725	1690.4683	1696.1999
1703.9087	3057.2593	3058.1840
3058.8478	3060.5573	3060.8265
3064.4556	3065.3343	3067.1786
3070.7334	3071.3013	3138.0503
3138.6567	3139.1826	3140.5733
3140.9949	3141.4247	3142.3685
3142.6057	3143.2095	3145.3243
3146.7434	3149.5046	3150.0151
3150.1009	3173.3377	3176.8848
3186.4247	3194.3686	3198.4649
3207.2592	3215.8796	3220.8690
3225.9405	3273.1531	3307.9661

29a-ts

Zero-point correction= 0.615737
Thermal correction to Energy= 0.647367
Thermal correction to Enthalpy= 0.648137
Thermal correction to Gibbs Free Energy= 0.556297
Sum of electronic and zero-point Energies= -3055.539810
Sum of electronic and thermal Energies= -3055.508180
Sum of electronic and thermal Enthalpies= -3055.507410
Sum of electronic and thermal Free Energies= -3055.599249

Cartesian coordinates

C	-0.302967	-0.045880	-0.068202
N	-1.232085	0.280567	-0.981465

H	2.983944	0.355766	-0.218816
N	-0.597135	0.984739	-1.919241
N	0.654555	1.077739	-1.602662
N	0.881777	0.444707	-0.444764
C	-0.502635	-0.846503	1.153777
C	0.217469	-0.533377	2.312556
C	-1.358608	-1.952529	1.159414
C	0.083786	-1.314245	3.458067
H	0.876135	0.329592	2.317610
C	-1.492382	-2.731690	2.305484
H	-1.914246	-2.204347	0.263403
C	-0.771298	-2.416184	3.457532
H	0.643466	-1.057873	4.352677
H	-2.160163	-3.587835	2.297281
H	-0.877002	-3.024362	4.351074
C	4.719228	1.370640	0.232820
C	4.583970	-0.921062	-0.457763
C	5.958770	-1.029598	-0.361326
C	6.748664	0.055792	0.039214
C	6.100202	1.256055	0.332574
H	6.422855	-1.977512	-0.598530
H	6.666872	2.121319	0.642811
N	4.016396	0.277840	-0.152753
C	3.957107	2.658588	0.513855
C	3.318431	3.146003	-0.799355
C	2.867071	2.391397	1.565675
C	4.894020	3.748606	1.043091
H	2.605261	2.426223	-1.211105
H	2.772395	4.074982	-0.605496
H	4.086031	3.350655	-1.553482
H	3.295503	1.974715	2.483882
H	2.372487	3.335472	1.814510
H	2.101356	1.713664	1.182546
H	4.300710	4.644839	1.244614
H	5.379785	3.452771	1.979118
H	5.664120	4.019117	0.313672
C	3.666738	-2.061573	-0.876663
C	2.677106	-2.343099	0.267295
C	2.924072	-1.662183	-2.165245
C	4.463039	-3.340077	-1.155464
H	3.206382	-2.674898	1.167221
H	2.080608	-1.464857	0.518994
H	1.986179	-3.135724	-0.037932
H	3.632701	-1.515702	-2.987344

H	2.235987	-2.466488	-2.444233
H	2.336382	-0.749059	-2.049104
H	3.759882	-4.127104	-1.443032
H	5.172815	-3.212360	-1.979557
H	5.006096	-3.686311	-0.269769
C	8.260524	-0.111794	0.148514
C	8.553331	-1.191319	1.206685
C	8.814312	-0.560988	-1.215099
C	8.957847	1.187906	0.559171
H	8.155871	-0.900353	2.184728
H	8.119016	-2.157549	0.932075
H	9.635801	-1.323973	1.302914
H	8.601136	0.182621	-1.990214
H	9.900449	-0.679218	-1.144047
H	8.394001	-1.519809	-1.533496
H	10.035926	1.011171	0.619128
H	8.792393	1.986492	-0.171981
H	8.623757	1.537658	1.541699
O	-5.320054	0.963279	-0.726729
S	-6.375786	-0.089161	-0.198202
S	-3.525538	0.748657	-0.685112
C	-6.773084	0.661104	1.448114
C	-3.570904	-0.533007	-2.109727
F	-5.693659	0.698220	2.210736
F	-7.702362	-0.090388	2.027862
F	-7.241094	1.889492	1.278212
F	-4.809230	-0.712012	-2.539088
F	-3.100835	-1.676244	-1.658280
F	-2.843900	-0.067574	-3.097141
O	-5.759161	-1.372719	0.051457
O	-7.574356	0.037732	-0.991754
O	-3.366109	0.205045	0.635784
O	-3.227997	2.076396	-1.144168

Vibrational frequencies

-102.0016	10.9675	14.7867
21.9392	26.1955	32.4293
38.9432	39.5639	45.0081
47.8773	51.7350	57.5526
64.5037	70.8433	76.6564
79.3650	88.9783	98.2662
106.6379	116.1897	123.0773
131.7732	135.5059	140.8412
144.5764	156.0729	163.7287

174.5405	189.7170	194.2370
208.7322	217.2793	226.4397
231.0665	232.8280	247.9061
250.6312	262.3128	263.4758
275.0610	281.0415	293.3425
298.3732	305.9672	309.5070
311.2870	312.6688	320.5809
321.7085	327.2425	335.1661
344.1574	351.7749	353.6278
365.7057	369.2112	369.5563
372.9345	380.2193	388.9529
391.1067	392.1273	398.8192
412.7891	420.6703	437.5009
459.4083	461.2131	465.9277
517.2094	539.5762	544.4891
547.9709	552.4923	555.2270
563.5520	566.7037	570.5884
571.4037	580.5515	615.1795
625.4185	626.3271	688.5809
693.1746	703.2522	709.3022
764.2518	768.1107	782.0304
782.6343	785.6492	786.1734
793.5418	813.0573	846.8851
859.6390	875.3061	911.4284
924.6929	926.6609	940.8917
947.9062	950.4192	951.9874
952.8430	955.3673	960.8438
963.4458	965.1869	966.8829
977.2303	981.9122	1009.5138
1015.0753	1022.1472	1026.9693
1044.1772	1045.2241	1045.9198
1048.8406	1052.1429	1057.7813
1057.9681	1071.9140	1081.0155
1087.9119	1113.5957	1148.5785
1161.4692	1166.5992	1168.1581
1180.6573	1201.3056	1201.8464
1203.7732	1220.2528	1229.7499
1238.8891	1240.8502	1243.2734
1244.7123	1257.8786	1262.0374
1263.6071	1270.4557	1285.0978
1285.6331	1287.1161	1289.9365
1308.1794	1322.2856	1328.6745
1356.9933	1358.5352	1367.0219
1390.9270	1393.3971	1399.7292

1401.2726	1402.1438	1402.4439
1409.1311	1419.8934	1426.0673
1431.7273	1434.5661	1443.1329
1445.9056	1471.6690	1473.8241
1474.8878	1476.7071	1478.7290
1481.9867	1483.7198	1487.0226
1489.0854	1492.4201	1499.1044
1499.5273	1500.0381	1501.2337
1502.5873	1503.1711	1505.0440
1505.9410	1510.6936	1518.6132
1521.9075	1564.1030	1590.8835
1667.2476	1693.3080	1699.3295
1699.6623	3057.2930	3057.6274
3058.2378	3058.5223	3061.8879
3062.5244	3064.9626	3065.1241
3068.8334	3137.3006	3138.4936
3139.0035	3139.6193	3140.1449
3140.7611	3141.0033	3141.6001
3142.0895	3142.6007	3143.0045
3144.7300	3145.1316	3149.0852
3166.3413	3173.7417	3175.3100
3192.5764	3201.9939	3218.8469
3224.2186	3237.9555	3246.6698
3256.8939	3258.1361	3301.6116

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Zero-point correction= 0.163251
Thermal correction to Energy= 0.170520
Thermal correction to Enthalpy= 0.171290
Thermal correction to Gibbs Free Energy= 0.134390
Sum of electronic and zero-point Energies= -603.483889
Sum of electronic and thermal Energies= -603.476620
Sum of electronic and thermal Enthalpies= -603.475850
Sum of electronic and thermal Free Energies= -603.512750

Cartesian coordinates

C	-1.920926	-0.029361	-0.000207
N	-2.755092	1.041412	0.006390
N	-3.967213	0.565600	0.004758
N	-3.842773	-0.736564	-0.002173
N	-2.600306	-1.171116	-0.005828
C	-0.457676	0.069965	-0.000812
C	0.334294	-1.078493	0.001459
C	0.162055	1.327647	-0.003227

C	1.724868	-0.989817	0.001536
H	-0.136731	-2.057198	0.003576
C	1.543027	1.428043	-0.003309
H	-0.446684	2.226584	-0.005302
C	2.333218	0.269631	-0.000734
H	2.314676	-1.898839	0.003585
H	2.034805	2.395735	-0.005337
O	3.673890	0.467206	-0.000666
C	4.515449	-0.676931	0.002396
H	4.352622	-1.286846	-0.892995
H	5.536926	-0.297301	0.001637
H	4.352216	-1.282332	0.900757
H	-4.647113	-1.356887	-0.005234

Vibrational frequencies

29.3715	61.2652	123.9356
126.6530	202.9945	257.5229
259.2961	312.9715	388.8553
424.2834	449.5051	513.0624
541.3480	631.6055	647.0899
647.7023	732.1477	736.9060
781.8292	829.2931	844.9813
866.4320	982.8296	1003.9290
1012.3562	1039.2288	1073.2922
1097.4350	1139.5225	1155.5768
1188.1438	1200.6382	1212.4200
1218.5132	1251.6646	1315.6395
1320.4225	1339.2613	1356.0730
1407.3590	1476.4708	1487.5521
1488.7574	1498.4478	1511.0926
1559.1123	1612.3341	1665.7719
1702.9878	3066.7823	3143.4283
3189.9589	3209.3006	3213.3669
3239.2455	3257.7550	3613.3276

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Zero-point correction= 0.163372
Thermal correction to Energy= 0.170512
Thermal correction to Enthalpy= 0.171282
Thermal correction to Gibbs Free Energy= 0.135201
Sum of electronic and zero-point Energies= -603.483706
Sum of electronic and thermal Energies= -603.476566
Sum of electronic and thermal Enthalpies= -603.475796
Sum of electronic and thermal Free Energies= -603.511878

Cartesian coordinates

C	-1.920430	-0.074992	-0.009057
N	-2.609019	-1.197405	-0.147572
H	-2.680173	1.909896	0.290563
N	-3.909106	-0.858675	-0.079221
N	-4.051357	0.405524	0.093273
N	-2.816644	0.916247	0.141870
C	-0.464421	0.064510	-0.013560
C	0.152934	1.322220	-0.083281
C	0.330164	-1.081694	0.049810
C	1.532790	1.425937	-0.080753
H	-0.438913	2.231091	-0.152419
C	1.718872	-0.989397	0.050984
H	-0.144093	-2.056826	0.104445
C	2.325090	0.270394	-0.012591
H	2.022111	2.392790	-0.138821
H	2.310130	-1.895879	0.102640
O	3.661758	0.471656	-0.015952
C	4.510215	-0.667623	0.045435
H	4.347414	-1.324154	-0.815921
H	5.528956	-0.281971	0.021248
H	4.352100	-1.224162	0.975504

Vibrational frequencies

65.9375	68.9068	125.8292
136.8171	208.8762	264.9448
269.7977	314.9752	390.1575
423.0986	440.5977	516.2351
534.4233	630.8038	647.6423
650.4650	719.7929	742.5155
766.2943	831.4169	838.1285
858.6562	975.7410	995.2405
1015.3489	1046.9762	1057.7439
1098.1197	1126.7616	1151.7804
1173.9544	1184.6264	1213.1863
1220.0794	1222.2711	1318.5950
1340.2210	1359.5724	1362.5869
1437.4393	1447.2468	1488.4076
1490.7746	1498.6928	1509.6299
1559.4583	1646.5387	1665.4892
1702.1453	3065.3283	3143.1788
3191.6365	3208.4057	3226.1114
3229.4735	3253.8220	3639.1483

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Zero-point correction= 0.133298
Thermal correction to Energy= 0.140499
Thermal correction to Enthalpy= 0.141269
Thermal correction to Gibbs Free Energy= 0.104208
Sum of electronic and zero-point Energies= -693.463804
Sum of electronic and thermal Energies= -693.456604
Sum of electronic and thermal Enthalpies= -693.455834
Sum of electronic and thermal Free Energies= -693.492894

Cartesian coordinates

C	-2.174629	0.001043	-0.001976
N	-2.931563	1.121786	-0.091006
N	-4.171449	0.729374	-0.055684
N	-4.132890	-0.575819	0.049800
N	-2.925677	-1.089408	0.089723
C	-0.705702	-0.003076	-0.003891
C	-0.009690	-1.217098	-0.014487
C	-0.011035	1.211182	0.006108
C	1.378594	-1.223487	-0.015776
H	-0.555687	-2.154490	-0.025030
C	1.377939	1.217859	0.011532
H	-0.559146	2.147113	0.014434
C	2.043752	-0.002346	-0.000900
H	1.936859	-2.151803	-0.026516
H	1.935496	2.146610	0.023476
H	-4.977592	-1.139176	0.103480
N	3.513056	-0.002288	0.002403
O	4.085099	1.071690	0.088653
O	4.085443	-1.076468	-0.081172

Vibrational frequencies

49.0760	59.7971	69.8950
119.8109	189.4068	260.3178
271.9385	347.1538	417.9233
457.6629	508.9911	516.4189
546.9036	636.6077	683.0250
711.1802	746.8988	749.6384
759.8892	801.2749	863.4137
889.0533	895.7831	1007.7715
1019.6788	1020.2663	1040.5346
1074.1242	1133.2549	1147.4987
1158.5518	1200.3929	1208.4451

1267.7163	1313.4301	1341.5640
1372.1609	1400.8483	1469.2254
1472.3224	1497.9131	1557.1727
1600.2610	1662.2087	1696.9974
1715.2988	3229.8280	3233.7682
3256.3557	3256.5906	3604.9517

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Zero-point correction= 0.133283
Thermal correction to Energy= 0.140448
Thermal correction to Enthalpy= 0.141218
Thermal correction to Gibbs Free Energy= 0.104302
Sum of electronic and zero-point Energies= -693.461111
Sum of electronic and thermal Energies= -693.453946
Sum of electronic and thermal Enthalpies= -693.453176
Sum of electronic and thermal Free Energies= -693.490093

Cartesian coordinates

C	2.178459	-0.040272	-0.001609
N	2.931084	-1.123746	-0.083680
N	4.206906	-0.703213	-0.055427
N	4.269470	0.577416	0.038584
N	3.010025	1.013065	0.073577
C	0.711325	-0.003530	0.003524
C	0.015983	1.210583	-0.006058
C	0.015313	-1.217928	0.013087
C	-1.372922	1.217429	-0.009530
H	0.542812	2.159479	-0.015790
C	-1.372843	-1.223505	0.014965
H	0.565437	-2.152511	0.021189
C	-2.037240	-0.002558	0.001440
H	-1.929815	2.146491	-0.020644
H	-1.930533	-2.152235	0.024134
N	-3.508535	-0.000445	-0.002030
O	-4.080235	-1.073872	0.079417
O	-4.076881	1.075122	-0.086489
H	2.817929	2.005931	0.155600

Vibrational frequencies

45.8764	65.5095	71.0504
139.3197	192.7132	265.1847
277.5104	345.7022	414.7419
452.2341	504.2099	519.0389
548.3408	637.0908	668.9295

705.4358	737.2386	746.6208
755.2441	781.7570	857.1036
889.4287	890.7449	1000.9301
1020.5432	1023.6874	1047.6844
1059.0007	1133.8747	1144.1653
1148.9335	1170.6102	1216.9503
1234.0733	1337.4575	1347.9421
1381.7779	1432.7600	1438.1057
1472.6051	1510.2512	1545.9935
1636.3466	1666.4541	1702.4113
1719.4239	3228.5941	3237.1570
3257.2678	3257.5764	3621.0701

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Zero-point correction= 0.135343
Thermal correction to Energy= 0.143236
Thermal correction to Enthalpy= 0.144006
Thermal correction to Gibbs Free Energy= 0.105187
Sum of electronic and zero-point Energies= -825.981526
Sum of electronic and thermal Energies= -825.973633
Sum of electronic and thermal Enthalpies= -825.972863
Sum of electronic and thermal Free Energies= -826.011682

Cartesian coordinates

C	2.561302	-0.001353	0.000801
N	3.318587	-1.123257	0.073993
N	4.559165	-0.729886	0.054505
N	4.521254	0.576417	-0.025687
N	3.313345	1.090710	-0.064742
C	1.091722	0.002759	-0.006540
C	0.394308	1.214517	0.022302
C	0.395293	-1.208819	-0.045003
C	-0.995299	1.216060	0.009888
H	0.939969	2.151980	0.055639
C	-0.994982	-1.209526	-0.058006
H	0.942899	-2.145098	-0.071588
C	-1.681805	0.003150	-0.033389
H	-1.540542	2.154183	0.031971
H	-1.539751	-2.147534	-0.093627
C	-3.182182	0.001982	0.000127
F	-3.660522	-0.035648	1.263338
F	-3.707343	-1.061726	-0.634171
F	-3.708268	1.101293	-0.570141
H	5.366028	1.140688	-0.061191

Vibrational frequencies

39.2327	55.5675	65.7606
112.8550	157.7262	211.6821
238.7503	284.6369	393.7997
414.7134	423.1493	467.1027
472.6873	518.4838	584.4673
607.5368	641.4282	671.5433
710.5916	742.8013	753.2095
795.2873	805.6423	870.4369
883.8064	1002.2191	1015.7836
1017.1345	1042.3119	1073.8350
1105.2888	1138.7763	1158.1789
1178.4395	1202.3870	1210.7827
1212.8384	1263.2147	1322.7913
1343.0738	1359.0676	1369.7445
1403.0181	1470.8156	1508.4772
1563.9559	1611.8787	1676.2837
1713.7643	3220.6502	3222.6569
3232.3337	3234.6070	3611.4116

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Zero-point correction= 0.135330
Thermal correction to Energy= 0.143179
Thermal correction to Enthalpy= 0.143949
Thermal correction to Gibbs Free Energy= 0.105344
Sum of electronic and zero-point Energies= -825.979642
Sum of electronic and thermal Energies= -825.971793
Sum of electronic and thermal Enthalpies= -825.971023
Sum of electronic and thermal Free Energies= -826.009629

Cartesian coordinates

C	2.563822	-0.041501	0.003315
N	3.318218	-1.125788	0.060507
H	3.201023	2.007684	-0.103357
N	4.594152	-0.703048	0.043811
N	4.655923	0.578952	-0.019335
N	3.395021	1.013749	-0.046134
C	1.096516	-0.003927	-0.005195
C	0.400094	1.208407	0.018170
C	0.398439	-1.215772	-0.039726
C	-0.989991	1.210610	0.004596
H	0.926607	2.157529	0.049065
C	-0.990622	-1.215108	-0.052639

H	0.947996	-2.150774	-0.061791
C	-1.676149	-0.001260	-0.033345
H	-1.533629	2.149505	0.022154
H	-1.535819	-2.152892	-0.083388
C	-3.177796	-0.000463	0.000241
F	-3.652648	-0.033675	1.263655
F	-3.702112	-1.064981	-0.631225
F	-3.700269	1.098210	-0.573222

Vibrational frequencies

39.2784	62.3473	66.1002
128.8409	161.3177	221.3168
241.6314	286.2393	393.6739
411.6652	416.4541	462.8439
477.0292	514.7032	585.0032
605.6778	641.9096	653.9177
710.2816	734.4085	751.9158
770.0142	807.0295	862.1160
880.9820	995.9315	1017.6146
1020.4978	1048.3917	1059.2440
1108.4287	1132.5416	1149.1409
1172.6874	1183.0616	1214.3311
1217.5302	1234.3398	1337.7438
1348.4704	1366.6791	1383.1923
1435.4720	1437.2589	1508.2748
1564.6871	1643.3353	1678.8086
1717.4460	3220.7511	3225.7651
3233.4850	3238.0372	3623.2093

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Zero-point correction= 0.049003
Thermal correction to Energy= 0.052324
Thermal correction to Enthalpy= 0.053268
Thermal correction to Gibbs Free Energy= 0.022992
Sum of electronic and zero-point Energies= -258.131633
Sum of electronic and thermal Energies= -258.128312
Sum of electronic and thermal Enthalpies= -258.127368
Sum of electronic and thermal Free Energies= -258.157644

Cartesian coordinates

C	-1.057521	-0.311888	0.000000
N	-0.655251	0.976315	0.000001
N	0.647923	0.945894	-0.000001
N	0.974776	-0.321482	0.000001

N	-0.040044	-1.155179	0.000000
H	-2.090682	-0.620627	0.000000
H	1.943976	-0.626881	0.000001

Vibrational frequencies

706.2348	734.4804	772.4563
922.6290	1010.8385	1063.2979
1169.9948	1209.9919	1232.8353
1305.2755	1386.9106	1450.8675
1585.8254	3338.0246	3620.1971

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Zero-point correction= 0.048286
Thermal correction to Energy= 0.051666
Thermal correction to Enthalpy= 0.052611
Thermal correction to Gibbs Free Energy= 0.022240
Sum of electronic and zero-point Energies= -258.132237
Sum of electronic and thermal Energies= -258.128856
Sum of electronic and thermal Enthalpies= -258.127912
Sum of electronic and thermal Free Energies= -258.158283

Cartesian coordinates

C	-0.905320	-0.608060	0.000001
N	0.295388	-1.145479	0.000001
H	-1.453204	1.459163	-0.000003
N	1.164516	-0.114358	-0.000003
N	0.545069	1.011437	0.000003
N	-0.756802	0.721814	-0.000002
H	-1.852079	-1.124695	0.000001

Vibrational frequencies

650.0576	702.7923	753.2852
910.5056	1011.6228	1033.9251
1132.8028	1137.4796	1170.3344
1313.8689	1367.7186	1512.8941
1561.7032	3312.0724	3623.9154

38

Zero-point correction= 0.076098
Thermal correction to Energy= 0.079907
Thermal correction to Enthalpy= 0.080677
Thermal correction to Gibbs Free Energy= 0.052996
Sum of electronic and zero-point Energies= -297.408292
Sum of electronic and thermal Energies= -297.404483

Sum of electronic and thermal Enthalpies= -297.403713
Sum of electronic and thermal Free Energies= -297.431394

Cartesian coordinates

C	-0.605985	-0.014265	-0.002608
N	0.135714	1.121211	-0.001244
N	1.384843	0.748735	0.001164
N	1.369321	-0.558527	0.001281
N	0.164771	-1.093477	-0.001471
H	2.222781	-1.109063	0.001757
C	-2.093238	-0.035749	0.001169
H	-2.477553	0.405827	0.924198
H	-2.482841	0.541715	-0.840554
H	-2.449591	-1.063981	-0.074873

Vibrational frequencies

30.4824	271.4714	352.7295
652.2435	702.3758	720.8461
746.9806	1004.9990	1066.6288
1072.6352	1089.7261	1214.7968
1232.6532	1325.0066	1391.5308
1418.4084	1468.6010	1474.9258
1523.1082	1592.6377	3085.1629
3162.9529	3182.3029	3620.1364

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Zero-point correction= 0.076086
Thermal correction to Energy= 0.079833
Thermal correction to Enthalpy= 0.080603
Thermal correction to Gibbs Free Energy= 0.053417
Sum of electronic and zero-point Energies= -297.409497
Sum of electronic and thermal Energies= -297.405751
Sum of electronic and thermal Enthalpies= -297.404981
Sum of electronic and thermal Free Energies= -297.432167

Cartesian coordinates

C	-0.593438	-0.061933	-0.000044
N	0.180304	-1.131647	0.000049
H	-0.008882	1.996707	-0.000064
N	1.452772	-0.683442	-0.000075
N	1.490590	0.599097	0.000082
N	0.218600	1.008261	-0.000029
C	-2.078164	-0.020559	0.000008
H	-2.449645	0.496349	0.888361

H	-2.449679	0.498542	-0.887043
H	-2.458042	-1.042534	-0.001234

Vibrational frequencies

57.8493	282.2511	343.9685
664.9502	701.6452	712.8626
758.1433	1007.1208	1052.2623
1071.5667	1105.1479	1143.6562
1174.0441	1337.3093	1406.4274
1437.3883	1443.8343	1468.5869
1509.0183	1639.2929	3086.4923
3164.6134	3191.3300	3638.2965

40-ts

Zero-point correction= 0.139120
Thermal correction to Energy= 0.150200
Thermal correction to Enthalpy= 0.150970
Thermal correction to Gibbs Free Energy= 0.103713
Sum of electronic and zero-point Energies= -1374.358948
Sum of electronic and thermal Energies= -1374.347868
Sum of electronic and thermal Enthalpies= -1374.347098
Sum of electronic and thermal Free Energies= -1374.394355

Cartesian coordinates

C	-1.341872	0.556026	-0.100962
N	-0.184769	0.130947	-0.032252
N	0.885175	0.843449	-0.284405
N	-0.215565	2.692730	-0.451207
N	-1.225827	2.189318	-0.391920
C	-2.686968	0.021062	-0.051008
C	-3.802509	0.857026	-0.161751
C	-2.840422	-1.361354	0.134346
C	-5.077121	0.303933	-0.082034
H	-3.678088	1.924102	-0.314939
C	-4.118826	-1.897125	0.216266
H	-1.963545	-1.995999	0.215231
C	-5.237152	-1.067661	0.108289
H	-5.945671	0.948480	-0.168709
H	-4.242725	-2.965257	0.362555
H	-6.233930	-1.492981	0.169894
S	2.221584	0.434937	0.595080
O	3.145082	1.544887	0.477463
O	1.911241	-0.181754	1.872453
C	2.944111	-0.931832	-0.432205

F	4.050375	-1.379795	0.151149
F	3.239586	-0.487728	-1.646971
F	2.067761	-1.927807	-0.532155

Vibrational frequencies

-395.2137	12.7802	29.5806
43.9568	53.4329	70.8474
111.4186	132.4381	170.3907
197.1496	246.7857	269.2641
276.1342	311.5016	342.8516
350.0399	403.9458	407.0062
444.4954	464.0874	488.5301
524.6351	544.6142	566.0447
589.2749	595.1288	624.6645
639.0100	672.3404	699.9094
776.2899	780.7355	852.4575
859.9116	862.5768	956.4718
1007.8130	1014.7391	1032.0053
1061.8714	1122.8866	1134.5760
1176.0441	1184.1567	1202.1744
1232.9232	1259.1950	1267.3089
1320.7498	1350.8431	1365.8106
1382.3262	1494.7232	1534.3910
1662.6036	1681.7294	1867.7210
2205.7706	3214.7015	3221.9748
3226.7545	3232.6950	3237.5553

18b-ts

Zero-point correction= 0.649919
Thermal correction to Energy= 0.682977
Thermal correction to Enthalpy= 0.683747
Thermal correction to Gibbs Free Energy= 0.589416
Sum of electronic and zero-point Energies= -3169.994514
Sum of electronic and thermal Energies= -3169.961456
Sum of electronic and thermal Enthalpies= -3169.960686
Sum of electronic and thermal Free Energies= -3170.055016

Cartesian coordinates

C	-2.092295	-2.486762	0.184674
N	-1.143869	-1.574984	-0.106251
H	1.964159	-1.771707	0.140162
N	0.005059	-2.251983	-0.143791
N	-0.228971	-3.505565	0.098007
N	-1.528316	-3.692914	0.307030

C	-3.542600	-2.284919	0.342675
C	-4.409491	-3.324935	-0.028381
C	-4.086990	-1.120814	0.884051
C	-5.779546	-3.195649	0.128509
H	-3.996547	-4.238492	-0.445000
C	-5.465230	-0.976781	1.045622
H	-3.433906	-0.311037	1.189192
C	-6.316092	-2.018004	0.666024
H	-6.455341	-3.994163	-0.161506
H	-5.854915	-0.058137	1.467816
C	3.287345	-0.868298	1.434622
C	3.688264	-1.314527	-0.885864
C	4.890205	-0.633356	-0.807564
C	5.305575	-0.025717	0.383533
C	4.493309	-0.181915	1.507132
H	5.514403	-0.580772	-1.689908
H	4.797914	0.225200	2.459381
N	2.912692	-1.362232	0.229840
C	2.405705	-1.146916	2.649358
C	2.151745	-2.663336	2.737539
C	3.100962	-0.694067	3.937969
C	1.068695	-0.398348	2.528483
H	3.093672	-3.215669	2.824315
H	1.549587	-2.871653	3.627366
H	1.598341	-3.046211	1.874668
H	3.248973	0.390469	3.966031
H	2.463373	-0.961349	4.785177
H	4.068439	-1.187167	4.079495
H	0.497993	-0.543711	3.451409
H	1.225015	0.675644	2.383612
H	0.470520	-0.783461	1.703508
C	3.215064	-2.052212	-2.133532
C	4.322897	-2.091477	-3.191256
C	2.854333	-3.499815	-1.751557
C	1.987759	-1.342088	-2.725734
H	4.585230	-1.091444	-3.550590
H	5.228043	-2.582908	-2.818569
H	3.959899	-2.664093	-4.049570
H	2.005300	-3.557005	-1.064432
H	2.571598	-4.045378	-2.657244
H	3.709754	-4.011807	-1.297577
H	1.682491	-1.863815	-3.638908
H	1.152779	-1.356698	-2.026619
H	2.217163	-0.301655	-2.979643

C	6.620721	0.746223	0.420627
C	7.771404	-0.214575	0.070169
C	6.556427	1.876370	-0.622278
C	6.893632	1.359286	1.797122
H	7.831665	-1.035706	0.792201
H	7.655811	-0.644053	-0.929403
H	8.720138	0.331691	0.093584
H	5.731482	2.563658	-0.407906
H	7.491407	2.445510	-0.600367
H	6.423584	1.487009	-1.636051
H	7.838244	1.910247	1.761331
H	6.108287	2.063674	2.091854
H	6.987165	0.593185	2.574303
O	-0.666201	2.451390	-0.887535
S	-1.819745	3.526509	-0.828137
S	-0.829084	0.707847	-0.374790
C	-1.358401	4.387883	0.744946
C	-1.792711	0.278467	-1.978457
F	-1.406970	3.547805	1.765550
F	-2.217547	5.380629	0.945102
F	-0.131476	4.881338	0.636949
F	-1.933441	1.342815	-2.746235
F	-2.974151	-0.178631	-1.638414
F	-1.090440	-0.623541	-2.629484
O	-3.109704	2.906876	-0.621767
O	-1.600196	4.488432	-1.881481
O	-1.587947	0.899721	0.833610
O	0.576886	0.432968	-0.505286
O	-7.667962	-1.979502	0.781016
C	-8.252924	-0.811936	1.337774
H	-8.034392	0.069917	0.725259
H	-9.328103	-0.990844	1.345581
H	-7.903492	-0.646752	2.363135

Vibrational frequencies

-96.1115	10.2194	15.8949
21.6136	23.8277	34.4748
36.4727	43.7465	46.0772
47.9495	55.7801	62.7562
64.8848	68.3820	80.0780
81.4406	85.6429	87.8527
95.5819	106.1716	106.7516
122.3078	130.4654	136.6210
139.0755	145.2383	159.6037

170.3037	178.5307	186.8278
203.2224	211.0286	215.5717
219.6646	221.2370	226.5556
245.9335	252.5615	261.4652
263.6291	267.0831	273.4310
280.0168	284.7141	294.6095
300.3321	309.7202	313.1563
315.5150	320.5901	322.7492
325.8977	327.6480	339.2415
343.9602	354.9976	359.6268
364.7486	367.7373	374.1348
377.1670	382.8224	387.7370
392.6989	394.3204	409.6418
411.0364	420.5558	426.1294
437.8304	465.2385	470.0417
470.3170	513.0669	517.1779
541.9800	547.1182	554.6991
556.4048	558.0624	565.8708
568.9433	570.3972	577.4962
579.1588	615.0113	622.1302
632.1879	649.5361	680.3066
695.9567	735.5872	766.9813
778.2655	779.9800	784.9456
787.0585	794.2352	802.1168
831.4082	847.4334	849.3624
867.7375	873.2895	908.5702
919.5810	927.6378	930.0903
940.1968	950.3939	955.2019
957.1010	961.8848	963.2263
965.3600	968.0250	971.5790
975.4793	987.6904	1005.7034
1020.2076	1030.7491	1043.2888
1051.1804	1051.3265	1054.8462
1055.4418	1056.4942	1063.3608
1078.4974	1087.3044	1100.4714
1141.6782	1151.3479	1173.7489
1182.3301	1186.1689	1187.5518
1204.1823	1207.5136	1210.3900
1213.3989	1222.9420	1239.4865
1243.7904	1245.5585	1246.4350
1249.7091	1259.8425	1264.2287
1266.0244	1266.4191	1282.3139
1286.7385	1288.1449	1295.8651
1311.4071	1314.7596	1323.2769

1330.1848	1348.2222	1357.9047
1365.7289	1394.5713	1396.3730
1399.8653	1401.0580	1402.5456
1405.2533	1407.8824	1420.9081
1424.1097	1429.1303	1429.9330
1435.9151	1443.7363	1471.0807
1475.3916	1477.4518	1479.0186
1479.6209	1481.4934	1482.5688
1484.0113	1485.3238	1485.9424
1488.8749	1495.9376	1498.3436
1500.1659	1502.2951	1505.2762
1506.9703	1508.0048	1511.1590
1511.8418	1515.8049	1516.2294
1517.7809	1526.1019	1564.6080
1603.9054	1662.1029	1693.7468
1702.4413	1702.7927	3057.2610
3058.1526	3059.7318	3060.2661
3061.2624	3062.6148	3063.5235
3064.0135	3069.3393	3069.8984
3136.8529	3137.6759	3138.1045
3138.8396	3139.9036	3140.4318
3140.9375	3142.2317	3142.4078
3143.3541	3143.4443	3145.7860
3147.3467	3151.7630	3152.5549
3153.0306	3160.2664	3184.4581
3201.2864	3206.1350	3212.2026
3233.6857	3234.1682	3243.1221
3255.9624	3273.4582	3285.3892

19b-ts

Zero-point correction= 0.649543
Thermal correction to Energy= 0.682605
Thermal correction to Enthalpy= 0.683375
Thermal correction to Gibbs Free Energy= 0.588939
Sum of electronic and zero-point Energies= -3169.998449
Sum of electronic and thermal Energies= -3169.965387
Sum of electronic and thermal Enthalpies= -3169.964617
Sum of electronic and thermal Free Energies= -3170.059053

Cartesian coordinates

C	3.456067	-0.295480	0.127116
N	2.758555	0.840114	0.251175
H	-0.114742	-2.028531	0.138180
N	1.516199	0.438063	0.446083

N	1.445018	-0.868869	0.434053
N	2.655564	-1.366866	0.239816
C	4.905965	-0.358582	-0.106358
C	5.576259	-1.581594	-0.088858
C	5.640364	0.810004	-0.357742
C	6.951530	-1.655532	-0.312329
H	5.017953	-2.492607	0.105679
C	7.006361	0.750146	-0.582553
H	5.129686	1.768167	-0.377674
C	7.670611	-0.483507	-0.561005
H	7.441990	-2.621464	-0.288673
H	7.581820	1.649316	-0.780201
C	-1.566839	-2.495358	-1.251937
C	-1.732629	-2.845473	1.110821
C	-3.054282	-3.226926	0.961082
C	-3.674132	-3.222211	-0.294424
C	-2.893830	-2.880309	-1.400284
H	-3.606977	-3.536385	1.837862
H	-3.313013	-2.914053	-2.395057
N	-1.057542	-2.447411	0.001625
C	-0.648082	-2.174627	-2.427845
C	-0.325199	-0.671604	-2.455221
C	0.647398	-2.995183	-2.288291
C	-1.316766	-2.553322	-3.754146
H	0.238890	-0.363530	-1.574947
H	0.287599	-0.455178	-3.336399
H	-1.239450	-0.071699	-2.516738
H	0.429893	-4.068631	-2.266187
H	1.288953	-2.793095	-3.151662
H	1.220536	-2.734165	-1.394080
H	-0.602622	-2.377161	-4.563528
H	-1.601288	-3.610476	-3.781910
H	-2.202128	-1.943298	-3.959601
C	-0.981332	-2.895973	2.436965
C	0.354807	-3.633243	2.228544
C	-0.720570	-1.469375	2.946142
C	-1.798273	-3.652281	3.490798
H	0.192447	-4.638327	1.823789
H	1.031772	-3.091342	1.561373
H	0.861242	-3.730974	3.193777
H	-1.658552	-0.920233	3.080321
H	-0.209750	-1.526005	3.913506
H	-0.084921	-0.915458	2.256168
H	-1.202442	-3.721480	4.405484

H	-2.725906	-3.128932	3.743966
H	-2.042302	-4.670543	3.169494
C	-5.146998	-3.602333	-0.410010
C	-5.355829	-5.010380	0.175003
C	-5.971002	-2.581276	0.395406
C	-5.635924	-3.596720	-1.861140
H	-4.754784	-5.752877	-0.360681
H	-5.096239	-5.058019	1.236669
H	-6.409849	-5.290139	0.077757
H	-5.839950	-1.569703	-0.002871
H	-7.033280	-2.839790	0.333111
H	-5.686585	-2.572797	1.452148
H	-6.695663	-3.868392	-1.881550
H	-5.539003	-2.607805	-2.321697
H	-5.094580	-4.324097	-2.475863
O	-3.031316	4.860596	1.150978
S	-2.034702	4.327414	0.256732
S	-0.508694	1.747878	0.300998
C	-2.801051	4.323448	-1.430821
C	0.312261	2.409040	1.898368
F	-3.985276	3.730647	-1.377840
F	-2.021750	3.683978	-2.285736
F	-2.951494	5.583358	-1.816355
F	-0.471567	3.304468	2.478996
F	1.447058	2.968542	1.559716
F	0.487914	1.406081	2.730649
O	-1.960003	2.754137	0.502022
O	-0.716487	4.902657	0.140084
O	0.058335	2.278935	-0.907163
O	-1.184031	0.490273	0.482062
O	9.008940	-0.440884	-0.792717
C	9.728105	-1.663154	-0.753452
H	9.367649	-2.360305	-1.518480
H	10.767496	-1.407319	-0.959466
H	9.656453	-2.131110	0.235067

Vibrational frequencies

-74.2712	9.6391	14.0932
20.2265	26.9542	34.3752
40.2201	42.3677	48.1730
55.9581	58.6098	60.8318
65.3873	67.2195	75.0370
78.9612	83.0161	86.5301
95.3191	98.7296	117.8674

121.5306 126.2799 138.6353
141.9292 152.3527 156.0367
172.2454 173.4060 185.4560
192.6259 221.3792 222.9884
226.3502 234.6916 242.6949
245.8239 255.9349 257.0784
268.5959 271.5251 279.1139
285.9087 290.4468 293.9321
298.8043 299.9430 308.7978
311.0596 314.9542 320.0654
321.9034 325.8141 329.2373
336.9628 347.6546 354.6805
360.8036 364.1539 370.6352
375.3808 383.6943 388.8059
390.3480 392.8277 403.4435
407.0727 421.0704 426.5872
430.1822 463.1650 467.4852
469.2258 510.8363 520.2528
543.2143 543.4518 548.8078
555.7490 555.8474 564.5673
566.5537 569.7226 574.6691
581.3229 615.3739 630.3256
634.3657 648.5652 687.7993
693.2710 732.7391 763.9702
782.4555 783.3959 785.9923
786.8165 787.2972 793.5290
828.6693 839.7436 848.2070
848.9661 867.0413 913.8919
923.4773 928.3255 942.5884
949.4012 951.1085 955.2651
957.1143 962.1148 963.8123
965.7056 969.7502 971.2421
974.9165 979.6630 999.7052
1017.5012 1035.2571 1046.3353
1047.1558 1050.2571 1052.1060
1052.8108 1056.0807 1059.9497
1084.8919 1096.9544 1099.3549
1133.4109 1149.6207 1172.9402
1182.7687 1187.0218 1190.0216
1191.1941 1207.4079 1220.7573
1224.4047 1239.3147 1243.7646
1244.8339 1247.8167 1250.4337
1253.5802 1257.8655 1265.3761
1268.1620 1277.1429 1284.5913

1286.0347	1289.3211	1291.9895
1306.6511	1311.4341	1315.1341
1321.7924	1328.7225	1353.3126
1367.6916	1393.7650	1398.9723
1400.5968	1402.1565	1404.1303
1405.2430	1410.0338	1422.7043
1428.8277	1431.4781	1432.2967
1437.9940	1443.9191	1472.0532
1474.8369	1476.2899	1478.4724
1479.3304	1480.6202	1483.0994
1484.6003	1486.2127	1486.9152
1493.6518	1495.7277	1499.8080
1500.2865	1501.2861	1501.9524
1503.2100	1506.3155	1506.6589
1512.7151	1513.2014	1515.1415
1516.6754	1520.1151	1563.7271
1601.1357	1663.9218	1692.7215
1705.0270	1705.0689	3057.6395
3058.2945	3060.9434	3062.3873
3062.4874	3063.0643	3065.0803
3065.7437	3065.8128	3072.4091
3134.9461	3135.4608	3136.1387
3137.6781	3138.8386	3141.2276
3143.2625	3143.4250	3143.4643
3144.6694	3145.4122	3147.6301
3148.9997	3149.8263	3150.6909
3152.3395	3159.0927	3161.6119
3192.7902	3199.6458	3212.2069
3213.2501	3215.1601	3226.3141
3232.4700	3278.2308	3278.7692

20b-ts

Zero-point correction= 0.649321
Thermal correction to Energy= 0.682625
Thermal correction to Enthalpy= 0.683395
Thermal correction to Gibbs Free Energy= 0.587628
Sum of electronic and zero-point Energies= -3169.993549
Sum of electronic and thermal Energies= -3169.960245
Sum of electronic and thermal Enthalpies= -3169.959475
Sum of electronic and thermal Free Energies= -3170.055242

Cartesian coordinates

C	0.653480	1.532276	-0.325190
N	0.832753	0.221435	-0.586722

H	-3.132773	0.273984	-0.132452
N	-0.382443	-0.313579	-0.636194
N	-1.254031	0.621146	-0.417520
N	-0.650716	1.793241	-0.221512
C	1.686796	2.568527	-0.166325
C	1.411721	3.685371	0.625453
C	2.926171	2.499087	-0.817654
C	2.344234	4.710131	0.784651
H	0.454021	3.754639	1.132578
C	3.863378	3.508257	-0.667538
H	3.159742	1.650040	-1.448188
C	3.578992	4.619570	0.136387
H	2.098288	5.559718	1.410658
H	4.824922	3.455840	-1.168584
C	-4.544289	-0.269659	1.276354
C	-4.982136	0.125999	-1.044161
C	-6.318141	-0.171425	-0.841640
C	-6.800007	-0.523773	0.425373
C	-5.886280	-0.566536	1.478831
H	-6.995922	-0.127254	-1.683506
H	-6.210834	-0.832465	2.473527
N	-4.145161	0.059909	0.024744
C	-3.498726	-0.286453	2.383710
C	-2.441900	-1.359494	2.062943
C	-2.861320	1.111470	2.492571
C	-4.131689	-0.629068	3.736405
H	-1.944215	-1.197312	1.104715
H	-1.671894	-1.345189	2.840999
H	-2.898499	-2.355019	2.052016
H	-3.615962	1.857597	2.764797
H	-2.098451	1.093457	3.277553
H	-2.374039	1.431495	1.569239
H	-3.345386	-0.616365	4.496844
H	-4.893005	0.100685	4.031579
H	-4.577930	-1.628848	3.738633
C	-4.391592	0.524355	-2.390294
C	-3.745890	1.917368	-2.267293
C	-3.353080	-0.530999	-2.813166
C	-5.477731	0.591860	-3.468961
H	-4.494665	2.666294	-1.987221
H	-2.934266	1.944881	-1.537147
H	-3.325415	2.201397	-3.237168
H	-3.829020	-1.508747	-2.943390
H	-2.911604	-0.234291	-3.770016

H	-2.540015	-0.633614	-2.091050
H	-5.009472	0.888697	-4.411965
H	-5.958114	-0.378940	-3.628424
H	-6.247698	1.333886	-3.232024
C	-8.281636	-0.838232	0.607391
C	-9.103260	0.394256	0.186595
C	-8.647200	-2.031490	-0.293809
C	-8.624620	-1.189433	2.057960
H	-8.847244	1.266280	0.797507
H	-8.941005	0.652261	-0.864283
H	-10.169220	0.183469	0.320792
H	-8.072177	-2.922485	-0.020721
H	-9.711331	-2.262193	-0.178459
H	-8.462383	-1.814168	-1.350070
H	-9.694896	-1.404903	2.130838
H	-8.082934	-2.077610	2.400337
H	-8.405631	-0.360812	2.740048
O	3.852483	-2.532040	0.164922
S	5.366526	-2.316420	-0.245163
S	2.556636	-1.283568	0.006934
C	6.095106	-1.970099	1.422654
C	2.470692	-1.507886	-1.895427
F	5.579067	-0.868208	1.938224
F	7.406591	-1.822696	1.277378
F	5.853068	-2.994741	2.228918
F	3.323961	-2.435548	-2.297687
F	2.772245	-0.364756	-2.471615
F	1.253268	-1.895513	-2.196659
O	5.526291	-1.124951	-1.048255
O	5.907677	-3.589401	-0.655536
O	3.264939	-0.126721	0.482450
O	1.548945	-2.050399	0.684665
O	4.558833	5.555259	0.225045
C	4.311351	6.700357	1.025132
H	4.125363	6.421815	2.068538
H	5.215827	7.306033	0.968587
H	3.462724	7.275646	0.637887

Vibrational frequencies

-110.5556	11.4745	14.3198
17.7237	21.5485	29.2871
32.9051	36.4104	38.2478
43.6122	53.6375	60.7917
61.5099	63.7355	75.7541

80.1673 86.5991 93.7311
95.6383 109.8302 112.3974
118.1717 135.8429 138.1894
146.2381 148.8145 156.9230
159.0973 167.7056 190.7210
195.6483 204.6164 209.3083
210.9094 228.4700 234.9459
238.9800 247.1763 248.0968
255.0791 261.6074 268.7953
272.6084 280.9519 285.3647
293.0139 300.1835 305.7613
307.2448 312.1307 317.6083
323.2198 334.4678 338.3453
351.6313 353.9324 359.4296
360.2887 362.5867 363.7093
370.1137 383.5861 389.8628
390.8456 394.2651 401.8216
414.4375 422.5469 426.7284
443.8082 463.7913 467.6268
468.2271 510.2736 518.1702
542.8147 548.3355 553.1088
553.2181 556.8566 566.1958
568.3671 569.2110 570.9212
580.2298 616.0770 627.3383
630.7351 651.5293 684.1606
694.0239 732.4583 770.3348
782.3208 784.9561 786.1511
789.8540 793.3800 798.1553
830.8656 839.1369 846.9268
862.7629 865.4919 915.7564
925.1318 927.6207 938.5889
950.2465 951.6577 952.7743
958.1346 961.8730 964.7814
967.1151 968.0285 973.8795
975.0570 993.0085 1020.5631
1023.7035 1040.3947 1045.1380
1047.8394 1051.2863 1052.0622
1053.4529 1056.5458 1059.6627
1083.0521 1089.7810 1101.1585
1141.8534 1149.4500 1177.9610
1179.0967 1180.9531 1190.0844
1199.6650 1207.9586 1211.2631
1217.8083 1223.5552 1239.8220
1241.6146 1243.0274 1249.4214

1252.9553	1256.4130	1263.2577
1266.9853	1270.2394	1287.2228
1288.7034	1290.0165	1293.6015
1312.8825	1319.2562	1319.4347
1329.6424	1350.3430	1357.5186
1369.5699	1395.7010	1399.1328
1402.2749	1402.4865	1402.7835
1406.0814	1406.6579	1424.2955
1429.5628	1430.8222	1434.7303
1443.6010	1451.4704	1473.5207
1475.7569	1477.8239	1478.7921
1480.3755	1481.7223	1481.9382
1484.4136	1484.8268	1485.9021
1486.7675	1494.7634	1495.5386
1499.1657	1500.4723	1502.2363
1503.2000	1504.2478	1506.3922
1512.0913	1513.6495	1515.4702
1519.2649	1520.0228	1570.9109
1606.6184	1661.5842	1698.9156
1703.1693	1707.9379	3044.7167
3057.1158	3057.2651	3060.4513
3060.5909	3063.3171	3063.5908
3063.8325	3066.4803	3067.1304
3070.0754	3136.0385	3136.4793
3136.6298	3137.5508	3139.9766
3140.6560	3141.4268	3141.6969
3143.9349	3144.0364	3145.6808
3147.0109	3149.9393	3151.1247
3151.6062	3175.5230	3176.0297
3180.3514	3182.1608	3186.9659
3217.5078	3219.2807	3253.5097
3266.0698	3273.6978	3293.2611

27b-ts

Zero-point correction= 0.651461
Thermal correction to Energy= 0.683796
Thermal correction to Enthalpy= 0.684566
Thermal correction to Gibbs Free Energy= 0.593749
Sum of electronic and zero-point Energies= -3169.991679
Sum of electronic and thermal Energies= -3169.959345
Sum of electronic and thermal Enthalpies= -3169.958575
Sum of electronic and thermal Free Energies= -3170.049391

Cartesian coordinates

C	3.176182	-1.643327	-0.239604
N	3.191440	-2.961404	-0.498079
H	1.029260	0.655945	0.050978
N	1.925020	-3.335398	-0.508410
N	1.174573	-2.300362	-0.258977
N	1.918488	-1.202565	-0.091584
C	4.410051	-0.842520	-0.142404
C	4.398710	0.544872	0.063278
C	5.649561	-1.479161	-0.252301
C	5.578517	1.266715	0.155221
H	3.457208	1.074537	0.151197
C	6.845132	-0.768191	-0.162221
H	5.681027	-2.552499	-0.410010
C	6.811889	0.613882	0.044323
H	5.566503	2.340481	0.315333
H	7.785667	-1.299164	-0.250951
C	-0.080540	1.828202	1.330754
C	-0.033127	2.040805	-1.058441
C	-1.019992	3.008422	-0.982752
C	-1.564054	3.409817	0.242007
C	-1.060222	2.811989	1.395192
H	-1.370695	3.466096	-1.897241
H	-1.429617	3.107388	2.365155
N	0.385943	1.469813	0.106863
C	0.479482	1.158473	2.584735
C	-0.020971	-0.292925	2.656791
C	2.014378	1.153417	2.541907
C	0.027776	1.903048	3.847361
H	0.392674	-0.882940	1.838964
H	0.315158	-0.734619	3.601117
H	-1.113147	-0.348277	2.611406
H	2.423871	2.153662	2.361241
H	2.397420	0.798318	3.503490
H	2.381975	0.465421	1.779282
H	0.497096	1.424815	4.711482
H	0.335093	2.954477	3.837300
H	-1.055368	1.851494	3.995010
C	0.602142	1.626423	-2.386497
C	2.131292	1.609662	-2.254501
C	0.124433	0.223834	-2.795118
C	0.218447	2.614245	-3.496368
H	2.518135	2.546851	-1.839030
H	2.462178	0.773575	-1.637821
H	2.574822	1.467851	-3.244837

H	-0.968438	0.163166	-2.820765
H	0.506632	-0.000467	-3.796476
H	0.509838	-0.536335	-2.114689
H	0.754340	2.330318	-4.405996
H	-0.851212	2.584525	-3.726288
H	0.499643	3.643105	-3.247121
C	-2.644419	4.486295	0.274249
C	-2.074170	5.775430	-0.344351
C	-3.848753	4.007689	-0.555759
C	-3.117357	4.788117	1.698558
H	-1.195513	6.122543	0.209504
H	-1.787698	5.633282	-1.390904
H	-2.834963	6.562043	-0.307749
H	-4.287130	3.101932	-0.125167
H	-4.616875	4.788028	-0.563486
H	-3.572796	3.797092	-1.593604
H	-3.901120	5.550767	1.660207
H	-3.538968	3.900882	2.182628
H	-2.306419	5.176344	2.324280
O	-3.391265	-1.403432	1.501793
S	-4.017677	-1.797692	0.260342
S	-1.180393	-2.246422	-0.625336
C	-4.455878	-0.246424	-0.653462
C	-1.067243	-3.598999	0.727800
F	-3.391760	0.527774	-0.799699
F	-5.378606	0.399208	0.051039
F	-4.944527	-0.556372	-1.845182
F	-0.386173	-4.595108	0.216484
F	-2.274412	-4.020271	1.064315
F	-0.475433	-3.096908	1.787662
O	-5.200869	-2.620885	0.230091
O	-2.966992	-2.416089	-0.751096
O	-1.091857	-0.887803	-0.159149
O	-0.907157	-2.762480	-1.937741
O	7.913736	1.399527	0.150860
C	9.184817	0.773515	0.060668
H	9.920016	1.570149	0.174479
H	9.319787	0.036959	0.860634
H	9.319413	0.292068	-0.914352

Vibrational frequencies

-79.0695	11.6895	26.6824
29.2310	35.8884	43.9085
44.6895	50.9798	52.6162

55.1150 63.5379 69.7004
73.9148 75.6641 82.9205
89.1466 96.7488 97.1611
104.7898 105.5415 119.2521
126.1731 140.2581 149.0429
158.5158 163.2885 167.0871
177.1418 181.7301 192.8831
195.1129 221.7466 229.5821
232.6903 244.9690 249.4602
252.9471 262.8575 267.1016
275.7835 276.6692 283.6932
286.6783 292.4471 301.0724
307.6362 310.8736 315.4449
320.2579 323.4614 326.0929
329.0819 331.5503 334.5247
341.2751 358.2968 363.0515
365.0033 369.2295 382.0863
386.7862 390.4826 393.4772
395.6831 406.7919 412.5616
418.2302 426.2155 434.3771
441.3940 461.9832 465.5877
486.2048 511.0288 518.4822
545.5510 548.3164 553.5074
556.1671 562.3321 566.5978
568.0766 570.3268 579.5096
580.0419 613.6727 629.0251
633.6196 652.2771 682.2916
692.0999 730.2996 759.3902
772.9923 782.5271 785.6118
789.1465 794.4658 797.0716
830.9190 844.2400 852.2079
853.8601 868.2528 879.0034
920.9811 923.6161 928.8478
939.6314 951.1592 957.5517
959.8498 961.0483 963.1128
965.0584 975.4948 978.4945
982.6940 984.0604 1019.4961
1027.2625 1031.2932 1046.4336
1047.0776 1049.3431 1054.6361
1058.1714 1059.3200 1061.3410
1080.8079 1089.5835 1099.9546
1139.1791 1150.3648 1169.0512
1181.1311 1187.6961 1194.7342
1202.4679 1208.8815 1215.5099

1217.4117	1220.2070	1239.6299
1246.1156	1247.4019	1254.1929
1254.7920	1262.1225	1265.4855
1266.7204	1269.7923	1281.8487
1282.8150	1290.6607	1291.8877
1312.0986	1318.9627	1322.3845
1326.4795	1328.6025	1348.4213
1362.0918	1392.5727	1394.6005
1400.9653	1402.0093	1403.6558
1405.8661	1406.7849	1426.9991
1429.8932	1431.2722	1435.7104
1437.5858	1448.5733	1473.0445
1476.2526	1477.9394	1480.2682
1483.8567	1485.9176	1486.0389
1487.4997	1491.8249	1492.9468
1494.3215	1495.1903	1500.3793
1502.9929	1503.8706	1505.5581
1508.2963	1509.7967	1511.8488
1512.1811	1514.9342	1520.9884
1527.5790	1531.6573	1571.6055
1598.7113	1661.8043	1696.1528
1700.7124	1701.0744	3055.6083
3060.3768	3062.6247	3063.8479
3064.8795	3065.3179	3067.4108
3067.5709	3070.2494	3076.1212
3135.5639	3138.1990	3140.3466
3141.6502	3143.2407	3144.1546
3144.3883	3144.6681	3145.3890
3145.5072	3145.6550	3148.0293
3151.3881	3151.7625	3153.7653
3187.1925	3187.8157	3194.1028
3196.2858	3197.2000	3211.2963
3215.5256	3220.7070	3240.4044
3250.2709	3278.1760	3295.9405

28b-ts

Zero-point correction= 0.649558
Thermal correction to Energy= 0.682509
Thermal correction to Enthalpy= 0.683279
Thermal correction to Gibbs Free Energy= 0.589175
Sum of electronic and zero-point Energies= -3169.994479
Sum of electronic and thermal Energies= -3169.961528
Sum of electronic and thermal Enthalpies= -3169.960758
Sum of electronic and thermal Free Energies= -3170.054862

Cartesian coordinates

C	0.424973	1.940762	-0.012645
N	-0.882322	2.198862	0.066768
H	2.077117	-0.640891	0.097753
N	-1.443837	1.008303	0.234267
N	-0.546187	0.066138	0.258186
N	0.652785	0.619688	0.106297
C	1.462383	2.964224	-0.209076
C	2.819226	2.621744	-0.311015
C	1.110671	4.312029	-0.304958
C	3.788615	3.594950	-0.498343
H	3.122309	1.580368	-0.244475
C	2.074055	5.302230	-0.494631
H	0.064328	4.592676	-0.231562
C	3.421295	4.943216	-0.592104
H	4.839254	3.332753	-0.577256
H	1.762148	6.337740	-0.563869
C	3.386068	-1.674552	-1.129800
C	3.625698	-1.416766	1.238966
C	4.848907	-2.061366	1.182500
C	5.383711	-2.505808	-0.032754
C	4.616171	-2.319763	-1.182449
H	5.391804	-2.227919	2.102755
H	4.966952	-2.683879	-2.136373
N	2.957713	-1.212138	0.070947
C	2.486689	-1.492915	-2.348672
C	1.093362	-2.067552	-2.033586
C	2.384257	-0.000348	-2.706987
C	3.052177	-2.242736	-3.560251
H	0.598138	-1.556645	-1.203990
H	0.453761	-1.949719	-2.913893
H	1.157376	-3.135704	-1.799270
H	3.374080	0.431733	-2.889835
H	1.790897	0.103401	-3.621290
H	1.885308	0.569741	-1.922447
H	2.346635	-2.135798	-4.388986
H	4.012338	-1.833041	-3.890490
H	3.173116	-3.312689	-3.361026
C	2.978299	-0.961005	2.542919
C	2.918766	0.574997	2.590239
C	1.561366	-1.556293	2.635690
C	3.788290	-1.448112	3.749777
H	3.916946	1.013916	2.486115

H	2.270153	0.976844	1.811217
H	2.508390	0.884595	3.556923
H	1.596851	-2.650944	2.626666
H	1.103697	-1.237045	3.577355
H	0.907275	-1.221391	1.826600
H	3.266711	-1.142414	4.661106
H	3.882685	-2.538928	3.768320
H	4.789589	-1.005654	3.778944
C	6.751477	-3.180872	-0.053956
C	7.791528	-2.196386	0.511797
C	6.701280	-4.440459	0.829803
C	7.174231	-3.587384	-1.468395
H	7.831683	-1.279458	-0.085705
H	7.571188	-1.922310	1.548016
H	8.782255	-2.661889	0.490352
H	5.957451	-5.152932	0.457990
H	7.679903	-4.931357	0.816782
H	6.459881	-4.201866	1.870058
H	8.163251	-4.053519	-1.425383
H	6.483249	-4.315431	-1.906409
H	7.243163	-2.722768	-2.137361
O	-5.507441	-1.898486	0.982397
S	-6.409217	-0.981461	0.329350
S	-3.907655	0.567927	-0.153112
C	-6.785679	-1.654582	-1.356459
C	-3.718954	0.707276	1.740624
F	-7.489473	-2.768179	-1.204813
F	-5.661061	-1.919353	-1.997425
F	-7.494287	-0.767549	-2.036826
F	-4.907649	0.586152	2.317757
F	-3.229432	1.890472	2.031110
F	-2.937332	-0.263977	2.153759
O	-5.648369	0.359728	-0.104959
O	-7.669700	-0.590045	0.905758
O	-3.886606	1.850757	-0.794014
O	-3.434472	-0.680998	-0.676997
O	4.437700	5.824455	-0.777657
C	4.108220	7.200442	-0.895659
H	3.623662	7.569530	0.015246
H	5.053843	7.723002	-1.040260
H	3.457195	7.377256	-1.759109

Vibrational frequencies

-39.2820	12.0067	16.4473

22.1638	25.5830	28.6755
39.1265	41.2317	47.3267
48.5707	56.3897	57.3953
62.4270	72.9184	76.4257
83.4123	91.0556	97.3816
103.6205	105.3763	117.0982
131.7961	134.7660	142.5820
145.1414	155.1166	158.5733
168.2941	171.5578	181.4594
192.7600	221.8816	225.1061
230.2714	239.6601	244.9168
245.7849	253.6651	256.6065
260.3692	268.0638	277.2213
284.0606	287.1972	290.4357
297.5879	301.1246	306.8620
310.2644	315.0613	322.5845
324.0202	330.7273	331.0843
343.2880	352.5738	355.9131
358.2401	360.0628	368.2316
373.9326	378.3739	388.3567
390.3954	393.1542	404.2268
421.9730	423.3963	438.4398
441.8213	456.6323	459.7237
467.6934	515.4164	522.1045
540.2125	548.6966	550.9759
554.5259	556.0603	564.1746
565.6361	571.7298	572.8120
582.5537	613.4504	630.9569
648.0450	649.6347	682.4880
695.7064	732.4684	770.1034
784.0612	784.5139	786.3583
788.9868	792.7344	794.0809
828.7070	834.2024	844.5556
846.4824	866.1546	922.2202
924.6903	927.9369	947.4426
951.2632	951.9381	953.7615
958.5580	958.9852	963.8353
966.9566	967.9211	978.2192
982.9816	1000.6396	1007.9925
1020.0612	1044.6227	1048.8451
1049.6031	1050.6946	1051.9785
1052.7032	1053.6173	1065.6847
1091.5025	1098.1076	1099.7614
1136.9188	1146.2410	1177.0813

1180.2533	1185.4532	1190.7468
1198.3244	1205.0686	1215.0329
1230.0318	1234.4062	1239.0622
1242.6408	1245.5126	1248.9595
1250.3325	1257.0137	1261.9826
1265.7773	1277.2554	1279.6363
1285.1637	1291.3032	1293.0988
1310.7975	1315.7782	1323.9476
1324.6282	1325.3815	1350.6548
1366.6116	1392.8239	1397.8615
1400.2156	1402.6644	1403.4467
1405.1044	1417.2386	1424.1278
1429.3753	1431.4198	1434.5728
1442.8403	1457.9840	1473.8992
1474.3337	1476.2059	1478.8798
1479.9723	1480.6938	1481.9217
1483.0569	1486.3214	1487.7777
1493.2070	1494.9417	1496.3091
1500.0500	1500.3535	1501.3010
1501.8911	1503.2776	1506.7063
1512.6734	1514.0102	1515.7431
1517.1464	1521.9929	1559.8675
1601.6860	1663.7490	1689.9814
1700.3474	1701.0320	2975.5226
3057.7175	3059.4034	3060.0621
3061.1614	3062.3964	3063.4052
3064.2085	3066.0699	3068.7604
3069.4068	3136.5807	3136.9227
3137.1797	3138.8519	3139.4295
3140.0763	3140.4512	3140.8389
3141.1370	3142.7879	3145.6533
3146.0605	3147.6401	3154.1983
3155.4320	3164.1177	3176.4067
3188.0032	3193.0048	3197.5533
3203.6105	3219.4693	3223.3742
3242.8911	3262.8831	3307.4329

29b-ts

Zero-point correction= 0.649443
Thermal correction to Energy= 0.682799
Thermal correction to Enthalpy= 0.683569
Thermal correction to Gibbs Free Energy= 0.587761
Sum of electronic and zero-point Energies= -3169.990615
Sum of electronic and thermal Energies= -3169.957260

Sum of electronic and thermal Enthalpies= -3169.956490
Sum of electronic and thermal Free Energies= -3170.052298

Cartesian coordinates

C	-0.217743	-0.190117	0.220400
N	-1.113918	-1.091025	0.658208
H	3.041453	-0.496400	-0.033925
N	-0.429814	-2.215834	0.875569
N	0.816650	-2.015018	0.592928
N	0.993222	-0.754929	0.174737
C	-0.478912	1.219127	-0.115659
C	0.267938	1.861176	-1.114707
C	-1.433003	1.961858	0.579770
C	0.061718	3.199825	-1.408801
H	1.013906	1.302202	-1.672380
C	-1.653579	3.308917	0.296235
H	-2.017183	1.488009	1.360335
C	-0.902525	3.932243	-0.703670
H	0.630390	3.698216	-2.187793
H	-2.406558	3.851321	0.855531
C	4.736246	-0.989641	-1.101099
C	4.693162	0.261831	0.942870
C	6.071668	0.365556	0.905929
C	6.818607	-0.210358	-0.130008
C	6.121399	-0.885727	-1.132109
H	6.573006	0.903202	1.699116
H	6.651051	-1.344616	-1.953392
N	4.077170	-0.414044	-0.065873
C	3.931857	-1.738013	-2.156488
C	3.334122	-2.999526	-1.507199
C	2.809142	-0.836052	-2.695945
C	4.823728	-2.161932	-3.328307
H	2.673817	-2.762279	-0.668550
H	2.741374	-3.537700	-2.254156
H	4.127806	-3.666889	-1.154240
H	3.208855	0.107959	-3.082519
H	2.300923	-1.353243	-3.515562
H	2.059464	-0.626732	-1.929788
H	4.199011	-2.668994	-4.068937
H	5.294320	-1.302700	-3.818286
H	5.603497	-2.865024	-3.019225
C	3.828037	0.850538	2.049740
C	2.796879	1.807598	1.427924
C	3.126556	-0.300086	2.795489

C	4.676045	1.635792	3.055327
H	3.291908	2.642959	0.920840
H	2.147508	1.299877	0.714036
H	2.157344	2.214980	2.217807
H	3.863053	-0.959107	3.267438
H	2.488049	0.119326	3.579729
H	2.493647	-0.902216	2.139617
H	4.009576	2.052321	3.816162
H	5.404492	0.997760	3.566101
H	5.204034	2.470071	2.581583
C	8.338691	-0.082105	-0.127856
C	8.710339	1.411496	-0.155053
C	8.887159	-0.726233	1.158440
C	8.979258	-0.771697	-1.335434
H	8.317792	1.898806	-1.053748
H	8.326849	1.943347	0.720832
H	9.800405	1.513693	-0.159676
H	8.621591	-1.787126	1.211535
H	9.979137	-0.646597	1.166427
H	8.508102	-0.231321	2.057527
H	10.064463	-0.641034	-1.286398
H	8.773996	-1.847440	-1.345833
H	8.635646	-0.340079	-2.281531
O	-5.180357	-1.619301	-0.122892
S	-6.290322	-0.531531	0.180173
S	-3.404935	-1.354211	0.045605
C	-6.653380	0.042043	-1.543843
C	-3.497209	-1.410634	1.958555
F	-5.581001	0.594665	-2.083816
F	-7.631123	0.938975	-1.480634
F	-7.045482	-0.987073	-2.281058
F	-4.736858	-1.646429	2.357886
F	-3.105589	-0.247940	2.434011
F	-2.727172	-2.387749	2.372260
O	-5.737434	0.592479	0.902407
O	-7.478565	-1.215599	0.628998
O	-3.284121	-0.048883	-0.542745
O	-3.021789	-2.620178	-0.512767
O	-1.034366	5.235915	-1.058083
C	-2.006027	6.013874	-0.374787
H	-1.783342	6.070215	0.696750
H	-1.949100	7.012086	-0.808879
H	-3.012302	5.606939	-0.523450

Vibrational frequencies

-109.6545	10.9521	12.7633
19.8381	23.1636	29.4614
34.4438	37.7032	43.5074
45.7827	49.8065	52.8643
61.7284	64.6567	71.1002
77.3834	82.0104	89.3781
101.6837	110.6983	115.9512
123.4490	128.8959	134.5827
144.6577	148.4401	151.1068
160.6688	164.2130	183.3200
194.0383	197.1527	212.5152
214.1154	228.3881	233.5145
243.2281	247.8171	248.1917
254.2884	262.7888	263.9718
266.7342	279.1123	291.6854
292.5313	298.0925	304.9038
313.1108	320.7171	322.9080
325.2052	332.0472	337.5126
342.0831	349.8792	356.2380
362.2856	366.5408	370.1703
377.1958	378.7090	383.8281
389.4325	390.5590	403.5444
414.2505	423.1202	432.1186
438.3057	459.6507	463.8168
467.2450	510.8530	518.1658
539.8537	547.7532	553.2386
555.2608	559.4992	566.1537
567.3960	569.6528	571.8354
580.6593	614.5772	627.0477
631.7199	648.8010	686.6292
697.0952	737.8269	764.9168
782.5102	784.4112	786.4009
786.5211	787.8401	793.7953
831.6157	844.8553	847.9309
859.1849	864.5720	915.3117
924.5597	927.3867	946.9562
951.2276	952.3393	955.3218
960.0910	960.9539	966.2269
969.6899	972.2455	975.0643
982.7029	997.7884	1001.9525
1019.8901	1024.0873	1044.2759
1047.9435	1050.1744	1053.1185
1056.1425	1059.5140	1061.6473

1080.0434	1089.8742	1099.9659
1144.9602	1147.4024	1163.0715
1180.1604	1191.0332	1191.6344
1201.3124	1202.3861	1210.1153
1220.6634	1222.2788	1232.7507
1238.3836	1240.3322	1243.9415
1249.1779	1257.1723	1263.7732
1263.9794	1269.3103	1284.1854
1288.3822	1288.6795	1289.5545
1313.4928	1316.0064	1322.8098
1334.3953	1351.7951	1364.2711
1366.6956	1393.6871	1397.5924
1399.4596	1401.2278	1401.9029
1403.0509	1409.4071	1423.3063
1426.4442	1427.1399	1433.6985
1444.3177	1447.3260	1474.5650
1474.6846	1475.8790	1478.2197
1478.3157	1482.0650	1482.8602
1483.7122	1485.1603	1488.6457
1489.8942	1494.6945	1498.0615
1499.5799	1500.9962	1503.0476
1504.2940	1508.9075	1510.4225
1511.3842	1513.5158	1515.8629
1519.0664	1519.6932	1558.0706
1605.2122	1662.4417	1688.6629
1702.7857	1704.3643	3056.2453
3057.2387	3059.0994	3059.9370
3062.5092	3063.2682	3063.8842
3065.0672	3069.3103	3070.9098
3135.5697	3137.6720	3138.2302
3138.3953	3139.7587	3140.1279
3141.4097	3141.7237	3144.6383
3145.1870	3146.2419	3146.3619
3147.1841	3150.9037	3151.1955
3157.7016	3172.6048	3179.0058
3186.8582	3190.2099	3212.7379
3216.0188	3230.9918	3239.9359
3257.1802	3291.4019	3295.3683

18c-ts

Zero-point correction= 0.619786
Thermal correction to Energy= 0.652958
Thermal correction to Enthalpy= 0.653728
Thermal correction to Gibbs Free Energy= 0.557945

Sum of electronic and zero-point Energies= -3259.975976
Sum of electronic and thermal Energies= -3259.942804
Sum of electronic and thermal Enthalpies= -3259.942034
Sum of electronic and thermal Free Energies= -3260.037817

Cartesian coordinates

C	-2.138295	-2.284089	0.267763
N	-1.086070	-1.496046	-0.034157
H	2.032662	-1.953307	0.259294
N	-0.017616	-2.291300	-0.016061
N	-0.393915	-3.496740	0.273873
N	-1.711651	-3.533185	0.452071
C	-3.568044	-1.935352	0.372627
C	-4.501597	-2.894255	-0.043267
C	-4.007527	-0.716506	0.900802
C	-5.862973	-2.639726	0.054199
H	-4.153388	-3.839682	-0.445220
C	-5.367030	-0.447892	1.002889
H	-3.290300	0.022911	1.234826
C	-6.267379	-1.415928	0.574906
H	-6.595736	-3.369216	-0.269338
H	-5.722592	0.492383	1.406890
C	3.361541	-0.964488	1.470287
C	3.715992	-1.525400	-0.834058
C	4.896682	-0.805339	-0.825573
C	5.317260	-0.111985	0.316846
C	4.544015	-0.235289	1.472534
H	5.499921	-0.786822	-1.723267
H	4.858950	0.232644	2.393635
N	2.972849	-1.529616	0.303342
C	2.517608	-1.211942	2.718114
C	2.234612	-2.720850	2.837054
C	3.269485	-0.756557	3.974075
C	1.191800	-0.438558	2.634587
H	3.166238	-3.294181	2.891730
H	1.665711	-2.904376	3.753573
H	1.636395	-3.104013	2.004161
H	3.423758	0.327087	3.991088
H	2.667505	-1.016825	4.849152
H	4.239913	-1.253868	4.073839
H	0.657003	-0.551280	3.583177
H	1.361143	0.628263	2.456943
H	0.552789	-0.831624	1.844108
C	3.230788	-2.353747	-2.019260

C	4.331898	-2.475797	-3.078570
C	2.865750	-3.766426	-1.526395
C	2.001103	-1.688073	-2.657096
H	4.573583	-1.509725	-3.533145
H	5.248335	-2.915811	-2.671021
H	3.971154	-3.131233	-3.876330
H	2.021767	-3.766853	-0.829337
H	2.571933	-4.377279	-2.385458
H	3.720677	-4.248479	-1.040157
H	1.690212	-2.276614	-3.526786
H	1.170964	-1.649026	-1.953205
H	2.228072	-0.669862	-2.990062
C	6.596572	0.718111	0.267177
C	7.774847	-0.190676	-0.126976
C	6.418434	1.819168	-0.794806
C	6.911851	1.375481	1.613340
H	7.907185	-1.001060	0.597503
H	7.639122	-0.633326	-1.118015
H	8.696060	0.400657	-0.149382
H	5.574917	2.471933	-0.547729
H	7.325108	2.431426	-0.838688
H	6.246641	1.398488	-1.790219
H	7.829490	1.963337	1.516591
H	6.113899	2.054299	1.932434
H	7.076694	0.632519	2.401233
O	-0.279122	2.384671	-0.889941
S	-1.348951	3.523161	-0.876695
S	-0.600098	0.611014	-0.342852
C	-0.904481	4.381242	0.702129
C	-1.578628	0.304082	-1.970859
F	-1.019406	3.562320	1.735837
F	-1.724740	5.414242	0.865775
F	0.346534	4.822643	0.629730
F	-1.542652	1.341802	-2.778088
F	-2.821829	0.038230	-1.636030
F	-1.016741	-0.722971	-2.575422
O	-2.686226	2.989956	-0.714044
O	-1.047702	4.476098	-1.921649
O	-1.336266	0.945462	0.850814
O	0.793216	0.268230	-0.467421
N	-7.705885	-1.137220	0.680110
O	-8.484180	-1.977468	0.258805
O	-8.049868	-0.080850	1.184018

Vibrational frequencies

-104.0504	4.1816	13.8475
20.8425	27.0660	32.8470
37.8133	41.7182	43.3226
51.5567	55.7756	56.1566
59.5069	65.1714	66.9846
74.1843	83.9859	89.7711
92.2722	95.0142	107.3433
113.5387	123.0720	133.4111
138.7530	143.3490	160.0236
165.4523	170.8169	188.6292
192.1377	196.8121	199.5991
213.8708	236.1154	241.8786
246.4214	251.7770	256.5894
260.6730	269.5537	271.9177
286.6626	290.2191	290.7226
298.2733	301.4496	307.4424
311.5825	318.3933	321.2062
323.0708	334.6062	339.1508
350.5422	355.2614	360.3249
366.5629	370.3976	378.1062
382.3993	389.9039	390.2768
393.8819	397.4852	402.9634
421.0811	421.5169	428.7164
464.3237	470.1688	477.7155
514.2710	521.2735	527.5107
544.5412	549.2893	550.5542
554.1329	555.5045	563.6385
568.4476	571.2065	576.2811
578.3621	612.6029	617.0026
640.6691	681.5707	691.5316
713.7796	747.6439	759.4031
764.3116	775.6424	778.6676
786.1303	787.8296	794.7018
802.3322	850.1850	867.2320
891.2209	893.8222	898.2249
903.6585	915.1562	925.9593
931.9314	939.8199	952.4258
954.1677	955.7303	961.9284
964.0964	965.5825	973.5037
974.0940	975.5760	1008.7928
1023.7288	1027.3280	1036.3266
1047.3360	1051.1221	1052.8872
1053.9373	1056.3990	1056.8432

1060.3615	1078.4317	1087.2900
1138.8412	1148.1397	1150.4085
1172.5922	1177.2332	1182.1506
1201.2426	1207.8260	1211.6217
1216.7607	1239.0179	1243.1771
1244.1352	1245.9320	1248.5860
1257.6597	1258.7141	1262.0938
1263.3089	1277.5780	1283.4986
1285.4005	1301.8075	1313.3073
1318.3959	1322.7222	1355.8989
1365.0745	1366.8315	1383.0755
1394.8585	1399.4221	1400.8363
1403.6231	1408.0821	1409.2462
1417.7619	1418.8151	1422.4002
1431.9689	1434.8208	1439.5613
1469.7249	1472.0351	1475.3141
1478.2570	1480.4549	1481.0106
1481.4973	1483.0141	1485.6218
1486.7114	1487.3856	1497.4559
1500.5967	1501.4291	1502.8276
1503.1855	1506.1082	1509.9517
1510.6783	1511.4900	1517.2211
1519.5740	1556.0519	1588.6794
1656.2017	1688.4706	1696.1029
1701.8286	1711.5550	3057.2858
3058.6622	3061.0181	3061.2019
3064.7289	3065.7158	3068.1056
3070.3961	3071.6162	3138.4794
3138.9595	3140.1859	3141.4476
3141.9966	3142.5410	3143.8650
3143.9894	3144.1629	3144.2923
3146.8353	3146.9647	3149.9129
3150.4587	3155.0556	3158.0976
3202.4448	3203.8937	3248.1515
3258.3176	3263.7992	3273.8472
3280.6251	3285.6074	3345.0889

19c-ts

Zero-point correction= 0.619420
Thermal correction to Energy= 0.652547
Thermal correction to Enthalpy= 0.653317
Thermal correction to Gibbs Free Energy= 0.558782
Sum of electronic and zero-point Energies= -3259.983847
Sum of electronic and thermal Energies= -3259.950721

Sum of electronic and thermal Enthalpies= -3259.949951
Sum of electronic and thermal Free Energies= -3260.044486

Cartesian coordinates

C	3.562556	-0.006805	0.185425
N	2.912767	1.106722	-0.167460
H	-0.120223	-1.623311	0.462953
N	1.652776	0.836107	0.100841
N	1.522830	-0.378534	0.581090
N	2.715267	-0.936806	0.654630
C	5.014417	-0.192660	0.066506
C	5.616683	-1.346652	0.583797
C	5.797344	0.780194	-0.568071
C	6.987388	-1.534000	0.469590
H	5.005629	-2.095218	1.076971
C	7.169117	0.605436	-0.690129
H	5.325053	1.670936	-0.968888
C	7.738511	-0.551747	-0.167960
H	7.468707	-2.420316	0.865466
H	7.788561	1.346790	-1.180827
C	-1.432371	-2.418703	-0.904212
C	-1.899778	-2.002012	1.409708
C	-3.222856	-2.351628	1.204010
C	-3.689166	-2.712914	-0.066167
C	-2.761818	-2.765930	-1.108137
H	-3.899389	-2.350439	2.048390
H	-3.065964	-3.088571	-2.092679
N	-1.071501	-2.007226	0.333763
C	-0.358426	-2.526356	-1.983394
C	0.063524	-1.125582	-2.456958
C	0.856577	-3.277975	-1.410845
C	-0.885442	-3.311378	-3.190968
H	0.560068	-0.567541	-1.663083
H	0.771396	-1.229419	-3.285737
H	-0.798167	-0.548088	-2.808014
H	0.570575	-4.272582	-1.051892
H	1.602414	-3.402080	-2.201904
H	1.343180	-2.735820	-0.594577
H	-0.066400	-3.436997	-3.904719
H	-1.241006	-4.307890	-2.908243
H	-1.691484	-2.782068	-3.708845
C	-1.311185	-1.659014	2.773870
C	-0.018261	-2.468359	2.986872
C	-1.003125	-0.154646	2.843581

C	-2.299847	-2.015352	3.889602
H	-0.203327	-3.544235	2.896289
H	0.774001	-2.186478	2.285806
H	0.360545	-2.271495	3.994510
H	-1.894312	0.446304	2.636318
H	-0.644224	0.087226	3.849901
H	-0.226679	0.116294	2.128766
H	-1.821677	-1.813695	4.852318
H	-3.209312	-1.408077	3.842221
H	-2.579653	-3.074290	3.868142
C	-5.160463	-3.068575	-0.256234
C	-5.496600	-4.277487	0.635566
C	-6.018687	-1.863328	0.168541
C	-5.486782	-3.419424	-1.710685
H	-4.892548	-5.149450	0.363164
H	-5.328848	-4.060273	1.694680
H	-6.552101	-4.539852	0.508882
H	-5.796708	-0.986591	-0.448128
H	-7.078201	-2.109659	0.044467
H	-5.855114	-1.594739	1.216584
H	-6.554034	-3.645984	-1.793977
H	-5.269883	-2.585874	-2.387593
H	-4.933088	-4.300986	-2.051309
O	-2.705437	2.646645	1.304015
S	-2.933518	3.234126	0.003587
S	-0.262498	2.013043	-0.585502
C	-4.090755	2.113985	-0.914603
C	0.422091	3.143490	0.800214
F	-5.266536	2.143731	-0.298285
F	-3.628492	0.873707	-0.924773
F	-4.232247	2.544037	-2.159841
F	-0.333664	4.218159	0.942512
F	1.630061	3.511392	0.441806
F	0.433560	2.466497	1.927029
O	-1.646981	3.109052	-0.914876
O	-3.464265	4.565012	-0.153479
O	0.391527	2.232231	-1.846114
O	-0.970883	0.841106	-0.141001
N	9.185825	-0.745178	-0.297813
O	9.675468	-1.757881	0.177272
O	9.830909	0.115208	-0.875780

Vibrational frequencies

-70.0251	12.8750	17.2720

20.0683	27.8560	34.0684
39.2931	39.5328	51.9107
53.6966	58.1341	61.2504
62.7080	64.8580	71.2840
73.6123	79.4980	84.9355
89.0922	95.2619	104.1141
117.9514	121.4153	136.4831
142.6534	144.3059	155.9114
172.5000	175.2234	182.9457
191.7369	202.4743	221.2513
230.3917	232.6092	235.8329
244.4353	245.7465	253.2908
258.2308	269.6406	276.6764
278.7426	280.4212	282.7711
298.9189	302.0134	306.7815
315.2123	316.1258	318.9495
326.3019	331.3786	339.7826
350.2109	355.2009	361.9446
364.2052	365.9570	370.1618
374.1559	385.3755	389.9816
390.4486	391.5686	404.1295
415.8189	420.0404	437.1392
464.9301	467.9610	474.6965
516.6131	518.1411	523.2248
544.0979	547.4988	550.0159
553.1898	557.0198	562.5941
567.2831	570.0380	573.2485
580.8425	613.3667	633.1988
638.4830	682.6454	693.3306
710.0407	744.3667	757.4829
768.2547	779.7911	783.2001
784.8679	785.5203	792.1806
800.7036	846.9040	858.9751
860.6601	888.4678	893.6601
917.5169	925.6949	926.1733
938.5263	951.3164	953.2781
956.8744	957.8352	961.6658
963.4817	964.4604	972.2201
973.9408	975.5850	1003.4268
1017.3767	1021.8390	1033.6593
1043.1200	1047.1583	1049.4215
1050.3053	1053.2488	1054.0196
1056.9255	1084.0204	1097.1514
1131.0391	1146.3689	1150.5815

1176.3927	1181.7506	1183.3125
1200.8405	1206.3327	1217.2795
1235.3424	1241.0448	1243.5226
1244.2091	1249.5515	1257.3429
1264.8295	1265.6683	1271.2541
1271.6690	1282.3354	1282.9005
1287.8579	1292.8638	1313.5134
1316.0435	1318.4840	1322.0922
1365.5159	1367.7510	1391.8679
1398.5084	1401.3018	1402.0941
1402.9959	1404.7579	1405.8005
1421.1457	1427.1057	1430.2577
1431.4084	1436.2599	1440.0663
1464.9276	1469.1156	1472.9276
1476.9834	1478.5522	1479.9452
1480.2206	1483.7796	1484.5726
1486.3999	1492.4049	1494.6040
1499.2715	1501.2798	1502.1653
1502.6658	1503.6928	1507.6302
1511.9425	1516.7303	1517.1374
1521.2706	1560.6897	1583.7628
1652.8505	1689.9871	1691.5308
1701.7881	1707.3501	3057.0351
3058.2472	3061.3832	3062.3571
3064.4592	3064.9212	3065.8447
3067.7846	3069.6736	3136.4030
3139.7025	3139.8858	3141.0668
3141.5786	3141.8490	3142.5399
3144.5949	3144.9956	3145.1804
3146.2439	3148.8707	3149.2411
3149.9045	3153.0292	3159.0369
3199.0213	3210.3614	3226.9130
3229.7977	3248.7012	3250.7669
3267.1735	3289.3383	3294.1690

20c-ts

Zero-point correction= 0.619178
Thermal correction to Energy= 0.652573
Thermal correction to Enthalpy= 0.653343
Thermal correction to Gibbs Free Energy= 0.556469
Sum of electronic and zero-point Energies= -3259.975835
Sum of electronic and thermal Energies= -3259.942440
Sum of electronic and thermal Enthalpies= -3259.941670
Sum of electronic and thermal Free Energies= -3260.038544

Cartesian coordinates

C	-0.622696	1.310317	0.303427
N	-0.789987	-0.012475	0.510117
H	3.244719	0.131539	0.137920
N	0.426909	-0.536654	0.567829
N	1.291352	0.417038	0.415061
N	0.678075	1.587626	0.247455
C	-1.651388	2.355182	0.155424
C	-1.344755	3.474696	-0.630622
C	-2.885023	2.286016	0.811346
C	-2.258988	4.509883	-0.771930
H	-0.385691	3.528180	-1.134546
C	-3.810390	3.313502	0.680515
H	-3.128351	1.432403	1.429794
C	-3.477823	4.406381	-0.111276
H	-2.035386	5.378541	-1.379354
H	-4.768634	3.270016	1.184072
C	4.701894	-0.221221	-1.276575
C	5.081145	0.064396	1.071990
C	6.439657	-0.099345	0.870873
C	6.962249	-0.332315	-0.408237
C	6.065432	-0.393149	-1.476045
H	7.103547	-0.049325	1.723408
H	6.420630	-0.571677	-2.479952
N	4.266080	0.001275	-0.013701
C	3.667234	-0.259761	-2.393093
C	2.672263	-1.402782	-2.118163
C	2.950770	1.101977	-2.454172
C	4.328683	-0.514999	-3.751239
H	2.157945	-1.300612	-1.159883
H	1.908176	-1.409102	-2.901964
H	3.186510	-2.369498	-2.133815
H	3.662853	1.901776	-2.684357
H	2.198306	1.073357	-3.248821
H	2.437483	1.353020	-1.523534
H	3.547875	-0.531490	-4.517133
H	5.038448	0.275305	-4.016851
H	4.844658	-1.480036	-3.781601
C	4.439177	0.306355	2.431186
C	3.715576	1.665385	2.413210
C	3.453638	-0.838442	2.730756
C	5.496772	0.333237	3.538957
H	4.426959	2.479361	2.238064

H	2.934280	1.716150	1.651223
H	3.240176	1.829057	3.385533
H	3.976120	-1.800480	2.758668
H	2.997030	-0.669272	3.711124
H	2.644915	-0.901884	1.998841
H	4.993577	0.506816	4.494430
H	6.034290	-0.617761	3.615544
H	6.223312	1.139686	3.395145
C	8.466961	-0.506483	-0.586901
C	9.169294	0.775955	-0.106600
C	8.930299	-1.699692	0.268201
C	8.852012	-0.764342	-2.046074
H	8.848521	1.644394	-0.691575
H	8.967074	0.980082	0.949003
H	10.251985	0.664360	-0.226281
H	8.424662	-2.621652	-0.037606
H	10.008207	-1.842524	0.140629
H	8.736955	-1.538009	1.332871
H	9.937899	-0.880047	-2.113113
H	8.396203	-1.682554	-2.431782
H	8.567077	0.069077	-2.697147
O	-3.791003	-2.672728	-0.209867
S	-5.292708	-2.427760	0.192002
S	-2.447718	-1.429591	-0.048517
C	-6.017379	-2.057227	-1.471575
C	-2.393360	-1.693782	1.852601
F	-5.486230	-0.959111	-1.982540
F	-7.327241	-1.889719	-1.326762
F	-5.792705	-3.079085	-2.287582
F	-3.260950	-2.607649	2.243448
F	-2.672874	-0.548623	2.441330
F	-1.181060	-2.101491	2.154588
O	-5.435643	-1.235855	1.000780
O	-5.873876	-3.686508	0.596796
O	-3.170288	-0.282916	-0.535555
O	-1.480439	-2.238952	-0.739010
N	-4.448853	5.498432	-0.249832
O	-4.159388	6.434402	-0.978130
O	-5.496680	5.417104	0.370053

Vibrational frequencies

-109.8609	6.3442	13.9233
17.2815	20.4518	28.3012
35.1124	37.8747	38.4571

41.7652 52.3480 52.7237
57.6219 63.7055 65.4298
77.4807 81.7259 86.7561
99.4461 108.2317 109.4663
118.5214 129.3616 136.6860
140.0372 144.9393 151.0714
157.8663 162.7598 191.4956
194.5995 203.3645 209.1326
212.0086 219.2085 221.6748
235.5497 248.2151 254.9462
255.1990 265.4123 268.0823
274.6109 279.0911 285.9938
294.0138 295.4893 300.2462
311.5743 318.9536 321.9570
326.2601 332.1974 337.7142
340.4626 349.4029 350.3981
351.8726 365.6521 368.7393
381.1286 386.5163 387.8632
393.1074 393.9916 400.0249
418.1900 421.2963 442.9584
459.1528 466.1972 471.4037
517.2427 520.0662 529.6607
542.3883 547.6089 552.4857
553.8320 556.7317 566.2280
567.2851 570.6131 571.9552
580.1718 617.6508 621.5503
640.5477 684.0676 693.9284
711.3038 748.5554 764.0728
770.7026 780.7382 783.8232
785.9613 786.4916 792.9247
806.4431 847.1631 856.9625
876.3040 891.0831 892.4954
901.2279 924.9916 928.7696
940.3903 950.9547 953.3159
955.7155 958.4407 958.7765
961.0429 966.2268 966.6210
969.0032 1000.6341 1013.6307
1022.0083 1024.3173 1028.4378
1045.7964 1046.6612 1049.3538
1049.7690 1051.7366 1055.2693
1057.4729 1080.5738 1089.5795
1143.6940 1150.2952 1153.1086
1179.5245 1181.4384 1191.8372
1206.8187 1210.1806 1213.0530

1233.0621	1239.5003	1243.0645
1243.9177	1248.7277	1249.6837
1257.6996	1261.6978	1266.6474
1267.2178	1285.8583	1290.8950
1292.8459	1296.2291	1310.2648
1320.3241	1325.5218	1356.8938
1367.6964	1368.1482	1396.4806
1397.1555	1400.6613	1401.5613
1401.8022	1403.5507	1404.5376
1422.2688	1426.3959	1431.6523
1433.9315	1434.6378	1450.0477
1470.5717	1474.7033	1475.3894
1476.5357	1477.3575	1479.7391
1480.4190	1482.3242	1482.9046
1483.8723	1487.5097	1495.2732
1500.1926	1501.0390	1501.2856
1502.3622	1505.3791	1509.9677
1513.0719	1513.5237	1515.7949
1517.0595	1566.9139	1590.5364
1656.0903	1696.9448	1698.5538
1706.3015	1711.2019	3056.8772
3057.5562	3058.6918	3060.2904
3065.1573	3065.5795	3067.7756
3067.9027	3070.8006	3136.0725
3137.8257	3138.1635	3140.4358
3141.8705	3142.2062	3143.2598
3143.6819	3145.3036	3145.8739
3147.0063	3148.0149	3148.4305
3150.5733	3152.0977	3171.9684
3174.7144	3175.5512	3176.9098
3231.8529	3251.0876	3266.7492
3274.6353	3288.3741	3290.3934

27c-ts

Zero-point correction= 0.621371
Thermal correction to Energy= 0.653776
Thermal correction to Enthalpy= 0.654546
Thermal correction to Gibbs Free Energy= 0.563250
Sum of electronic and zero-point Energies= -3259.974517
Sum of electronic and thermal Energies= -3259.942112
Sum of electronic and thermal Enthalpies= -3259.941342
Sum of electronic and thermal Free Energies= -3260.032638

Cartesian coordinates

C	3.071359	-1.560329	-0.497865
N	3.069148	-2.723245	-1.170587
H	0.705812	0.763675	0.041436
N	1.809380	-3.102066	-1.212903
N	1.083567	-2.215113	-0.586966
N	1.829888	-1.212782	-0.129644
C	4.316762	-0.823048	-0.224792
C	4.316564	0.499873	0.233458
C	5.541748	-1.472891	-0.440898
C	5.508791	1.166285	0.485270
H	3.382078	1.023409	0.389638
C	6.742409	-0.821056	-0.196826
H	5.544942	-2.497533	-0.795509
C	6.702886	0.490346	0.264898
H	5.516043	2.190166	0.839560
H	7.692149	-1.317681	-0.356147
C	-0.535187	1.883678	1.233321
C	-0.348711	2.064541	-1.153429
C	-1.389195	2.976000	-1.158058
C	-2.037514	3.353489	0.023355
C	-1.567673	2.812219	1.220287
H	-1.696655	3.407401	-2.100668
H	-2.013854	3.099251	2.160762
N	0.011345	1.526446	0.043911
C	0.022263	1.274923	2.516366
C	-0.320130	-0.221797	2.572318
C	1.551212	1.436646	2.532778
C	-0.565711	1.969489	3.749108
H	0.174489	-0.761233	1.763344
H	0.038375	-0.629210	3.523767
H	-1.398329	-0.394743	2.500226
H	1.858105	2.471279	2.343539
H	1.933157	1.138161	3.513714
H	2.016961	0.777124	1.797198
H	-0.107503	1.532369	4.640635
H	-0.355489	3.044474	3.756435
H	-1.646666	1.817855	3.828352
C	0.420479	1.674859	-2.414080
C	0.101668	2.643363	-3.559946
C	1.928947	1.732086	-2.129826
C	0.033392	0.253461	-2.852598
H	-0.939564	2.565835	-3.888774
H	0.312536	3.683905	-3.290678
H	0.731983	2.382948	-4.414849

H	2.224784	0.970102	-1.406195
H	2.479143	1.524792	-3.052669
H	2.234866	2.717199	-1.760498
H	0.517887	0.032405	-3.809177
H	0.368783	-0.490624	-2.130113
H	-1.049379	0.157619	-2.983355
C	-3.198307	4.340360	-0.038535
C	-2.691278	5.665706	-0.634957
C	-4.294986	3.752878	-0.945683
C	-3.796247	4.615079	1.343330
H	-1.893701	6.094937	-0.019313
H	-2.308639	5.537660	-1.652042
H	-3.516171	6.384707	-0.674083
H	-4.665404	2.801238	-0.550270
H	-5.136328	4.451662	-0.996500
H	-3.935738	3.585432	-1.965568
H	-4.627274	5.318912	1.239417
H	-4.187206	3.701525	1.804572
H	-3.064880	5.064669	2.023257
O	-3.280859	-1.932512	1.748837
S	-3.948393	-2.036563	0.471111
S	-1.241998	-2.359388	-0.699696
C	-4.150891	-0.287790	-0.187140
C	-0.847365	-3.702717	0.612666
F	-3.439859	0.556417	0.543128
F	-5.434949	0.031944	-0.092919
F	-3.771338	-0.214419	-1.453992
F	-0.096580	-4.607214	0.028848
F	-1.953878	-4.274423	1.046441
F	-0.223411	-3.133734	1.621532
O	-5.236917	-2.667701	0.329263
O	-2.997301	-2.689391	-0.618471
O	-1.252782	-0.994408	-0.222781
O	-1.068011	-2.831736	-2.045342
N	7.965426	1.187298	0.529307
O	7.912177	2.343309	0.919604
O	9.006705	0.577523	0.348092

Vibrational frequencies

-67.5026	16.2810	21.7776
32.4401	36.8436	43.8757
44.6441	47.3589	49.4702
56.7981	61.7312	65.9471
69.2240	71.4550	73.6089

78.9162 86.4214 91.7543
98.8596 109.0340 121.0172
125.0304 131.6607 143.6314
147.4125 154.9013 163.7139
175.5911 185.0067 192.5952
217.7972 223.0372 227.1101
233.7247 243.2447 250.8849
254.8391 261.6341 262.7128
269.1492 276.1004 277.0143
284.0113 288.4739 296.1647
301.1733 311.8791 317.8147
318.3481 323.3291 327.7409
330.8238 337.8009 344.9537
354.5733 358.8844 361.3076
362.7475 371.6562 373.9773
381.4787 389.9388 393.1085
394.1749 396.6440 406.0735
421.2843 434.5264 453.0905
466.5844 471.1513 473.3740
520.2354 523.4117 525.4061
541.5469 548.1930 549.7107
554.9953 556.2934 567.0168
569.4128 571.6126 576.3671
582.5104 601.2724 641.7706
653.2782 684.4960 693.8560
717.6291 746.8895 758.6561
762.4382 778.7533 780.5596
781.0863 787.3098 795.7369
807.7015 851.3355 857.0416
877.5647 890.2429 904.9863
905.7663 918.4855 925.9135
928.8754 938.2193 949.9118
956.5632 959.0195 960.1838
961.7794 966.7855 974.1463
974.5174 991.7134 1016.1770
1024.8590 1029.1277 1035.9938
1044.8716 1046.8934 1049.4233
1051.2602 1053.9462 1057.9855
1074.6822 1078.0930 1086.8895
1141.4032 1141.8682 1152.6729
1169.4691 1180.7894 1191.9782
1203.4438 1208.6701 1211.1166
1228.7884 1238.3307 1243.6016
1244.2890 1246.3752 1251.9358

1254.5640	1261.0865	1268.4474
1270.2549	1283.1984	1284.2160
1287.0559	1300.7208	1317.7137
1319.5496	1320.1008	1322.0326
1362.4060	1367.2710	1394.5912
1397.1199	1399.9224	1402.3957
1404.0136	1405.0515	1414.5397
1423.4768	1423.9759	1425.6850
1429.6099	1435.4007	1444.7199
1467.1550	1472.5837	1475.3301
1478.0657	1481.6722	1482.7098
1486.7754	1486.9301	1490.2154
1490.3735	1491.5203	1496.2900
1498.2893	1499.3461	1503.2469
1504.4835	1506.7819	1507.3984
1512.5978	1514.2074	1520.9970
1523.5941	1561.5615	1581.2563
1655.6917	1691.3761	1691.8504
1701.9622	1711.5137	3056.0606
3059.0099	3061.2888	3061.9192
3065.6448	3067.9944	3069.1334
3072.6975	3073.1087	3136.3992
3138.8166	3140.4963	3140.8741
3141.4643	3142.8367	3143.8806
3144.1139	3145.3249	3145.9693
3147.7213	3150.4773	3152.3452
3157.5863	3174.9624	3177.4216
3201.3895	3209.1302	3243.3447
3256.5326	3261.1464	3271.2185
3272.4707	3281.9173	3363.2317

28c-ts

Zero-point correction= 0.619091
Thermal correction to Energy= 0.652208
Thermal correction to Enthalpy= 0.652978
Thermal correction to Gibbs Free Energy= 0.556665
Sum of electronic and zero-point Energies= -3259.976932
Sum of electronic and thermal Energies= -3259.943816
Sum of electronic and thermal Enthalpies= -3259.943046
Sum of electronic and thermal Free Energies= -3260.039359

Cartesian coordinates

C	0.292914	1.904713	-0.070360
N	-1.005303	2.206864	-0.007869

H	1.878497	-0.834347	0.064133
N	-1.603543	1.037461	0.129478
N	-0.737079	0.060848	0.147933
N	0.477333	0.574853	0.025531
C	1.358986	2.903375	-0.221331
C	2.707455	2.522271	-0.258166
C	1.022872	4.260934	-0.322914
C	3.708705	3.475445	-0.387964
H	2.978759	1.474540	-0.179397
C	2.012207	5.225375	-0.453697
H	-0.020978	4.554692	-0.296814
C	3.340734	4.813090	-0.481186
H	4.754309	3.192907	-0.414451
H	1.764255	6.277400	-0.530339
C	3.197273	-1.876125	-1.129470
C	3.344263	-1.672762	1.254824
C	4.551048	-2.349114	1.235337
C	5.120866	-2.788215	0.033285
C	4.407212	-2.558969	-1.144115
H	5.052525	-2.545857	2.173511
H	4.784456	-2.920423	-2.088954
N	2.735193	-1.426657	0.063241
C	2.352158	-1.633917	-2.375782
C	0.922517	-2.145992	-2.120654
C	2.330290	-0.131338	-2.708183
C	2.929398	-2.387826	-3.578848
H	0.421994	-1.623249	-1.301101
H	0.322825	-1.982963	-3.021544
H	0.926520	-3.218764	-1.900454
H	3.344450	0.259846	-2.843050
H	1.781551	0.016002	-3.643965
H	1.822030	0.445969	-1.934209
H	2.260578	-2.238141	-4.430986
H	3.917144	-2.013304	-3.866876
H	2.998136	-3.464598	-3.392869
C	2.649464	-1.220095	2.534360
C	2.644638	0.316169	2.611122
C	1.208769	-1.763093	2.542549
C	3.377422	-1.765693	3.767623
H	3.662625	0.717630	2.561749
H	2.046417	0.756882	1.811946
H	2.201714	0.623127	3.564087
H	1.204395	-2.857674	2.506246
H	0.716198	-1.450770	3.468740

H	0.606430	-1.384339	1.712280
H	2.817226	-1.468285	4.658529
H	3.435166	-2.859111	3.758490
H	4.388903	-1.358214	3.862808
C	6.467532	-3.503858	0.054380
C	7.512378	-2.559630	0.676158
C	6.344790	-4.773889	0.915517
C	6.934862	-3.901279	-1.348689
H	7.608364	-1.638953	0.090905
H	7.255723	-2.288376	1.704553
H	8.487072	-3.057799	0.693370
H	5.591350	-5.456314	0.508256
H	7.306767	-5.296510	0.928733
H	6.076451	-4.541976	1.950708
H	7.907294	-4.397169	-1.273667
H	6.241625	-4.602179	-1.825691
H	7.056153	-3.029192	-2.000395
O	-5.653582	-1.676592	1.199005
S	-6.449766	-0.903939	0.276373
S	-4.029849	0.722395	-0.126410
C	-6.329996	-1.727062	-1.407967
C	-3.772199	0.824672	1.762875
F	-7.474311	-2.360931	-1.621450
F	-5.337581	-2.595202	-1.419275
F	-6.146991	-0.811555	-2.345751
F	-4.940960	0.787057	2.381166
F	-3.185920	1.967932	2.044517
F	-3.040531	-0.201517	2.137497
O	-5.761107	0.515981	-0.010078
O	-7.846028	-0.625989	0.494850
O	-4.019781	2.024154	-0.731007
O	-3.636812	-0.532278	-0.715605
N	4.393677	5.824709	-0.607167
O	5.555126	5.446290	-0.618013
O	4.058716	6.994996	-0.693436

Vibrational frequencies

-56.6338	10.1635	11.1620
15.1468	19.8412	22.6667
34.8137	37.0263	40.9923
41.7437	47.1379	54.4956
59.0290	62.6952	71.4406
75.6731	82.1152	92.0749
94.6517	100.6010	102.5823

127.6048	133.1770	137.4357
145.0032	153.3238	154.9018
163.9219	167.8293	185.4518
216.5630	221.1188	228.9084
233.6416	234.5183	235.3326
252.3283	254.5838	262.8200
264.9842	275.5407	279.5884
282.2763	284.8386	292.5036
297.3597	298.1668	305.2323
314.8052	318.5961	322.7857
324.1922	325.4922	337.0134
344.3874	349.4493	353.5661
360.0613	366.2577	366.9779
372.0960	381.0754	385.3694
389.9868	391.1093	399.9033
420.5482	427.9754	450.4483
456.9774	466.9975	472.3213
519.8941	520.4898	525.9146
540.4757	547.4711	548.5662
553.5908	553.7183	563.0514
566.9797	571.7791	573.8506
584.4326	600.1351	639.5464
669.3787	685.2295	693.8103
712.6674	745.5360	756.7924
772.9526	778.4844	783.8802
784.3173	785.8996	793.0478
801.4271	831.8696	846.4161
862.4774	888.9848	894.2409
922.4550	924.8373	926.1192
944.3387	949.4089	952.5940
953.9873	956.5431	958.2566
965.2172	966.2562	970.7152
972.9459	986.0389	1002.1933
1020.5079	1023.8742	1032.6781
1045.0516	1046.0404	1048.0995
1049.7886	1052.3717	1053.5931
1054.6497	1088.0438	1097.5744
1135.0204	1135.9651	1151.1729
1176.6950	1178.2962	1180.8914
1201.4876	1201.5857	1219.2949
1233.9160	1238.4238	1242.2329
1245.7756	1247.8489	1255.4779
1256.6634	1262.0604	1264.2251
1277.1925	1283.3261	1284.5752

1285.8630	1296.1412	1311.8054
1314.3250	1317.9249	1320.0705
1365.5800	1366.2788	1392.5732
1399.0052	1400.0613	1402.1659
1402.8842	1403.6011	1411.1937
1421.2612	1424.1418	1428.7730
1431.2847	1439.2252	1440.2995
1463.2270	1472.0115	1473.2460
1474.8496	1478.8944	1479.4147
1479.9521	1482.8236	1484.8686
1486.3641	1492.2982	1493.1213
1498.0239	1499.6157	1501.2736
1502.8802	1503.4187	1505.6292
1508.4461	1513.7596	1515.2205
1518.6791	1560.9974	1583.7976
1651.8908	1687.8175	1690.8335
1699.8468	1707.0582	3056.2651
3058.0291	3060.3905	3060.4217
3061.6201	3063.3489	3064.2444
3065.4777	3068.4878	3129.4875
3135.4475	3136.6826	3136.9462
3137.7150	3138.4921	3139.5007
3139.8628	3140.5505	3141.9544
3146.8390	3147.1453	3151.9224
3153.1892	3155.5580	3161.1869
3170.2169	3183.9754	3185.9150
3228.5041	3247.2339	3257.4957
3269.4642	3269.5270	3304.8411

29c-ts

Zero-point correction= 0.619348
Thermal correction to Energy= 0.652673
Thermal correction to Enthalpy= 0.653443
Thermal correction to Gibbs Free Energy= 0.557446
Sum of electronic and zero-point Energies= -3259.972513
Sum of electronic and thermal Energies= -3259.939187
Sum of electronic and thermal Enthalpies= -3259.938417
Sum of electronic and thermal Free Energies= -3260.034414

Cartesian coordinates

C	0.284475	-0.200685	0.660049
N	1.109133	-1.243753	0.468629
H	-3.079290	-0.356694	0.571188
N	0.406865	-2.332224	0.776379

N	-0.789849	-1.976753	1.120986
N	-0.909048	-0.646272	1.060187
C	0.562935	1.231511	0.457363
C	-0.063408	2.158528	1.301000
C	1.372899	1.684543	-0.589767
C	0.104656	3.522491	1.101343
H	-0.679651	1.804866	2.121147
C	1.553064	3.045233	-0.802154
H	1.858361	0.975973	-1.248967
C	0.909524	3.938323	0.046887
H	-0.370450	4.249941	1.748694
H	2.175669	3.407244	-1.611665
C	-5.001284	-0.477315	1.268837
C	-4.363970	-0.207045	-1.028654
C	-5.695054	-0.234925	-1.398927
C	-6.711547	-0.398792	-0.447268
C	-6.338273	-0.505058	0.893972
H	-5.946694	-0.127913	-2.445775
H	-7.087106	-0.613350	1.664629
N	-4.072857	-0.347024	0.291962
C	-4.510510	-0.590562	2.705171
C	-3.768608	-1.929456	2.866489
C	-3.564980	0.585068	3.011268
C	-5.680914	-0.547981	3.691653
H	-2.904988	-2.013581	2.200827
H	-3.402620	-2.012381	3.894924
H	-4.441512	-2.771598	2.672878
H	-4.067990	1.546048	2.857888
H	-3.252089	0.525242	4.058364
H	-2.658512	0.552467	2.400403
H	-5.279118	-0.601377	4.707412
H	-6.253464	0.381566	3.605450
H	-6.360448	-1.396474	3.562427
C	-3.202902	-0.019197	-1.994396
C	-2.369633	1.191387	-1.536048
C	-2.349286	-1.300435	-2.008743
C	-3.705113	0.246113	-3.416562
H	-2.968388	2.108290	-1.557698
H	-1.969052	1.063226	-0.527254
H	-1.519517	1.319075	-2.213952
H	-2.925632	-2.143223	-2.404071
H	-1.480607	-1.143106	-2.656735
H	-1.981836	-1.573612	-1.016755
H	-2.838015	0.395960	-4.066362

H	-4.273641	-0.600563	-3.814552
H	-4.324308	1.147755	-3.471012
C	-8.165243	-0.452695	-0.905731
C	-8.510488	0.862836	-1.626220
C	-8.325296	-1.631799	-1.882820
C	-9.134384	-0.644629	0.264203
H	-8.391707	1.721606	-0.957311
H	-7.881696	1.023705	-2.507106
H	-9.552984	0.830705	-1.959004
H	-8.069094	-2.580520	-1.399846
H	-9.366659	-1.687221	-2.216152
H	-7.694953	-1.517127	-2.770039
H	-10.157372	-0.683730	-0.121688
H	-8.945727	-1.581105	0.800020
H	-9.081073	0.184112	0.978663
O	5.178901	-1.713938	0.291374
S	6.131690	-0.845322	-0.617807
S	3.395538	-1.415111	0.520652
C	6.940608	0.197549	0.680613
C	3.011060	-2.103404	-1.228026
F	6.041302	0.938160	1.306411
F	7.827947	0.985836	0.083972
F	7.561719	-0.582134	1.554734
F	4.113199	-2.480335	-1.850295
F	2.420910	-1.157838	-1.932023
F	2.228396	-3.146075	-1.077232
O	5.378247	0.043312	-1.475696
O	7.171133	-1.699096	-1.141638
O	3.422282	0.017844	0.655072
O	3.247401	-2.408013	1.547794
N	1.082232	5.378252	-0.182089
O	1.795173	5.730335	-1.107334
O	0.499357	6.150928	0.561906

Vibrational frequencies

-111.5439	9.0760	14.5355
19.7759	24.1114	27.9599
35.4603	40.5363	42.1807
45.5039	52.8884	54.7341
60.4293	63.4302	70.8529
77.5417	83.0499	85.4308
91.2900	95.7756	109.4592
115.6784	130.1414	137.7465
142.9735	145.0070	150.0619

154.9773 164.5011 193.2460
195.6422 206.7816 209.9778
218.3032 219.6155 224.2192
239.5250 248.3073 254.2741
260.4599 265.6867 268.0001
269.0127 275.8162 282.6103
296.0998 296.6364 305.1730
312.1776 313.6804 321.8192
322.8423 328.2663 341.8103
349.6083 350.0494 352.6883
361.1213 369.6849 371.2964
381.4115 385.0620 391.7813
392.5702 393.1058 398.7483
419.2826 421.9588 435.4682
464.1954 467.1083 471.2654
517.9616 518.2549 529.1253
543.7602 547.6074 550.0957
550.4955 556.5753 567.8735
570.0013 570.4383 572.5778
580.4059 617.3521 622.6207
639.3339 688.2260 693.5735
714.4336 745.8754 763.7969
767.0822 781.1414 785.1428
786.9536 787.6085 794.7874
804.4762 849.3881 855.1002
864.9277 887.4794 890.9045
924.5278 926.3506 928.5797
944.0621 950.3656 951.9801
952.9755 958.2813 959.0032
962.7672 971.7170 972.3526
976.5779 990.0272 999.5784
1011.8662 1026.7257 1029.1661
1045.0069 1047.3379 1049.5956
1052.3696 1057.5033 1058.5129
1071.0460 1082.0271 1087.3000
1140.0869 1146.1094 1150.4034
1163.8793 1181.2958 1185.5817
1206.9145 1209.9071 1212.6862
1217.0816 1230.5559 1238.5412
1241.2781 1242.7958 1249.3411
1256.4876 1261.9575 1269.9322
1271.1333 1286.0443 1287.6785
1290.1287 1292.1897 1313.8011
1316.8177 1323.7102 1358.1625

1366.7252	1368.7357	1394.0331
1394.9019	1395.3776	1399.7977
1402.8838	1405.2978	1414.2434
1422.9255	1426.3411	1429.9752
1436.2549	1441.1427	1446.8129
1469.3160	1471.3033	1472.1516
1473.2712	1476.2098	1477.7569
1480.2739	1481.0514	1482.0333
1484.5545	1490.0383	1496.5077
1499.3043	1500.7324	1501.3422
1504.7209	1507.3805	1508.8710
1511.6983	1515.1445	1517.1457
1521.5032	1567.0711	1589.7341
1655.9684	1694.4059	1696.4527
1706.6366	1711.4724	3056.0089
3058.1565	3058.3031	3059.9150
3060.2090	3062.6239	3063.2566
3064.9588	3067.8640	3136.5167
3137.6405	3138.4522	3138.7870
3139.5419	3140.2425	3140.9951
3141.6504	3142.1250	3143.9265
3144.3054	3145.5887	3147.3434
3148.6121	3160.6493	3165.1988
3168.7877	3170.0881	3231.1224
3246.3844	3253.4936	3258.4931
3261.2724	3302.5055	3358.6427

18d-ts

Zero-point correction= 0.621972
Thermal correction to Energy= 0.655837
Thermal correction to Enthalpy= 0.656607
Thermal correction to Gibbs Free Energy= 0.559616
Sum of electronic and zero-point Energies= -3392.493392
Sum of electronic and thermal Energies= -3392.459527
Sum of electronic and thermal Enthalpies= -3392.458757
Sum of electronic and thermal Free Energies= -3392.555748

Cartesian coordinates

C	-1.946198	-2.239171	0.158336
N	-0.899005	-1.439066	-0.127614
H	2.208231	-1.905166	0.185261
N	0.173049	-2.230400	-0.127681
N	-0.196636	-3.444504	0.136141
N	-1.513701	-3.490613	0.316805

C	-3.377038	-1.895356	0.270676
C	-4.312066	-2.845885	-0.152540
C	-3.818186	-0.682744	0.813263
C	-5.675704	-2.588989	-0.046302
H	-3.965495	-3.786841	-0.567141
C	-5.178305	-0.421469	0.917451
H	-3.100535	0.052830	1.155342
C	-6.100693	-1.374837	0.485089
H	-6.397148	-3.326471	-0.381269
H	-5.521229	0.520776	1.335344
C	3.551031	-1.019910	1.463022
C	3.938902	-1.517190	-0.850663
C	5.153967	-0.858828	-0.785894
C	5.580877	-0.233846	0.392374
C	4.768309	-0.353236	1.521029
H	5.780969	-0.838653	-1.667315
H	5.082593	0.065389	2.465412
N	3.165729	-1.525070	0.266902
C	2.666736	-1.270839	2.681995
C	2.355221	-2.776925	2.765396
C	3.389590	-0.851048	3.966717
C	1.357508	-0.472789	2.576604
H	3.275620	-3.366412	2.836855
H	1.756999	-2.966709	3.661898
H	1.775840	-3.135136	1.908507
H	3.571318	0.228007	4.001452
H	2.753447	-1.105028	4.819067
H	4.342823	-1.375284	4.091811
H	0.789287	-0.603319	3.503217
H	1.550807	0.595660	2.436972
H	0.738466	-0.830610	1.754398
C	3.447490	-2.272561	-2.080936
C	4.565920	-2.391786	-3.122299
C	3.018618	-3.691538	-1.662759
C	2.258076	-1.529327	-2.708923
H	4.869926	-1.416416	-3.515038
H	5.447724	-2.901795	-2.719708
H	4.191625	-2.981566	-3.963826
H	2.152864	-3.693076	-0.993758
H	2.732589	-4.253045	-2.557493
H	3.841145	-4.224133	-1.173452
H	1.946366	-2.059553	-3.614988
H	1.414064	-1.496777	-2.021323
H	2.529385	-0.503810	-2.980854

C	6.911971	0.510295	0.412682
C	8.041554	-0.488516	0.102393
C	6.881150	1.605444	-0.668079
C	7.189425	1.162863	1.769830
H	8.074340	-1.289454	0.848535
H	7.923768	-0.943485	-0.885699
H	9.003083	0.035097	0.119678
H	6.069958	2.317747	-0.485051
H	7.828160	2.154735	-0.656783
H	6.748782	1.185529	-1.669616
H	8.143015	1.696879	1.720252
H	6.413982	1.888505	2.038139
H	7.267827	0.420674	2.571496
O	-0.065807	2.474097	-0.887804
S	-1.121914	3.630278	-0.845097
S	-0.397336	0.707867	-0.381725
C	-0.649736	4.444629	0.749345
C	-1.365419	0.420823	-2.018025
F	-0.754440	3.595840	1.759729
F	-1.463104	5.475620	0.952216
F	0.601830	4.881627	0.670489
F	-1.359067	1.487937	-2.789011
F	-2.600933	0.107572	-1.699756
F	-0.768273	-0.566085	-2.653812
O	-2.465533	3.115572	-0.683004
O	-0.808303	4.595020	-1.874645
O	-1.146513	1.003966	0.813198
O	0.992152	0.348633	-0.497153
C	-7.561927	-1.063946	0.622182
F	-7.893476	0.087958	0.003425
F	-8.349680	-2.023719	0.108339
F	-7.927645	-0.911201	1.912873

Vibrational frequencies

-93.7059	8.0975	12.9309
17.1953	24.6013	32.8021
37.2905	41.0419	42.1696
45.2537	54.0181	57.3423
61.7156	63.4246	70.6456
75.5988	78.9871	86.8357
88.7830	93.4176	103.3300
108.6744	123.8272	136.4733
139.5392	144.5856	153.5997
162.1659	172.3296	185.4693

189.3370	194.3303	198.6084
201.9809	219.4196	223.9713
230.1232	238.8054	247.9438
252.4680	253.4086	269.8531
271.9502	277.1611	283.9790
295.3259	296.5322	304.6900
309.0110	311.9281	323.4859
324.2350	331.8637	338.7250
342.6568	352.0394	360.1446
364.3950	371.3628	377.2658
379.9366	384.3456	386.4112
396.0182	396.8917	397.6917
406.3431	418.7818	421.4562
426.7110	444.9970	461.7346
470.8731	474.0144	493.4683
515.4322	534.5303	541.8369
545.9417	553.9903	555.3889
565.1367	567.7588	570.3917
575.7305	579.2321	586.7084
614.7261	616.3609	617.6554
645.1692	681.1014	696.2532
709.9512	755.7314	762.0682
778.1118	782.8512	785.3599
786.0701	794.6405	800.2574
806.6107	848.5924	876.4999
886.2904	888.2167	913.5747
920.1709	927.0121	934.1202
948.3026	951.1619	954.6026
958.0303	961.0648	962.3381
966.2042	971.7641	972.0116
977.8767	1004.7959	1023.4470
1025.2290	1033.6656	1041.8015
1050.4052	1051.8306	1052.8744
1055.8772	1056.2502	1063.0762
1079.1371	1087.0049	1108.5556
1147.4726	1150.3743	1173.2363
1177.1134	1181.7993	1189.2896
1207.6483	1209.8422	1214.0838
1214.9607	1215.3165	1240.1211
1244.3090	1244.8339	1245.4732
1249.5055	1259.8445	1260.4668
1263.8347	1266.1959	1278.3394
1285.6292	1289.0004	1302.2891
1317.3026	1317.6292	1332.8966

1352.3483	1357.4738	1366.1701
1372.4124	1387.0239	1393.7929
1398.8217	1399.8325	1401.1471
1402.2800	1409.9538	1421.6130
1422.6638	1425.7450	1428.9861
1434.0640	1444.0319	1471.3596
1473.6612	1477.4549	1479.2594
1480.1049	1480.9449	1481.2345
1483.5355	1484.0052	1487.2887
1496.0286	1498.9510	1501.4885
1503.1279	1505.8976	1507.9065
1509.5111	1515.2488	1516.6497
1523.3245	1525.8407	1561.7222
1606.5189	1666.4661	1693.0752
1703.8126	1713.1284	3057.4595
3059.7747	3059.9369	3060.0692
3062.5251	3063.9077	3066.6071
3069.7277	3070.4470	3136.9440
3138.2137	3139.1305	3139.4601
3139.9483	3141.9833	3142.1697
3143.5882	3144.3060	3146.9511
3148.4469	3149.4257	3150.7019
3151.8184	3152.5171	3154.0644
3202.3453	3204.9755	3228.4809
3234.9545	3247.3081	3267.7489
3283.2462	3285.3555	3309.3468

19d-ts

Zero-point correction= 0.621642
Thermal correction to Energy= 0.655398
Thermal correction to Enthalpy= 0.656168
Thermal correction to Gibbs Free Energy= 0.560526
Sum of electronic and zero-point Energies= -3392.500692
Sum of electronic and thermal Energies= -3392.466936
Sum of electronic and thermal Enthalpies= -3392.466166
Sum of electronic and thermal Free Energies= -3392.561808

Cartesian coordinates

C	3.314689	-0.001303	0.110313
N	2.659500	1.145902	-0.089638
H	-0.366259	-1.635498	0.355787
N	1.393087	0.823955	0.082088
N	1.267239	-0.452008	0.360024
N	2.465418	-1.002304	0.391399

C	4.775317	-0.146947	0.026693
C	5.374584	-1.385302	0.287510
C	5.571573	0.951073	-0.314775
C	6.754142	-1.524342	0.204234
H	4.754558	-2.235345	0.553286
C	6.953380	0.815863	-0.398283
H	5.103346	1.909077	-0.516626
C	7.538291	-0.422506	-0.140868
H	7.220341	-2.484898	0.402919
H	7.568464	1.668498	-0.666484
C	-1.767470	-2.404050	-0.935786
C	-2.090815	-2.017696	1.407047
C	-3.428076	-2.349394	1.275928
C	-3.974073	-2.686911	0.030921
C	-3.110845	-2.734057	-1.065185
H	-4.053847	-2.352712	2.158455
H	-3.474427	-3.039462	-2.034892
N	-1.328021	-2.015139	0.283253
C	-0.762439	-2.504150	-2.080237
C	-0.349895	-1.099165	-2.551644
C	0.473830	-3.285135	-1.597638
C	-1.373832	-3.256182	-3.268607
H	0.221843	-0.572194	-1.787750
H	0.283837	-1.195645	-3.439072
H	-1.225326	-0.497140	-2.816782
H	0.196627	-4.291153	-1.264352
H	1.178417	-3.382970	-2.429276
H	1.004961	-2.779602	-0.785711
H	-0.600256	-3.382828	-4.031354
H	-1.731358	-4.251480	-2.983795
H	-2.198287	-2.701632	-3.727906
C	-1.416546	-1.706073	2.738943
C	-0.132167	-2.547033	2.861918
C	-1.070139	-0.210416	2.813273
C	-2.344317	-2.055627	3.908119
H	-0.347826	-3.617070	2.768837
H	0.619260	-2.273467	2.114256
H	0.314375	-2.373103	3.845765
H	-1.956379	0.412799	2.656581
H	-0.657291	0.008738	3.803941
H	-0.322937	0.054341	2.065805
H	-1.800335	-1.888835	4.842151
H	-3.234382	-1.418406	3.930680
H	-2.658758	-3.104596	3.884733

C	-5.458948	-3.021012	-0.077363
C	-5.766653	-4.224484	0.831618
C	-6.274681	-1.802319	0.390632
C	-5.870802	-3.366401	-1.511143
H	-5.188479	-5.104843	0.531629
H	-5.544712	-4.008836	1.881063
H	-6.830760	-4.472463	0.758316
H	-6.071037	-0.928958	-0.237157
H	-7.343037	-2.032126	0.322171
H	-6.053686	-1.536178	1.428696
H	-6.943322	-3.581373	-1.532621
H	-5.684544	-2.534609	-2.199122
H	-5.347010	-4.253158	-1.883912
O	-2.975636	2.617577	1.305963
S	-3.196676	3.218465	0.010167
S	-0.518235	2.001390	-0.580533
C	-4.353153	2.110451	-0.922952
C	0.159663	3.131466	0.809505
F	-5.532862	2.139830	-0.313819
F	-3.896927	0.867754	-0.941197
F	-4.485767	2.551109	-2.165761
F	-0.606599	4.196971	0.963595
F	1.360764	3.513609	0.444869
F	0.185604	2.448208	1.931957
O	-1.909409	3.101427	-0.904278
O	-3.727982	4.551102	-0.133419
O	0.127926	2.232308	-1.843405
O	-1.229942	0.828420	-0.144431
C	9.028335	-0.581553	-0.190532
F	9.397161	-1.749973	-0.753103
F	9.631106	0.396538	-0.888961
F	9.584509	-0.569695	1.041799

Vibrational frequencies

-71.8353	14.2277	18.3969
23.9345	32.2485	35.0273
36.5855	36.7888	40.1631
52.0318	57.7978	60.4511
62.2154	66.5851	70.4068
75.3122	77.4879	84.2470
88.9183	93.0201	106.1831
115.9815	120.1862	138.6077
140.1073	140.9027	147.1796
165.3813	171.1538	179.8487

191.5508	204.5321	210.5909
216.7461	229.2208	235.7516
239.7097	242.4315	251.3229
253.9565	262.1325	263.8042
272.6236	281.4093	284.2655
296.2533	298.0638	301.6346
306.8302	314.4015	318.2778
319.2936	324.3713	331.5348
346.2063	352.2532	357.3544
362.7574	365.0926	367.3604
374.8600	383.7821	387.1188
389.2909	390.4685	399.7279
401.8559	413.6046	419.8970
427.2768	437.4957	464.1703
466.4301	476.4396	491.9152
518.4081	523.4077	542.5849
549.3990	552.3955	556.5690
561.9286	567.9148	569.8817
571.9307	580.7762	585.2565
610.6670	613.5544	630.7940
643.3010	684.6059	693.2954
708.6818	750.1826	762.2030
779.9185	783.0079	784.5306
785.6918	792.3964	792.8016
803.5756	846.8470	861.5844
877.0257	888.7485	917.5319
923.1612	926.2684	938.7410
948.8624	950.0685	956.5441
959.0170	960.9811	964.6149
964.9373	971.9593	972.4570
975.5337	1005.7340	1019.2486
1020.3151	1033.7053	1045.2910
1046.2939	1048.5939	1049.2317
1051.0675	1055.1449	1056.8797
1083.9386	1097.6469	1103.0680
1137.4582	1150.7029	1172.8184
1175.6486	1180.7871	1182.1288
1201.5098	1202.5942	1207.2991
1216.7555	1233.4154	1240.1530
1243.1006	1243.6309	1248.0396
1256.7614	1262.4982	1262.9916
1265.6913	1270.3930	1281.2981
1285.1947	1287.5326	1292.8848
1313.1519	1313.3308	1323.4474

1328.1818	1353.6225	1366.1219
1368.1249	1391.4433	1397.2799
1400.6028	1402.1373	1403.2061
1403.8606	1404.9456	1421.7949
1429.1543	1429.6908	1430.2729
1436.1135	1440.7732	1471.0004
1472.4220	1476.0008	1477.8640
1480.6067	1482.1891	1483.2374
1486.2122	1487.2326	1494.6791
1496.1912	1499.7018	1500.4625
1503.8809	1504.4721	1505.8210
1511.1845	1511.9007	1515.5020
1517.7481	1520.5936	1559.6136
1605.1942	1668.8573	1693.6266
1700.6769	1710.2495	3056.1097
3059.4850	3060.6801	3063.0665
3064.1600	3064.6061	3067.4142
3067.5997	3072.3199	3134.1872
3137.2551	3140.2663	3140.5350
3141.5188	3141.5596	3142.8465
3143.2437	3145.2416	3145.5620
3147.2450	3149.4843	3153.5800
3155.1975	3157.0162	3164.3212
3199.7368	3205.4074	3224.4495
3230.9461	3240.9867	3244.4300
3247.0010	3280.6248	3287.3932

20d-ts

Zero-point correction= 0.621240
Thermal correction to Energy= 0.655206
Thermal correction to Enthalpy= 0.655976
Thermal correction to Gibbs Free Energy= 0.558162
Sum of electronic and zero-point Energies= -3392.492680
Sum of electronic and thermal Energies= -3392.458714
Sum of electronic and thermal Enthalpies= -3392.457944
Sum of electronic and thermal Free Energies= -3392.555758

Cartesian coordinates

C	0.569488	1.278892	-0.172997
N	0.606002	-0.067526	-0.221404
H	-3.369236	0.370535	0.022010
N	-0.653222	-0.474321	-0.144330
N	-1.419472	0.569187	-0.065184
N	-0.695494	1.687522	-0.076631

C	1.706916	2.216667	-0.194521
C	1.577750	3.437402	0.479476
C	2.886546	1.936933	-0.891020
C	2.618071	4.359496	0.471850
H	0.660045	3.656419	1.015493
C	3.930198	2.854615	-0.901483
H	2.995206	1.003326	-1.427311
C	3.791072	4.062620	-0.220169
H	2.515735	5.301746	1.000596
H	4.843998	2.630362	-1.442567
C	-4.984102	0.279282	1.298525
C	-5.079177	0.002800	-1.078932
C	-6.445310	-0.198055	-0.998991
C	-7.113998	-0.168242	0.231477
C	-6.356250	0.077856	1.377612
H	-6.997228	-0.385267	-1.910277
H	-6.827813	0.114617	2.348531
N	-4.401540	0.231386	0.076920
C	-4.095126	0.548005	2.505370
C	-3.077302	-0.600084	2.643450
C	-3.383972	1.900830	2.316535
C	-4.922345	0.616195	3.793783
H	-2.433851	-0.703289	1.766833
H	-2.432845	-0.402031	3.505797
H	-3.591389	-1.552322	2.811373
H	-4.115439	2.712966	2.246411
H	-2.744334	2.091088	3.184262
H	-2.748376	1.927136	1.428879
H	-4.245196	0.822012	4.627637
H	-5.666182	1.419343	3.761141
H	-5.431343	-0.329743	4.005811
C	-4.287523	-0.029188	-2.379149
C	-3.553291	1.311572	-2.564870
C	-3.294661	-1.204937	-2.323340
C	-5.215314	-0.237808	-3.580284
H	-4.269614	2.138255	-2.619624
H	-2.840017	1.520827	-1.764537
H	-2.993544	1.282969	-3.505114
H	-3.830636	-2.156353	-2.238893
H	-2.708456	-1.223359	-3.247979
H	-2.592717	-1.129394	-1.489651
H	-4.608164	-0.249025	-4.489933
H	-5.747460	-1.193111	-3.526514
H	-5.947511	0.570667	-3.678837

C	-8.620739	-0.401209	0.272628
C	-9.311858	0.680515	-0.576928
C	-8.918855	-1.790938	-0.317914
C	-9.177642	-0.339859	1.697081
H	-9.105495	1.680980	-0.182387
H	-8.988264	0.649540	-1.621666
H	-10.394900	0.521389	-0.555800
H	-8.421354	-2.578188	0.258174
H	-9.997565	-1.976040	-0.289845
H	-8.592044	-1.869188	-1.359164
H	-10.256031	-0.522453	1.667124
H	-8.729473	-1.102601	2.342765
H	-9.020539	0.642661	2.154821
O	3.393562	-3.016813	0.439942
S	4.852988	-2.981221	-0.162397
S	2.195544	-1.649753	0.313314
C	5.818922	-2.665019	1.385560
C	1.899870	-2.026753	-1.546254
F	5.424288	-1.537420	1.952435
F	7.103887	-2.575190	1.063584
F	5.643738	-3.672613	2.229354
F	2.628233	-3.051098	-1.952524
F	2.222469	-0.961993	-2.250709
F	0.628962	-2.328732	-1.688497
O	5.032591	-1.837543	-1.030168
O	5.210199	-4.314226	-0.585555
O	3.068687	-0.550117	0.626398
O	1.211897	-2.275963	1.152894
C	4.942867	5.022827	-0.183577
F	5.673924	4.991281	-1.314083
F	4.547088	6.297440	-0.008361
F	5.798600	4.749233	0.826200

Vibrational frequencies

-108.1956	8.7146	15.2483
18.1641	18.4508	28.1450
30.7847	37.5687	39.5100
42.3741	47.5303	48.6538
57.6914	62.5815	69.0637
75.3970	78.1917	92.0705
99.6377	107.7376	111.4207
118.2311	122.6504	136.9023
141.7729	145.7372	152.7279
157.9024	165.0619	178.3153

191.2216	193.3170	200.5410
213.4109	217.9304	221.6388
225.3057	227.5907	245.1877
251.3856	251.6183	258.1072
269.0207	271.1861	281.9972
293.9540	294.6702	300.3906
303.2027	310.9299	321.6127
324.6332	329.7707	336.0082
347.2010	357.6418	361.8800
362.3980	367.0247	370.8395
379.7982	385.6389	391.1816
391.6256	396.8885	397.8199
405.3487	417.8740	422.8901
424.8348	443.9914	456.7769
469.5486	471.5997	486.1079
516.9422	532.1420	543.5754
546.1056	553.7866	554.2993
565.7655	566.5473	568.6109
574.2593	578.6335	584.6085
613.9045	617.1390	622.3529
643.5425	687.6433	693.8387
708.4423	756.7373	770.2704
778.6642	784.1188	787.8207
787.9056	792.9922	794.4860
804.8667	848.0682	867.3708
870.2722	883.4512	908.3916
927.2641	929.6660	943.6170
951.1988	952.6350	953.9197
957.0528	961.3327	963.3623
965.0494	965.7237	977.0601
1000.1497	1016.3775	1023.3349
1024.3584	1032.2457	1046.9437
1048.6481	1050.0489	1050.3985
1054.4291	1057.4847	1057.5920
1084.8599	1088.9014	1105.0499
1138.0350	1146.5398	1173.9743
1175.0115	1179.3037	1182.9745
1203.0918	1204.3393	1208.1003
1216.8348	1233.9350	1240.3358
1242.7965	1243.6492	1248.7734
1249.9069	1255.2631	1261.7087
1264.1465	1269.8942	1283.2470
1286.4915	1288.9223	1290.7170
1312.0781	1312.4529	1327.5433

1351.3062	1356.4966	1367.3738
1369.4290	1395.6130	1395.7026
1400.9066	1402.6871	1404.5484
1405.0063	1406.0906	1420.6060
1424.3840	1432.9288	1434.9957
1435.6582	1446.4005	1473.4163
1474.6913	1475.6940	1476.8246
1479.7090	1480.9292	1482.8611
1484.3190	1484.6929	1486.7376
1495.7442	1501.0745	1502.9351
1504.3221	1506.5366	1509.1873
1511.0020	1515.3158	1516.7801
1520.0192	1521.6650	1568.0816
1606.4410	1669.1667	1696.4283
1706.0803	1713.7772	3057.4552
3059.6128	3062.0897	3062.1163
3063.2621	3064.4135	3066.7482
3067.6530	3070.2489	3111.8740
3137.7246	3138.6021	3139.0463
3140.0524	3140.4869	3140.8862
3141.8824	3142.7420	3143.0876
3143.9734	3144.0993	3149.9564
3150.2838	3152.3846	3171.5372
3173.1729	3174.0287	3185.3990
3222.4388	3228.0617	3234.6475
3263.8602	3271.7016	3274.5448

27d-ts

Zero-point correction= 0.623301
Thermal correction to Energy= 0.656489
Thermal correction to Enthalpy= 0.657259
Thermal correction to Gibbs Free Energy= 0.563508
Sum of electronic and zero-point Energies= -3392.491659
Sum of electronic and thermal Energies= -3392.458471
Sum of electronic and thermal Enthalpies= -3392.457701
Sum of electronic and thermal Free Energies= -3392.551452

Cartesian coordinates

C	2.752082	-1.736778	-0.516995
N	2.696658	-2.907817	-1.172128
H	0.522630	0.657344	0.018087
N	1.421299	-3.239209	-1.193500
N	0.736527	-2.317680	-0.573508
N	1.528370	-1.337963	-0.139684

C	4.029844	-1.044142	-0.266077
C	4.092450	0.278060	0.182743
C	5.226441	-1.741577	-0.492218
C	5.318379	0.893616	0.419919
H	3.183439	0.842694	0.347471
C	6.452378	-1.132280	-0.263140
H	5.184917	-2.767987	-0.840183
C	6.494810	0.184379	0.198002
H	5.351904	1.918971	0.773106
H	7.373789	-1.680649	-0.436266
C	-0.621855	1.866418	1.221849
C	-0.461218	2.025385	-1.167601
C	-1.435484	3.007544	-1.160106
C	-2.033543	3.437844	0.029653
C	-1.583156	2.868936	1.220487
H	-1.728446	3.453118	-2.100823
H	-1.987708	3.192428	2.167924
N	-0.118179	1.467239	0.026577
C	-0.104373	1.218849	2.502999
C	-0.571508	-0.243683	2.564844
C	1.431805	1.249496	2.513213
C	-0.623379	1.964889	3.736775
H	-0.117976	-0.825341	1.761096
H	-0.253391	-0.675027	3.520002
H	-1.659766	-0.327644	2.485934
H	1.824327	2.256275	2.332016
H	1.790285	0.913805	3.491064
H	1.839284	0.558520	1.772672
H	-0.192643	1.498293	4.626931
H	-0.327944	3.019753	3.734488
H	-1.712176	1.902100	3.827922
C	0.255695	1.580419	-2.440703
C	1.770709	1.557432	-2.190731
C	-0.216820	0.177032	-2.852537
C	-0.033666	2.552721	-3.591146
H	2.140278	2.531582	-1.851849
H	2.039220	0.797477	-1.455052
H	2.286424	1.297394	-3.120114
H	-1.305353	0.138203	-2.963770
H	0.238765	-0.083325	-3.813421
H	0.090103	-0.574094	-2.124635
H	0.561963	2.247856	-4.456009
H	-1.084944	2.532277	-3.895375
H	0.242404	3.582024	-3.338322

C	-3.121129	4.505774	-0.016325
C	-2.531744	5.788442	-0.630158
C	-4.274231	3.996285	-0.899861
C	-3.671928	4.826539	1.374976
H	-1.688949	6.157608	-0.036189
H	-2.185529	5.627975	-1.655780
H	-3.301352	6.566848	-0.653162
H	-4.714060	3.083354	-0.484966
H	-5.058313	4.758784	-0.950153
H	-3.944849	3.784795	-1.921635
H	-4.461348	5.578468	1.283077
H	-4.107696	3.941511	1.851300
H	-2.900583	5.235683	2.036283
O	-3.629175	-1.814121	1.757872
S	-4.296796	-1.860875	0.477099
S	-1.621629	-2.346417	-0.693583
C	-4.374792	-0.097821	-0.167639
C	-1.288650	-3.702331	0.620727
F	-3.590034	0.686155	0.552905
F	-5.629592	0.316279	-0.047639
F	-4.015214	-0.047435	-1.441206
F	-0.565390	-4.634895	0.047733
F	-2.423101	-4.230920	1.038953
F	-0.657303	-3.156463	1.637297
O	-5.623825	-2.401470	0.320100
O	-3.386191	-2.573047	-0.613962
O	-1.549808	-0.982434	-0.220624
O	-1.462374	-2.833593	-2.035201
C	7.829593	0.831436	0.416326
F	7.743842	1.971996	1.123719
F	8.438734	1.147263	-0.748064
F	8.684292	0.023979	1.075039

Vibrational frequencies

-66.8520	12.5005	18.3259
29.8802	31.5227	34.6568
38.9489	43.7353	49.0045
51.9095	56.1374	61.0152
68.6465	69.2277	70.9796
75.7053	83.0322	95.2110
96.3780	106.3150	117.3916
122.7217	130.4603	143.4641
144.1119	153.3427	156.5965
169.7102	172.8989	183.5332

200.7609	221.4593	222.4572
226.4298	234.4479	242.7827
244.7055	255.9888	261.1583
264.9363	271.2977	273.3438
278.1318	287.9137	294.0428
300.3277	305.3963	312.0158
313.5564	316.8494	323.0206
326.7933	332.9714	336.0469
342.5712	357.1010	359.1565
360.4758	368.7630	381.9597
385.1026	389.0516	390.6425
392.5500	396.7391	399.7754
410.3841	417.2404	421.9566
441.4501	449.9422	466.0194
476.5403	476.9751	484.0232
522.5148	526.6801	543.0024
547.9206	554.7480	556.9758
567.9021	568.6790	571.9451
577.4186	583.4674	585.9883
600.3230	618.7121	645.4298
657.4520	682.5201	692.3924
709.0043	750.5716	762.0328
779.5560	779.8209	781.1845
788.1504	797.0281	802.4511
806.4184	852.0640	856.2242
880.2402	892.5857	908.8999
922.1921	927.4572	931.2307
940.6566	950.7011	956.9325
958.5305	959.1871	962.2505
970.4685	972.0663	974.3916
984.3445	1009.6686	1020.9675
1025.9936	1028.5671	1046.2286
1047.6397	1048.4959	1049.1458
1054.1986	1058.5308	1068.9868
1079.1538	1087.7164	1105.4670
1139.7417	1141.0644	1167.7056
1175.5860	1180.8821	1201.8630
1204.7921	1205.7094	1209.1863
1209.8551	1230.0096	1237.9091
1245.1722	1246.2403	1249.7877
1253.6597	1254.4200	1261.7311
1269.3640	1270.9505	1284.0945
1285.3464	1291.4358	1297.6227
1320.2567	1322.7935	1323.1779

1326.1202	1353.6002	1363.4351
1367.1299	1393.3164	1393.5692
1401.4050	1402.8768	1404.0091
1405.9093	1411.1116	1424.2265
1425.8567	1425.9021	1431.0072
1435.8068	1446.2057	1473.2334
1475.8002	1478.2649	1479.7592
1483.1459	1483.6406	1484.9830
1488.9605	1490.1964	1491.4475
1498.8690	1500.7146	1504.4191
1504.8370	1505.9948	1507.0839
1509.8232	1512.1723	1517.7561
1523.8489	1526.5915	1560.9461
1598.6212	1670.1969	1687.9644
1701.5011	1708.7486	3053.9675
3059.5528	3064.2983	3064.7333
3067.0898	3067.3142	3068.5956
3071.6857	3071.8316	3131.1907
3140.1334	3140.8920	3141.4341
3142.6044	3143.1435	3144.5578
3146.5839	3147.7081	3147.9242
3148.0339	3149.7420	3151.6445
3155.8519	3186.5207	3190.3386
3193.0472	3200.4844	3217.5057
3230.1833	3241.0827	3258.9825
3269.5814	3297.0628	3336.6278

28d-ts

Zero-point correction= 0.622138
Thermal correction to Energy= 0.655903
Thermal correction to Enthalpy= 0.656673
Thermal correction to Gibbs Free Energy= 0.559635
Sum of electronic and zero-point Energies= -3392.493239
Sum of electronic and thermal Energies= -3392.459474
Sum of electronic and thermal Enthalpies= -3392.458704
Sum of electronic and thermal Free Energies= -3392.555742

Cartesian coordinates

C	0.414037	1.859311	0.073253
N	-0.869829	2.219380	0.126960
H	1.815496	-0.981965	0.060584
N	-1.524276	1.072511	0.204731
N	-0.705337	0.058580	0.196452
N	0.534569	0.519928	0.116092

C	1.532053	2.808100	-0.036016
C	2.860936	2.361547	-0.027554
C	1.268123	4.176754	-0.156883
C	3.906445	3.268124	-0.143503
H	3.075900	1.301250	0.066466
C	2.312165	5.088716	-0.274325
H	0.239424	4.521675	-0.163058
C	3.627055	4.629869	-0.268950
H	4.935372	2.919746	-0.138186
H	2.101882	6.148461	-0.372336
C	2.950808	-2.180327	-1.180573
C	3.034075	-2.193474	1.215249
C	4.043781	-3.138348	1.171101
C	4.534387	-3.626333	-0.046546
C	3.961677	-3.132583	-1.219059
H	4.448259	-3.512065	2.101935
H	4.290228	-3.495730	-2.181240
N	2.543865	-1.728991	0.032467
C	2.259378	-1.647576	-2.431655
C	0.751649	-1.943253	-2.333019
C	2.501685	-0.133865	-2.557679
C	2.805157	-2.328802	-3.691193
H	0.279606	-1.458891	-1.474682
H	0.257651	-1.566689	-3.234347
H	0.569888	-3.021322	-2.268714
H	3.572566	0.097038	-2.570697
H	2.065376	0.218605	-3.497651
H	2.025342	0.419309	-1.747234
H	2.265597	-1.933191	-4.556302
H	3.869902	-2.123176	-3.842900
H	2.650918	-3.412429	-3.671828
C	2.417442	-1.681939	2.513071
C	2.654175	-0.168126	2.648557
C	0.910095	-1.993831	2.500246
C	3.042573	-2.376224	3.728115
H	3.723200	0.069418	2.616712
H	2.137683	0.393575	1.868922
H	2.259607	0.168850	3.612353
H	0.738433	-3.073788	2.439361
H	0.464878	-1.628857	3.431442
H	0.383022	-1.511188	1.673940
H	2.554429	-1.995194	4.629649
H	2.892571	-3.460421	3.704037
H	4.113485	-2.166017	3.816781

C	5.642678	-4.674409	-0.048171
C	6.876307	-4.088974	0.661181
C	5.151336	-5.915359	0.719412
C	6.039023	-5.095956	-1.465349
H	7.237853	-3.191794	0.147972
H	6.659389	-3.828564	1.701525
H	7.680903	-4.831389	0.661390
H	4.256082	-6.339847	0.253062
H	5.935570	-6.679481	0.713365
H	4.917692	-5.683436	1.762835
H	6.833012	-5.846414	-1.404731
H	5.199377	-5.544810	-2.006833
H	6.422232	-4.252371	-2.049373
O	-5.673962	-1.585140	0.946321
S	-6.521997	-0.628898	0.275493
S	-3.934508	0.797790	-0.178171
C	-6.904392	-1.297810	-1.410788
C	-3.774590	0.909291	1.721347
F	-7.646644	-2.386956	-1.259937
F	-5.785560	-1.604889	-2.043366
F	-7.578423	-0.392710	-2.103557
F	-4.973313	0.864926	2.283535
F	-3.209958	2.056570	2.024353
F	-3.060654	-0.112134	2.138386
O	-5.698925	0.672914	-0.142773
O	-7.776640	-0.188210	0.829971
O	-3.867870	2.087659	-0.804125
O	-3.546270	-0.472423	-0.723679
C	4.776737	5.582382	-0.403162
F	4.384927	6.859702	-0.537562
F	5.547930	5.296044	-1.475023
F	5.601573	5.538243	0.665986

Vibrational frequencies

-60.7472	11.3066	14.3297
18.2986	20.2466	27.7070
32.1904	35.8246	42.6337
44.8769	51.1952	54.0677
56.4588	61.8558	70.5533
74.3848	80.8880	90.2457
95.5195	103.1698	113.1678
114.9928	131.2712	143.2564
146.1676	149.2665	156.5041
160.7148	166.4423	172.8402

193.5570 200.4094 211.4127
213.6537 223.3194 237.9258
245.1380 246.8963 252.4779
256.8593 257.9916 263.0860
266.9121 276.5251 287.6234
294.0295 301.0941 303.6053
314.4142 315.3027 317.1651
323.8813 324.9613 333.9891
344.6309 354.9325 358.6102
359.5599 363.2452 365.7648
371.7004 376.6172 386.2998
388.6339 392.6876 399.5128
400.7299 420.5712 426.9804
430.5104 438.3967 457.1575
467.1136 477.7233 483.7083
522.0720 527.4458 540.0045
549.1570 555.0744 555.4143
566.7499 568.4968 571.7214
574.7722 583.0063 584.5589
614.7826 618.9844 639.9145
644.5340 689.8013 692.5914
709.4592 751.6079 769.2296
784.0729 784.8421 785.6536
788.0182 792.0197 798.3215
805.0272 837.4235 846.9149
881.9929 891.7887 922.5869
926.6761 928.2529 948.5518
953.1590 954.9115 955.9575
960.9891 963.4308 964.7056
971.2519 974.0499 979.5008
1008.6866 1011.6869 1022.2403
1025.2593 1038.9780 1044.7878
1048.7231 1050.6210 1052.4096
1054.2505 1054.6295 1059.9657
1090.5369 1097.4743 1106.9369
1145.7420 1146.7785 1168.0852
1176.5830 1181.2202 1194.0540
1207.2991 1210.3922 1212.2769
1224.8612 1240.5921 1242.8006
1244.5955 1245.4771 1250.3329
1256.1875 1258.6031 1264.3754
1265.1391 1277.9128 1280.6900
1285.0851 1291.7523 1295.1592
1322.3609 1323.2061 1324.2431

1329.9069	1353.6362	1365.2391
1372.0775	1394.6734	1398.8626
1400.3926	1403.8354	1405.3367
1406.2544	1413.6259	1426.0192
1426.3038	1430.5895	1433.0405
1449.2545	1449.7608	1474.2152
1476.6899	1477.9510	1480.1619
1482.3574	1483.0415	1484.8017
1486.2286	1491.2907	1493.0259
1500.8911	1501.6644	1502.8823
1503.3898	1505.1970	1506.2113
1512.0513	1513.8409	1515.0548
1519.9081	1523.0111	1567.3454
1603.7844	1668.1334	1699.5903
1704.7487	1709.0121	3058.2992
3058.4776	3058.7190	3060.0817
3062.8366	3064.1028	3066.4166
3069.6760	3070.6271	3117.1517
3138.3906	3138.8072	3139.4517
3139.8367	3139.9952	3141.0475
3141.2056	3142.3797	3142.5395
3145.9968	3146.2982	3147.7470
3150.7229	3153.6254	3170.1608
3181.8102	3189.3595	3199.3693
3217.9643	3228.0083	3230.5362
3242.1885	3287.3246	3300.4805

29d-ts

Zero-point correction= 0.621068
Thermal correction to Energy= 0.655084
Thermal correction to Enthalpy= 0.655854
Thermal correction to Gibbs Free Energy= 0.557614
Sum of electronic and zero-point Energies= -3392.489980
Sum of electronic and thermal Energies= -3392.455965
Sum of electronic and thermal Enthalpies= -3392.455195
Sum of electronic and thermal Free Energies= -3392.553435

Cartesian coordinates

C	0.270523	-0.583347	0.274120
N	1.092874	-1.619439	0.043198
H	-3.033968	-0.594965	0.381182
N	0.356031	-2.717703	0.201795
N	-0.856416	-2.373466	0.499824
N	-0.952663	-1.039728	0.555196

C	0.596194	0.853140	0.207815
C	0.000011	1.729899	1.123663
C	1.435538	1.363383	-0.785149
C	0.242230	3.095221	1.048176
H	-0.650212	1.337664	1.899330
C	1.684126	2.730597	-0.865265
H	1.893710	0.693924	-1.503105
C	1.083851	3.589657	0.050972
H	-0.214776	3.773209	1.763466
H	2.339610	3.119376	-1.637130
C	-4.883457	-0.706793	1.269751
C	-4.473470	-0.161506	-1.028975
C	-5.835285	-0.064615	-1.247403
C	-6.755718	-0.293725	-0.215408
C	-6.250623	-0.607086	1.047077
H	-6.183596	0.200579	-2.236796
H	-6.921131	-0.775441	1.876398
N	-4.052701	-0.496609	0.220788
C	-4.270378	-1.040125	2.623164
C	-3.642539	-2.443193	2.546622
C	-3.195175	0.004658	2.969780
C	-5.335342	-1.029274	3.724660
H	-2.851962	-2.502602	1.793538
H	-3.197094	-2.689184	3.516160
H	-4.402402	-3.197841	2.317220
H	-3.608469	1.019309	2.954253
H	-2.815974	-0.195571	3.976571
H	-2.345035	-0.048959	2.285491
H	-4.844338	-1.229386	4.681239
H	-5.835058	-0.057604	3.801905
H	-6.092774	-1.805613	3.576840
C	-3.415975	0.102381	-2.092252
C	-2.461416	1.194398	-1.576201
C	-2.657902	-1.205533	-2.385470
C	-4.053938	0.596821	-3.394308
H	-2.999107	2.133941	-1.408954
H	-1.967134	0.908292	-0.645797
H	-1.680226	1.373052	-2.322070
H	-3.332554	-1.948812	-2.822850
H	-1.857077	-1.002918	-3.104257
H	-2.203203	-1.639436	-1.492202
H	-3.256255	0.800737	-4.114499
H	-4.716432	-0.152493	-3.839421
H	-4.615379	1.525453	-3.246537

C	-8.250695	-0.176670	-0.495380
C	-8.556003	1.265028	-0.940868
C	-8.624826	-1.154129	-1.623751
C	-9.096164	-0.500767	0.739086
H	-8.293870	1.982948	-0.156706
H	-8.010663	1.535308	-1.849756
H	-9.626639	1.361796	-1.148882
H	-8.403452	-2.188352	-1.340243
H	-9.697698	-1.077826	-1.828054
H	-8.090662	-0.931296	-2.552152
H	-10.155614	-0.416026	0.479107
H	-8.921958	-1.522113	1.094509
H	-8.900291	0.195117	1.561917
O	5.175447	-2.006114	0.240314
S	6.128380	-0.882788	-0.357730
S	3.404165	-1.805568	0.317780
C	6.204746	0.356885	1.052199
C	3.188757	-2.360034	-1.504801
F	5.448076	1.404304	0.782267
F	7.467286	0.748270	1.171251
F	5.813039	-0.209444	2.182801
F	4.345839	-2.732534	-2.020417
F	2.703089	-1.354000	-2.203486
F	2.369949	-3.386766	-1.513820
O	5.499564	-0.220206	-1.478090
O	7.443723	-1.466911	-0.450505
O	3.361364	-0.386997	0.583613
O	3.156122	-2.888169	1.229033
C	1.326316	5.068949	-0.004791
F	2.137191	5.428206	-1.013108
F	1.885618	5.534092	1.131691
F	0.177805	5.763416	-0.163114

Vibrational frequencies

-91.3170	7.4031	13.7760
15.6622	16.5436	27.9691
31.3325	35.2062	38.6025
43.2554	47.6646	50.5344
63.2091	65.2216	70.2983
75.9941	76.9353	82.3401
86.6536	92.9272	101.4750
121.8962	128.4902	132.2548
136.6234	141.1879	146.0035
160.4447	174.9720	179.1774

197.6772 207.8220 212.1758
217.2827 218.0068 224.1980
227.5504 238.8867 249.3324
254.8592 262.6144 266.6079
269.0412 274.0703 279.2479
293.5161 297.4409 299.0341
307.4407 311.6808 313.4691
323.0119 324.0019 333.6588
334.8776 341.8120 349.3972
360.1564 360.9350 366.4684
371.1247 376.1790 389.1499
390.5479 392.8571 397.7344
399.8110 415.9115 423.2241
434.4475 459.5598 463.6766
467.5172 470.0770 480.6342
520.5338 534.5761 541.0281
549.2894 551.7443 555.4257
565.4117 566.4899 568.7402
570.0214 582.6348 584.1685
602.0211 613.3177 644.2800
656.3878 688.5426 693.5029
707.5371 756.0810 768.5524
780.3201 781.1641 785.0185
786.5723 794.0034 795.4163
805.6578 847.7527 852.4850
868.2158 878.8869 918.3213
924.3964 927.5073 940.8564
949.6937 952.5309 953.8153
956.9609 961.3268 964.0270
965.8367 967.7666 972.9483
988.3369 995.8591 1011.7584
1024.3260 1027.6248 1042.9454
1047.1168 1047.7421 1051.8333
1053.3343 1060.2673 1062.3561
1080.2151 1084.9304 1106.1145
1137.6434 1142.5802 1163.3446
1172.3312 1178.3682 1180.2813
1204.8742 1205.7714 1208.6671
1209.4578 1211.0462 1229.8683
1237.5949 1241.4113 1243.4015
1249.4116 1251.2906 1256.1466
1266.2520 1271.8621 1284.1560
1289.3369 1290.9068 1291.5246
1313.4932 1315.6429 1330.9789

1353.1556	1357.4572	1367.7501
1372.1521	1394.8737	1397.3121
1400.4713	1402.1455	1402.2019
1404.2989	1406.7975	1423.1890
1425.3371	1427.1152	1428.5042
1433.1532	1446.1487	1471.0525
1473.0187	1476.3143	1476.5786
1479.2197	1481.2540	1481.8769
1483.2415	1485.3932	1488.3310
1495.1509	1497.5882	1501.1004
1502.0995	1503.7436	1505.2678
1507.6981	1513.0131	1517.7121
1520.9248	1521.6542	1571.1530
1606.8482	1669.5186	1697.1479
1706.6016	1712.4808	3055.4929
3058.4054	3058.5480	3059.2779
3059.8960	3062.7734	3064.8888
3065.0607	3068.5750	3136.3186
3137.2036	3138.3375	3138.4818
3138.6824	3140.5542	3141.2499
3142.8153	3142.9424	3143.8987
3145.1098	3147.0533	3149.2458
3151.0742	3163.1734	3165.1291
3174.7843	3176.7048	3218.9146
3231.1814	3231.8567	3265.5087
3271.8189	3273.0876	3284.5125

18e-ts

Zero-point correction= 0.535110
Thermal correction to Energy= 0.563279
Thermal correction to Enthalpy= 0.564049
Thermal correction to Gibbs Free Energy= 0.481011
Sum of electronic and zero-point Energies= -2824.643203
Sum of electronic and thermal Energies= -2824.615033
Sum of electronic and thermal Enthalpies= -2824.614263
Sum of electronic and thermal Free Energies= -2824.697301

Cartesian coordinates

C	1.518872	3.432970	0.038998
N	1.037311	2.197104	0.193833
H	-2.040711	1.326554	0.363848
N	-0.243428	2.354031	0.529849
N	-0.518099	3.626078	0.567173
N	0.569331	4.336460	0.262586

C	-3.200899	-0.051950	1.343243
C	-3.394317	0.528262	-0.976855
C	-4.356330	-0.452982	-1.137309
C	-4.754302	-1.266503	-0.067780
C	-4.172872	-1.030683	1.178252
H	-4.811381	-0.580883	-2.110431
H	-4.475421	-1.606335	2.040082
N	-2.824765	0.659443	0.252387
C	-2.560613	0.284006	2.684430
C	-1.075481	-0.114778	2.657492
C	-2.701726	1.796040	2.942356
C	-3.253777	-0.470671	3.824363
H	-0.516835	0.466085	1.923920
H	-0.634384	0.082697	3.639928
H	-0.955597	-1.181465	2.438305
H	-3.755282	2.095277	2.951159
H	-2.270252	2.028997	3.920685
H	-2.170776	2.402403	2.203072
H	-2.801316	-0.155678	4.768803
H	-4.324690	-0.246600	3.874802
H	-3.121286	-1.554301	3.741323
C	-2.988620	1.504055	-2.076486
C	-3.248462	2.937640	-1.577611
C	-1.502323	1.330903	-2.427042
C	-3.816719	1.270442	-3.343877
H	-4.306988	3.083848	-1.336800
H	-2.649211	3.192743	-0.698737
H	-2.976967	3.642682	-2.369695
H	-1.286394	0.302969	-2.737606
H	-1.253368	1.999293	-3.257537
H	-0.856964	1.594355	-1.588606
H	-3.517882	2.011176	-4.090859
H	-3.641780	0.278557	-3.773900
H	-4.889504	1.394058	-3.162994
C	-5.804675	-2.348758	-0.294184
C	-7.087872	-1.695029	-0.838409
C	-5.255007	-3.348457	-1.327932
C	-6.146257	-3.103762	0.993743
H	-7.482348	-0.955695	-0.133453
H	-6.920977	-1.198755	-1.798993
H	-7.851917	-2.464632	-0.988611
H	-4.334752	-3.820145	-0.967746
H	-5.996461	-4.134674	-1.503658
H	-5.040967	-2.866089	-2.286337

H	-6.896481	-3.868408	0.770976
H	-5.271998	-3.611153	1.415385
H	-6.566472	-2.438007	1.755353
O	3.520273	-1.079287	0.557782
S	4.536198	-1.529585	-0.575218
S	2.533419	0.421048	0.510882
C	6.131721	-0.982032	0.192288
C	1.377894	-0.286442	-0.835279
F	6.155238	0.332794	0.320347
F	7.119988	-1.370480	-0.604550
F	6.270295	-1.550974	1.380745
F	1.703322	-1.531685	-1.140149
F	1.472919	0.464574	-1.908212
F	0.154983	-0.286469	-0.342148
O	4.343504	-0.757192	-1.781591
O	4.575657	-2.971463	-0.588902
O	3.519359	1.359007	0.043316
O	2.001261	0.266458	1.837022
H	2.542492	3.652270	-0.222801

Vibrational frequencies

-105.1491	13.0948	23.6098
26.8099	32.0637	35.9065
45.1278	53.4150	57.9450
58.9607	70.3104	73.5755
78.0922	80.6659	94.1583
99.1332	114.2461	120.8947
125.1245	138.1021	142.6400
149.0600	158.0802	169.2453
171.0793	192.4700	217.1498
223.2237	226.3376	238.7954
241.0626	246.4154	254.5132
263.7075	267.2903	276.0833
284.3083	294.7241	297.3165
301.9320	304.6381	314.1168
318.9472	320.4697	325.1674
330.7980	344.4395	346.6577
352.8159	359.8482	365.8580
368.7905	370.8382	379.9366
389.9938	392.7834	394.2733
401.2122	423.5285	443.1238
460.6304	465.5501	517.3978
542.0296	547.9145	553.6673
555.3478	562.5745	566.7057

568.6216	572.9757	579.2248
616.3594	633.8780	687.7223
691.7804	720.3656	770.1169
778.2390	781.7584	786.1673
787.0100	794.6733	847.9991
858.5598	897.9611	919.7728
923.7456	925.7262	931.4898
945.0532	951.0414	952.9321
956.9323	959.4338	960.1994
962.5813	970.6135	971.8822
973.3311	1027.3628	1033.6398
1048.1968	1048.9532	1051.3432
1052.7902	1053.5345	1055.5956
1073.4419	1086.3778	1145.5188
1172.6550	1176.5168	1180.7106
1191.0850	1199.6528	1217.8936
1230.0756	1239.5539	1242.0226
1245.4744	1248.2018	1257.2600
1261.9557	1262.2113	1272.7199
1281.5923	1283.0017	1287.4227
1289.2857	1303.7226	1310.3110
1316.6218	1366.2669	1392.2183
1398.4341	1399.2888	1399.5954
1401.3078	1402.7911	1404.4053
1405.4205	1420.1940	1430.0060
1432.5971	1438.3110	1441.9836
1472.8830	1474.8152	1477.2622
1478.7283	1479.2258	1482.2777
1484.5140	1485.9220	1486.9629
1495.1931	1499.3616	1500.5285
1503.7740	1504.5342	1507.2734
1510.2829	1515.2581	1517.4993
1518.3876	1520.5492	1556.9112
1688.7682	1697.6950	3055.1707
3060.1101	3061.7646	3062.1618
3062.5846	3064.5358	3068.3192
3068.6846	3068.9204	3134.9342
3137.5024	3138.9929	3139.4623
3139.8147	3142.1367	3142.6635
3144.7095	3147.1772	3147.3710
3147.8941	3149.1759	3150.0803
3151.4523	3159.4373	3160.6843
3194.8015	3198.4130	3284.0969
3286.2857	3297.2310	3326.4763

19e-ts

Zero-point correction= 0.534828
Thermal correction to Energy= 0.562847
Thermal correction to Enthalpy= 0.563617
Thermal correction to Gibbs Free Energy= 0.482499
Sum of electronic and zero-point Energies= -2824.649271
Sum of electronic and thermal Energies= -2824.621251
Sum of electronic and thermal Enthalpies= -2824.620481
Sum of electronic and thermal Free Energies= -2824.701599

Cartesian coordinates

C	3.345182	-3.832271	-0.523863
N	3.742088	-2.560231	-0.509073
H	-0.324780	-2.335097	-0.014636
N	2.629570	-1.885450	-0.275351
N	1.608705	-2.697809	-0.165313
N	2.029607	-3.944004	-0.313291
C	-1.854039	-1.501251	-1.107047
C	-1.689373	-1.507574	1.281472
C	-2.790761	-0.673405	1.360004
C	-3.423674	-0.198230	0.204762
C	-2.951202	-0.652842	-1.028096
H	-3.161679	-0.388599	2.335780
H	-3.439342	-0.355797	-1.944517
N	-1.241184	-1.849317	0.047367
C	-1.340219	-2.092759	-2.417708
C	-0.042147	-1.388576	-2.846702
C	-1.084003	-3.599006	-2.230401
C	-2.382940	-1.914085	-3.529283
H	0.771662	-1.589022	-2.148989
H	0.258096	-1.765624	-3.830049
H	-0.186312	-0.305568	-2.922888
H	-1.992821	-4.116012	-1.903506
H	-0.771872	-4.026984	-3.187944
H	-0.284913	-3.804460	-1.512117
H	-2.022195	-2.425403	-4.426255
H	-3.349819	-2.350525	-3.256417
H	-2.531956	-0.861822	-3.790723
C	-0.968062	-2.080761	2.495669
C	-0.720094	-3.585429	2.285061
C	0.371354	-1.349190	2.683124
C	-1.814739	-1.898304	3.760669
H	-1.660419	-4.121828	2.117499

H	-0.044804	-3.788709	1.448542
H	-0.248987	-3.995378	3.183758
H	0.223219	-0.268955	2.783967
H	0.856206	-1.721921	3.591928
H	1.037138	-1.532987	1.840108
H	-1.302141	-2.388178	4.593486
H	-1.936151	-0.843479	4.025964
H	-2.805640	-2.354314	3.659434
C	-4.618206	0.742520	0.332123
C	-5.754428	-0.007967	1.051584
C	-4.203870	1.969608	1.164115
C	-5.123589	1.221388	-1.031918
H	-6.061875	-0.892861	0.484349
H	-5.456052	-0.329475	2.054457
H	-6.622040	0.652523	1.152883
H	-3.372641	2.502722	0.692091
H	-5.051594	2.658111	1.242370
H	-3.901202	1.695015	2.178800
H	-5.954069	1.917818	-0.881919
H	-4.342499	1.748740	-1.590762
H	-5.493454	0.392688	-1.644891
O	0.854255	2.429127	1.519850
S	1.242364	3.150401	0.330916
S	2.162926	0.444697	-0.596580
C	-0.277296	3.410795	-0.696919
C	3.497019	0.490271	0.774108
F	-1.108604	4.195235	-0.022389
F	-0.867430	2.251918	-0.948194
F	0.055935	3.994863	-1.837756
F	3.728582	1.737938	1.148970
F	4.591081	-0.022198	0.264973
F	3.070547	-0.194807	1.810593
O	2.055369	2.225080	-0.672205
O	1.906807	4.428149	0.392296
O	2.719289	0.282805	-1.910737
O	0.841657	0.099417	-0.143350
H	4.007303	-4.669273	-0.686695

Vibrational frequencies

-82.0117	20.1230	28.3858
39.3875	42.3287	50.0411
54.0527	57.9850	59.7341
66.1422	70.9226	78.5844
82.4184	85.4601	94.9860

104.0905	108.5793	117.5975
131.4539	138.5158	140.6754
152.8935	163.8952	175.7386
177.5259	191.3752	209.6477
213.1644	226.6354	234.4782
242.7166	248.8086	251.9503
256.2937	263.0231	271.5253
277.6204	289.2428	295.8116
300.3696	310.3065	315.1296
317.3995	322.1912	326.8099
331.8009	333.6776	336.2636
342.1532	355.7091	361.7630
371.4459	381.3751	386.4298
390.4054	392.0103	393.9101
405.8841	423.2691	438.5955
466.1418	470.5511	520.8847
542.8913	548.9513	553.8847
554.9256	566.0108	567.9499
570.9631	572.4192	582.1356
613.3508	633.2705	681.2605
693.8482	732.1819	769.3552
778.0180	784.1616	785.1090
786.4599	794.0041	848.1168
854.9936	894.5242	903.0469
916.4425	927.6062	936.8259
940.9390	950.2963	954.0048
956.1506	960.3843	961.2228
963.7952	972.1807	973.2943
977.6256	988.7859	1039.6621
1047.1720	1049.2858	1049.6882
1051.0569	1053.0103	1059.6766
1061.5658	1086.8751	1149.4843
1171.2024	1181.4155	1190.8107
1211.7622	1215.1365	1219.9271
1239.3628	1239.6899	1243.9863
1246.5358	1249.5977	1257.3756
1258.3315	1264.8968	1265.5399
1276.5616	1282.3352	1288.7417
1291.0505	1292.1497	1318.3607
1331.4284	1366.8110	1372.3233
1393.3409	1399.1026	1400.1781
1403.3604	1404.4104	1404.8353
1406.4705	1426.3983	1429.0944
1432.7546	1441.3939	1444.8129

1471.7361	1473.5761	1475.2242
1476.1551	1478.5396	1479.7271
1483.9775	1485.4003	1488.7034
1493.8629	1498.0654	1499.8235
1500.5703	1502.6217	1505.1618
1508.0843	1513.3715	1515.5965
1516.3673	1521.5834	1566.4968
1697.8931	1702.7591	3056.4105
3057.3053	3058.4009	3059.9803
3063.3846	3063.4517	3065.5485
3066.2979	3066.5570	3136.7946
3136.8732	3137.6943	3138.0830
3138.4121	3139.1371	3140.3421
3141.7212	3142.9248	3143.1082
3144.6761	3146.6691	3151.7688
3153.5827	3155.6474	3162.0980
3194.2992	3198.1083	3204.1828
3261.2836	3286.1680	3287.3835

20e-ts

Zero-point correction= 0.534280
Thermal correction to Energy= 0.562754
Thermal correction to Enthalpy= 0.563524
Thermal correction to Gibbs Free Energy= 0.478166
Sum of electronic and zero-point Energies= -2824.645362
Sum of electronic and thermal Energies= -2824.616888
Sum of electronic and thermal Enthalpies= -2824.616118
Sum of electronic and thermal Free Energies= -2824.701476

Cartesian coordinates

C	0.842621	0.688788	1.861562
N	1.178664	0.624774	0.569293
H	-2.783338	0.225252	0.355596
N	0.034992	0.542180	-0.096758
N	-0.946064	0.561085	0.761586
N	-0.477728	0.654836	2.008922
C	-4.184811	-1.252618	-0.014356
C	-4.658921	1.083925	0.190119
C	-6.004825	0.827342	-0.003503
C	-6.473370	-0.476623	-0.208486
C	-5.535437	-1.509562	-0.214665
H	-6.699102	1.657296	0.001588
H	-5.847995	-2.530486	-0.375626
N	-3.800404	0.030408	0.186690

C	-3.111656	-2.332818	-0.014040
C	-2.097109	-2.027667	-1.131421
C	-2.429399	-2.368164	1.365878
C	-3.717957	-3.714053	-0.282416
H	-1.610905	-1.057034	-1.013117
H	-1.311685	-2.790136	-1.119111
H	-2.586923	-2.056901	-2.110778
H	-3.153325	-2.626608	2.146321
H	-1.647632	-3.134407	1.356306
H	-1.959731	-1.418778	1.629527
H	-2.909976	-4.451517	-0.277195
H	-4.437076	-4.004218	0.490580
H	-4.208468	-3.765094	-1.259929
C	-4.081691	2.477081	0.403324
C	-3.454673	2.550563	1.807560
C	-3.033464	2.762044	-0.688270
C	-5.176823	3.544742	0.305908
H	-4.219353	2.400660	2.577340
H	-2.661771	1.814708	1.957397
H	-3.015199	3.543049	1.951308
H	-3.490028	2.717884	-1.682783
H	-2.630735	3.769160	-0.541298
H	-2.193668	2.064710	-0.656993
H	-4.717664	4.526311	0.454381
H	-5.659910	3.548658	-0.677094
H	-5.944116	3.418433	1.076545
C	-7.965328	-0.720210	-0.414186
C	-8.718511	-0.237679	0.838400
C	-8.435166	0.083954	-1.639604
C	-8.283246	-2.200055	-0.643049
H	-8.395457	-0.788146	1.728302
H	-8.561928	0.829787	1.020435
H	-9.792429	-0.404036	0.704164
H	-7.894089	-0.220856	-2.541502
H	-9.502600	-0.094788	-1.805179
H	-8.291986	1.159546	-1.500186
H	-9.361779	-2.315712	-0.786785
H	-7.785545	-2.589887	-1.537549
H	-7.995473	-2.816631	0.215166
O	4.985612	-0.562137	-0.885616
S	6.363969	0.124691	-0.438403
S	3.419430	-0.215716	-0.184010
C	7.025599	-1.239683	0.629981
C	3.249432	1.488129	-1.026701

F	6.214705	-1.445996	1.652168
F	8.220975	-0.870607	1.069109
F	7.135898	-2.345677	-0.088431
F	4.308106	1.710405	-1.795086
F	3.189828	2.414140	-0.097814
F	2.175489	1.475356	-1.780518
O	6.116843	1.271496	0.401169
O	7.210463	0.183652	-1.601406
O	3.703949	-0.137567	1.222192
O	2.672419	-1.230766	-0.869348
H	1.558396	0.752570	2.667670

Vibrational frequencies

-65.1594	6.5913	11.7560
16.9552	28.2038	35.0979
46.3548	52.6286	53.2934
58.3048	60.2950	72.9830
78.1149	82.6323	96.4035
104.1470	110.6216	116.6542
130.8546	135.4535	141.2368
148.1092	156.8424	169.4889
175.7582	191.9835	196.2265
203.5738	205.0644	211.4387
245.1428	251.0728	252.9854
255.4346	261.8318	263.9559
268.9249	277.2698	293.7045
295.1593	300.1304	312.8224
316.0687	317.9313	324.3040
329.9545	340.3647	341.7375
352.7170	355.6546	358.4140
362.0077	373.9853	381.7481
388.9980	391.3272	392.5262
401.4611	421.4877	441.5646
459.2603	469.3751	522.5329
540.4015	548.7367	553.8383
554.4117	565.2494	567.3231
570.0624	573.1997	581.8297
613.4960	651.7911	683.6189
693.5942	728.3530	774.7951
783.1176	784.9356	785.7636
786.0550	792.6885	833.9780
847.2021	903.4282	914.2710
924.7924	928.1958	940.5403
950.2571	951.3003	955.6232

957.9577	958.2106	964.8048
966.0049	966.3805	977.3406
1020.1466	1030.6039	1044.5963
1046.8609	1048.8699	1050.8884
1051.6434	1055.4569	1064.3941
1069.6897	1091.8278	1148.2506
1170.9741	1177.6600	1181.9667
1197.2826	1207.6181	1225.9396
1238.3412	1240.0130	1242.3112
1243.3366	1250.1335	1254.1240
1267.2128	1267.3381	1277.8601
1278.3001	1283.8967	1292.5382
1293.3605	1294.1409	1316.9956
1330.9905	1368.4412	1392.3113
1395.1584	1399.1106	1401.2073
1402.0452	1406.3273	1406.9346
1420.3956	1423.2086	1433.1266
1435.5142	1446.2978	1449.5773
1473.0737	1474.8380	1475.9723
1476.7110	1479.6829	1481.6055
1482.8923	1483.8288	1486.3603
1494.1161	1500.3965	1500.8077
1502.4843	1503.2790	1505.8564
1510.7845	1512.2558	1513.5221
1515.9186	1517.5299	1570.7080
1697.2611	1707.3820	2986.7095
3056.4099	3058.4165	3059.8957
3063.1020	3063.3830	3063.4463
3066.2639	3067.6840	3072.8092
3136.9409	3138.0358	3139.9730
3140.3764	3140.4705	3141.0072
3141.2097	3142.5680	3145.5228
3145.9839	3146.6975	3146.7396
3147.8230	3157.4300	3171.8547
3176.4643	3182.0062	3185.6567
3265.0558	3279.5550	3297.5083

27e-ts

Zero-point correction= 0.534903
Thermal correction to Energy= 0.563003
Thermal correction to Enthalpy= 0.563773
Thermal correction to Gibbs Free Energy= 0.481598
Sum of electronic and zero-point Energies= -2824.645464
Sum of electronic and thermal Energies= -2824.617364

Sum of electronic and thermal Enthalpies= -2824.616594
Sum of electronic and thermal Free Energies= -2824.698769

Cartesian coordinates

C	-2.201546	-3.956317	-0.283434
N	-3.503825	-3.852359	-0.560951
H	0.319703	-2.269316	0.040651
N	-3.748675	-2.548044	-0.565834
N	-2.645307	-1.908544	-0.296307
N	-1.637114	-2.760765	-0.117363
C	1.674282	-1.420808	1.331520
C	1.881706	-1.481641	-1.052889
C	2.998708	-0.669358	-0.973082
C	3.472276	-0.199202	0.259018
C	2.799431	-0.608925	1.410410
H	3.519779	-0.410698	-1.884918
H	3.150797	-0.307385	2.386146
N	1.238747	-1.787988	0.104226
C	0.932437	-1.952709	2.552732
C	-0.434619	-1.259479	2.667396
C	0.739754	-3.472540	2.402152
C	1.732715	-1.688977	3.832903
H	-1.068743	-1.505356	1.816031
H	-0.933277	-1.606499	3.578782
H	-0.325443	-0.171443	2.721635
H	1.702677	-3.985929	2.306575
H	0.232247	-3.856641	3.292326
H	0.117582	-3.726412	1.539167
H	1.202825	-2.147685	4.672577
H	2.735400	-2.127448	3.787902
H	1.822242	-0.619141	4.045391
C	1.383119	-2.106253	-2.353061
C	1.206575	-3.619949	-2.136017
C	0.049184	-1.473684	-2.781599
C	2.403991	-1.895270	-3.477700
H	2.151142	-4.087549	-1.837344
H	0.452098	-3.842982	-1.376160
H	0.873460	-4.080045	-3.071301
H	0.144664	-0.388264	-2.890523
H	-0.246396	-1.891012	-3.749832
H	-0.746933	-1.688668	-2.068422
H	2.048073	-2.417918	-4.370043
H	2.513317	-0.837719	-3.738235
H	3.388651	-2.299946	-3.219847

C	4.706587	0.696590	0.299358
C	5.876256	-0.032838	-0.386682
C	4.392171	1.997046	-0.461643
C	5.118852	1.047822	1.731585
H	6.095664	-0.982543	0.112733
H	5.669590	-0.239062	-1.441130
H	6.773661	0.592721	-0.339123
H	3.573783	2.542706	0.018286
H	5.277749	2.641170	-0.463113
H	4.114904	1.801399	-1.502305
H	6.003639	1.690716	1.702436
H	4.330148	1.592748	2.260958
H	5.377187	0.154765	2.310972
O	-0.912475	2.413495	1.504936
S	-1.270505	3.135911	0.307154
S	-2.179751	0.434938	-0.629803
C	0.272704	3.378029	-0.689849
C	-3.530881	0.482105	0.725799
F	0.833077	2.208651	-0.957717
F	1.113882	4.122119	0.017661
F	-0.024593	3.996805	-1.822196
F	-4.617248	-0.036731	0.207791
F	-3.770793	1.731534	1.089829
F	-3.113193	-0.194343	1.771201
O	-1.926289	4.418603	0.352841
O	-2.071494	2.213608	-0.709390
O	-0.864058	0.090938	-0.159747
O	-2.720562	0.263523	-1.948673
H	-1.666276	-4.891761	-0.204643

Vibrational frequencies

-83.6175	15.1833	25.3975
29.9573	34.8764	41.3991
52.3889	54.1710	60.4752
63.1127	70.3642	71.9871
78.1354	80.3214	89.4423
97.2315	107.3429	116.2882
127.3088	139.3346	144.0590
152.6956	158.9310	177.6753
180.2844	193.6274	209.6618
213.0695	232.7201	239.7121
244.2143	249.8378	254.1099
255.4267	265.6417	278.6597
290.1190	293.7394	296.8555

302.3207	312.0604	317.3900
320.7020	323.1010	326.6095
330.3387	335.6051	344.9399
353.2766	360.5232	363.1835
371.3398	371.3886	383.3580
389.0550	391.6170	392.5272
400.1522	421.3065	438.2946
464.1060	469.3736	521.2753
541.8491	548.6771	552.1152
554.8216	563.8953	568.0935
570.9040	571.4322	582.6085
614.1221	633.8876	682.7055
689.5014	728.5823	767.3857
780.0544	784.2364	786.2764
786.5621	794.0664	848.5179
854.6590	888.7563	913.3319
923.5606	926.4801	938.2108
943.7001	952.2885	953.3635
954.2721	960.4193	964.1157
964.5185	971.4101	975.8504
981.9540	1019.5000	1035.1126
1046.5671	1050.1296	1051.3175
1052.8509	1054.0210	1058.8762
1060.4880	1087.1262	1148.5172
1175.2055	1180.8657	1181.2881
1200.5606	1203.3650	1219.8644
1230.2775	1238.9151	1242.5774
1243.3435	1249.7199	1257.6148
1264.6192	1265.6030	1275.3118
1283.0425	1283.9702	1284.2973
1288.6623	1291.2548	1311.7581
1332.5279	1367.2152	1376.3324
1390.1495	1396.4798	1401.1483
1404.8901	1405.7085	1406.3140
1406.8425	1422.4054	1429.1289
1433.2255	1439.8227	1442.4785
1469.0985	1471.2963	1475.4245
1478.7917	1480.1818	1480.4388
1484.0195	1485.1540	1486.7501
1495.3599	1499.7827	1500.1309
1500.9364	1503.4891	1504.7709
1509.7172	1511.9196	1513.0586
1516.1148	1517.8393	1564.4459
1693.6510	1700.4936	3055.4420

3059.3512	3061.0408	3062.7611
3063.0712	3064.8172	3068.0369
3068.1552	3068.8705	3135.9173
3139.4312	3139.6730	3140.3339
3140.6127	3142.1368	3143.3446
3144.1056	3145.6782	3146.7507
3148.2696	3150.0874	3150.2770
3154.5041	3155.1187	3155.3895
3197.1527	3200.9319	3212.1341
3268.9734	3281.3026	3290.4733

28e-ts

Zero-point correction= 0.533785
Thermal correction to Energy= 0.562460
Thermal correction to Enthalpy= 0.563230
Thermal correction to Gibbs Free Energy= 0.477251
Sum of electronic and zero-point Energies= -2824.642498
Sum of electronic and thermal Energies= -2824.613823
Sum of electronic and thermal Enthalpies= -2824.613053
Sum of electronic and thermal Free Energies= -2824.699032

Cartesian coordinates

C	-0.404092	2.062974	2.479318
N	0.924803	2.066969	2.423246
H	-2.650779	0.688491	0.836309
N	1.203565	1.297555	1.374780
N	0.113737	0.849393	0.822456
N	-0.931434	1.318975	1.499724
C	-4.032825	-0.842213	0.982108
C	-4.082355	0.912684	-0.645280
C	-5.211219	0.349899	-1.213641
C	-5.768944	-0.831563	-0.710070
C	-5.162647	-1.409341	0.405882
H	-5.666474	0.840803	-2.063401
H	-5.565476	-2.312122	0.841206
N	-3.526020	0.284959	0.425412
C	-3.338608	-1.412499	2.212056
C	-1.927708	-1.887636	1.819884
C	-3.276806	-0.326601	3.301965
C	-4.110689	-2.609801	2.777473
H	-1.311289	-1.086287	1.408425
H	-1.421695	-2.275196	2.709920
H	-1.986289	-2.693631	1.080763
H	-4.285394	-0.021188	3.601004

H	-2.765656	-0.731961	4.180780
H	-2.724242	0.557841	2.978677
H	-3.591847	-2.961481	3.673937
H	-5.132123	-2.341234	3.066987
H	-4.150625	-3.444932	2.070983
C	-3.430981	2.194136	-1.147323
C	-3.339314	3.204089	0.011192
C	-2.033423	1.862028	-1.699844
C	-4.258636	2.826871	-2.271102
H	-4.336354	3.450205	0.392185
H	-2.726604	2.834793	0.836346
H	-2.876190	4.125484	-0.355610
H	-2.107836	1.170671	-2.545851
H	-1.560583	2.784688	-2.052440
H	-1.377540	1.417971	-0.948316
H	-3.769318	3.755858	-2.577688
H	-4.318226	2.179656	-3.152097
H	-5.273915	3.075905	-1.944420
C	-7.004314	-1.424624	-1.379730
C	-8.149731	-0.399873	-1.294562
C	-6.679575	-1.710156	-2.857305
C	-7.455334	-2.726921	-0.713086
H	-8.397290	-0.172181	-0.252434
H	-7.895269	0.536570	-1.800130
H	-9.042468	-0.811520	-1.776750
H	-5.854719	-2.424405	-2.949132
H	-7.560611	-2.139369	-3.345545
H	-6.406761	-0.800085	-3.400217
H	-8.334852	-3.111133	-1.238539
H	-6.677944	-3.497228	-0.757680
H	-7.736351	-2.572751	0.334244
O	4.379110	-0.618273	-2.026527
S	5.530980	-0.594682	-1.159316
S	3.532751	0.384854	0.811825
C	5.863827	-2.331491	-0.601934
C	3.288550	1.897184	-0.327191
F	6.180476	-3.048273	-1.671561
F	4.787343	-2.835558	-0.025443
F	6.874015	-2.332787	0.252761
F	4.380949	2.085759	-1.056975
F	3.094352	2.958426	0.420625
F	2.272960	1.662372	-1.125381
O	5.159533	0.047506	0.263109
O	6.796823	-0.040334	-1.563213

O	3.848089	0.779795	2.153226
O	2.785934	-0.765096	0.391752
H	-0.985364	2.588958	3.223163

Vibrational frequencies

-37.9079	8.2472	13.9052
19.8190	25.0936	35.9418
37.8735	41.6779	45.5321
52.6714	59.3912	65.6887
71.2934	74.5514	97.1518
101.4361	114.3748	116.7292
133.4121	136.4187	146.2516
148.3932	151.5867	162.4471
168.4773	191.3792	194.1057
197.6386	212.9598	219.5869
240.7290	245.6998	249.0020
254.3731	260.9110	262.1295
266.6575	273.8605	290.2853
294.6614	301.0919	306.7671
313.8055	317.9458	320.2676
321.6222	324.7598	335.6497
346.2091	352.0247	354.6537
362.4554	373.3042	381.3919
386.3560	389.1740	392.8717
402.2765	422.9119	439.8532
461.2763	465.0347	520.1011
542.1570	550.1077	553.3471
554.1286	565.8944	568.1072
568.6916	572.1667	578.8724
611.5223	648.7040	687.4081
693.7259	730.6600	776.0724
782.1526	785.6679	786.8750
787.3567	794.3979	833.2998
846.0813	898.4629	912.8458
925.2001	926.7015	933.0189
949.0927	949.5065	951.3933
957.2186	958.8719	960.8848
964.3837	967.2012	968.1561
1014.5663	1023.4817	1041.1019
1043.4480	1046.9595	1047.7552
1050.4775	1052.0565	1055.6385
1067.4193	1097.9498	1144.9436
1175.5427	1180.1013	1196.3330
1199.4853	1207.1437	1231.8298

1234.2881	1238.4190	1242.0353
1242.6699	1249.0114	1256.8596
1264.8686	1266.8901	1279.6860
1281.4008	1290.4858	1290.7101
1292.2683	1293.4446	1323.1313
1328.7224	1370.5894	1379.7260
1394.0719	1398.0946	1399.6224
1399.9094	1402.3996	1403.9879
1415.8940	1423.8520	1427.2922
1430.3926	1449.5039	1460.3653
1469.4055	1474.8579	1476.8093
1478.5478	1480.1423	1481.9614
1482.4234	1483.4358	1485.4431
1497.0276	1499.7534	1500.3869
1501.7795	1503.6914	1505.0760
1509.5456	1512.0164	1512.9693
1516.2927	1520.1791	1567.4818
1697.7851	1708.8244	3027.2499
3055.6280	3057.7663	3059.2065
3060.9350	3062.1664	3062.6128
3064.4268	3066.2641	3067.8784
3135.5681	3136.1294	3137.3359
3138.9416	3139.3358	3139.4949
3140.6495	3141.0341	3142.0591
3142.1095	3145.8710	3146.3964
3146.7630	3147.0128	3172.9362
3174.9513	3182.0003	3182.8938
3271.1172	3280.8482	3289.9473

29e-ts

Zero-point correction= 0.534441
Thermal correction to Energy= 0.562977
Thermal correction to Enthalpy= 0.563747
Thermal correction to Gibbs Free Energy= 0.477873
Sum of electronic and zero-point Energies= -2824.642057
Sum of electronic and thermal Energies= -2824.613522
Sum of electronic and thermal Enthalpies= -2824.612752
Sum of electronic and thermal Free Energies= -2824.698625

Cartesian coordinates

C	-0.332548	-0.459738	-0.048572
N	-1.274333	-0.936684	-0.859901
H	2.790696	-0.293463	-0.168621
N	-0.621760	-1.525249	-1.862715

N	0.658013	-1.413859	-1.661656
N	0.879382	-0.746009	-0.521336
C	4.231638	1.165136	-0.422806
C	4.607509	-1.002659	0.520964
C	5.944397	-0.692569	0.695348
C	6.460582	0.549867	0.306754
C	5.576326	1.471397	-0.256257
H	6.594764	-1.433219	1.140709
H	5.925981	2.443598	-0.570629
N	3.800155	-0.058904	-0.033099
C	3.212730	2.133383	-1.009156
C	2.630453	1.532471	-2.301711
C	2.108733	2.380880	0.034945
C	3.859302	3.479762	-1.350318
H	2.151653	0.564396	-2.140142
H	1.873593	2.214294	-2.702351
H	3.414501	1.410982	-3.056503
H	2.527407	2.834023	0.940045
H	1.367263	3.068954	-0.383025
H	1.588910	1.461665	0.311343
H	3.087889	4.138213	-1.759753
H	4.279421	3.970295	-0.465998
H	4.643804	3.378747	-2.107280
C	3.988488	-2.338286	0.908334
C	2.856416	-2.094671	1.922104
C	3.452227	-3.023793	-0.360887
C	5.027166	-3.259041	1.556571
H	3.242306	-1.609753	2.825264
H	2.054898	-1.481733	1.504597
H	2.421092	-3.056927	2.209288
H	4.267403	-3.225511	-1.064206
H	2.995048	-3.979625	-0.085010
H	2.690475	-2.430646	-0.872089
H	4.536824	-4.200828	1.819270
H	5.850808	-3.492731	0.874112
H	5.439375	-2.830158	2.476111
C	7.940974	0.851098	0.518880
C	8.244864	0.766831	2.025739
C	8.777277	-0.198250	-0.235731
C	8.325553	2.244046	0.013223
H	7.642481	1.486905	2.589503
H	8.047426	-0.232754	2.424302
H	9.301623	0.995126	2.198425
H	8.561975	-0.176393	-1.309107

H	9.841744	0.016765	-0.095854
H	8.590001	-1.211879	0.131314
H	9.393921	2.404160	0.186427
H	8.142525	2.352098	-1.061169
H	7.783324	3.035591	0.541460
O	-5.352996	0.296693	-0.682179
S	-6.262571	0.152263	0.630941
S	-3.637332	-0.037242	-0.754204
C	-6.318839	1.933751	1.143014
C	-3.833792	-1.933539	-0.656288
F	-5.103559	2.359158	1.438365
F	-7.099234	2.024270	2.210854
F	-6.822598	2.659830	0.158137
F	-5.122865	-2.243468	-0.618810
F	-3.254811	-2.360019	0.442529
F	-3.303607	-2.461665	-1.732322
O	-5.564390	-0.582375	1.657308
O	-7.590457	-0.191026	0.193812
O	-3.137443	0.551179	0.458008
O	-3.405075	0.409991	-2.097078
H	-0.534647	0.089295	0.860054

Vibrational frequencies

-32.9246	2.9285	15.0482
20.4876	29.3846	33.9535
50.1049	55.0122	58.1248
59.5675	60.6795	67.8956
69.7012	75.7216	99.2752
102.2940	115.1056	116.7759
133.8917	137.5306	140.9539
144.9563	146.1147	160.3142
172.5036	183.6320	191.2966
196.2414	206.0777	208.7961
238.1979	244.3224	249.9682
250.6211	257.6315	261.4600
262.8337	270.8353	294.5428
296.2807	300.0870	310.2620
314.9174	317.4607	322.6789
334.2624	346.6999	357.4141
358.5531	360.6243	367.6325
372.5051	373.1302	379.8145
386.8411	389.0267	397.5409
403.0186	424.3282	442.5162
458.0740	466.7373	521.3857

541.2738	549.7499	554.2013
554.8209	566.0535	569.3124
569.8810	572.4722	580.6460
612.1436	649.9459	686.9415
697.1731	728.2384	770.9352
781.5402	784.9065	785.3520
789.9582	793.0327	831.2295
847.7531	914.8558	921.5814
925.6453	929.0056	949.5478
953.6414	955.0551	956.5941
957.9402	959.6070	961.2997
967.1991	969.1008	976.8840
1021.1130	1041.6439	1046.7935
1048.2697	1050.9973	1052.7436
1053.0787	1054.2528	1057.1861
1063.0721	1090.5782	1145.6792
1160.2212	1175.0952	1180.8419
1186.4268	1205.5223	1222.9490
1224.8188	1240.8130	1242.3454
1243.5768	1248.6645	1256.0638
1263.3276	1265.8314	1279.7596
1280.3641	1287.8324	1290.9680
1291.6113	1310.0462	1315.7965
1330.2201	1367.9092	1396.2532
1399.7626	1400.3208	1401.4296
1402.0674	1404.8059	1405.7136
1414.2496	1424.1670	1430.7064
1433.8069	1445.6023	1451.4151
1470.5178	1473.9937	1475.4041
1475.8894	1480.7779	1481.5439
1481.9614	1485.0748	1485.1704
1495.3801	1499.0223	1499.9652
1502.3208	1503.7127	1504.5393
1511.0714	1514.1786	1515.7381
1518.6463	1523.0313	1571.5175
1699.5525	1711.8400	3057.1861
3058.9319	3058.9629	3059.2197
3060.6499	3062.9346	3063.8868
3067.9717	3071.7644	3100.1992
3136.3560	3138.4536	3138.6383
3139.4909	3140.1124	3141.4973
3141.9376	3143.4545	3144.2234
3144.9865	3145.1520	3145.5334
3146.1103	3148.3577	3166.8264

3175.0732	3175.7575	3179.0883
3274.4055	3286.6545	3288.9948

18f-ts

Zero-point correction= 0.563565
Thermal correction to Energy= 0.592727
Thermal correction to Enthalpy= 0.593497
Thermal correction to Gibbs Free Energy= 0.509116
Sum of electronic and zero-point Energies= -2863.916699
Sum of electronic and thermal Energies= -2863.887537
Sum of electronic and thermal Enthalpies= -2863.886767
Sum of electronic and thermal Free Energies= -2863.971147

Cartesian coordinates

C	1.142885	3.485534	-0.071564
N	0.855676	2.245843	0.343292
H	-2.207205	1.380278	0.679977
N	-0.304476	2.346194	0.996941
N	-0.701713	3.587360	0.975414
N	0.180202	4.332431	0.308070
C	-3.175963	-0.270358	1.394956
C	-3.414338	0.633313	-0.815206
C	-4.213351	-0.440111	-1.164269
C	-4.486363	-1.471404	-0.254019
C	-3.979857	-1.346958	1.040019
H	-4.634513	-0.471013	-2.160312
H	-4.208432	-2.088537	1.791219
N	-2.889299	0.644484	0.439687
C	-2.609172	-0.061712	2.793790
C	-1.111328	-0.413354	2.781970
C	-2.803468	1.405847	3.216657
C	-3.328481	-0.961697	3.805419
H	-0.551604	0.261040	2.133482
H	-0.711268	-0.309508	3.796278
H	-0.950547	-1.446980	2.455621
H	-3.861072	1.689871	3.184495
H	-2.448575	1.524899	4.244738
H	-2.228023	2.103900	2.601485
H	-2.955163	-0.723566	4.805435
H	-4.411480	-0.797844	3.801930
H	-3.129827	-2.023218	3.627866
C	-3.130785	1.821124	-1.728134
C	-3.528464	3.114947	-0.994462
C	-1.639970	1.853178	-2.101771

C	-3.953193	1.722023	-3.017522
H	-4.588719	3.095953	-0.720033
H	-2.932612	3.292006	-0.094340
H	-3.361220	3.965998	-1.661969
H	-1.356420	0.946236	-2.646402
H	-1.452477	2.715524	-2.749721
H	-0.996635	1.950130	-1.225838
H	-3.749296	2.608960	-3.624196
H	-3.681564	0.844971	-3.614051
H	-5.029164	1.694517	-2.815079
C	-5.327099	-2.665566	-0.695005
C	-6.704043	-2.166671	-1.169205
C	-4.601670	-3.364219	-1.859966
C	-5.530508	-3.677457	0.435999
H	-7.233922	-1.648569	-0.363098
H	-6.622501	-1.484528	-2.020654
H	-7.310990	-3.022304	-1.482548
H	-3.611776	-3.716425	-1.551419
H	-5.187189	-4.230566	-2.184331
H	-4.477151	-2.699653	-2.720291
H	-6.125871	-4.515832	0.062229
H	-4.578557	-4.081634	0.796710
H	-6.068612	-3.239228	1.283265
O	3.331458	-1.217937	0.529647
S	4.314251	-1.662036	-0.655289
S	2.436717	0.292996	0.571157
C	5.940820	-1.254123	0.137270
C	1.205512	-0.234237	-0.789762
F	5.998794	0.033518	0.424122
F	6.898671	-1.567387	-0.724152
F	6.082080	-1.969038	1.241815
F	1.473058	-1.472088	-1.185502
F	1.325855	0.581142	-1.811517
F	-0.009810	-0.218846	-0.283399
O	4.153428	-0.799886	-1.801575
O	4.250572	-3.097609	-0.751093
O	3.410826	1.252193	0.134806
O	1.877514	0.142075	1.883079
C	2.347566	3.883812	-0.856616
H	3.236556	3.926316	-0.221507
H	2.544202	3.168976	-1.659146
H	2.182828	4.872427	-1.290203

Vibrational frequencies

-75.0824	16.2676	22.0629
31.9411	36.2630	38.8485
46.9768	50.4778	56.6752
60.3313	68.9541	74.3540
79.5628	83.3170	97.1888
104.5199	111.0053	112.6929
121.3971	135.0472	141.6928
146.5830	154.4800	158.9734
169.8855	189.9242	197.6946
213.1611	216.1815	225.0059
230.2704	233.7511	245.5809
254.0738	256.0533	266.2503
269.5238	273.8461	289.6136
292.5454	295.4399	304.8075
308.3374	315.3274	316.3875
319.0689	320.5605	322.9101
334.5148	351.0649	355.8412
361.0603	370.4537	373.2627
376.2952	384.4876	388.3003
389.1856	395.5179	397.3227
403.6539	424.9137	436.6819
467.5760	470.6967	520.8182
544.1608	548.8800	554.6290
555.2249	562.9977	569.6251
570.7244	573.1946	581.2575
614.3217	646.3155	685.5416
697.5711	709.5490	746.8916
767.5812	776.4737	782.7983
785.1856	786.8519	795.2553
836.5585	849.6471	870.8087
921.2475	926.9113	928.0987
948.1827	954.1211	954.9297
960.1284	961.2432	963.7313
965.5923	977.4702	981.8073
981.9073	1020.1729	1032.1067
1048.3137	1049.3332	1053.4021
1056.3001	1059.8605	1061.9235
1076.0790	1081.7789	1095.2692
1126.1103	1144.7355	1180.9971
1189.7109	1202.0973	1206.9495
1217.5281	1230.0294	1239.8302
1242.1694	1246.7592	1251.5527
1258.4572	1264.6479	1264.9536
1272.8956	1281.7215	1287.5737

1292.7987	1294.7084	1318.6363
1319.8595	1323.2312	1366.5127
1393.2114	1402.6005	1403.1050
1404.8054	1406.9235	1408.7468
1412.8137	1416.6656	1423.0546
1431.8718	1434.5790	1441.7266
1444.9173	1459.5610	1471.6442
1473.1679	1475.9279	1478.4006
1480.1247	1481.4851	1483.3581
1485.1943	1485.8414	1487.1071
1495.4194	1499.5748	1501.8631
1505.6420	1507.3631	1509.0130
1512.6279	1512.8557	1516.5083
1518.1200	1522.3150	1556.4122
1559.7469	1685.2891	1698.6353
3057.3056	3059.3301	3059.4393
3061.9617	3063.0628	3064.6714
3064.8299	3066.6221	3068.2229
3085.0727	3132.1518	3138.6576
3139.0431	3140.5216	3141.8766
3142.6185	3143.3938	3144.2567
3144.8276	3145.7512	3146.2721
3147.7604	3150.6471	3153.2293
3154.9858	3157.2318	3159.0585
3175.0457	3194.6463	3199.6634
3263.9455	3288.5183	3359.6066

19f-ts

Zero-point correction= 0.562766
Thermal correction to Energy= 0.592024
Thermal correction to Enthalpy= 0.592794
Thermal correction to Gibbs Free Energy= 0.508295
Sum of electronic and zero-point Energies= -2863.923735
Sum of electronic and thermal Energies= -2863.894477
Sum of electronic and thermal Enthalpies= -2863.893707
Sum of electronic and thermal Free Energies= -2863.978206

Cartesian coordinates

C	4.005090	-2.887204	-0.226223
N	4.120260	-1.559113	-0.318180
H	0.130114	-2.123680	0.148825
N	2.890394	-1.106342	-0.122364
N	2.064209	-2.101488	0.071441
N	2.734795	-3.242527	0.016296

C	-1.549438	-1.890087	-1.025307
C	-1.461275	-1.599895	1.349254
C	-2.763106	-1.129174	1.339387
C	-3.480229	-1.001670	0.143245
C	-2.856182	-1.417348	-1.033903
H	-3.231039	-0.867348	2.279254
H	-3.385507	-1.385353	-1.974279
N	-0.892978	-1.917898	0.157815
C	-0.845348	-2.430931	-2.267659
C	0.273905	-1.474690	-2.712159
C	-0.258400	-3.817006	-1.944156
C	-1.837807	-2.584400	-3.426442
H	1.077434	-1.426196	-1.977286
H	0.699756	-1.843031	-3.651242
H	-0.113220	-0.464490	-2.883070
H	-1.043607	-4.512491	-1.628060
H	0.213488	-4.220932	-2.845455
H	0.511076	-3.778172	-1.167427
H	-1.312941	-3.040664	-4.270536
H	-2.680123	-3.233724	-3.164825
H	-2.227497	-1.619239	-3.765870
C	-0.652236	-1.828235	2.622456
C	-0.055198	-3.247466	2.592882
C	0.473200	-0.786196	2.725788
C	-1.548740	-1.705637	3.859431
H	-0.842263	-4.004356	2.504963
H	0.660548	-3.387315	1.777268
H	0.483797	-3.423394	3.529013
H	0.077182	0.233520	2.681596
H	0.988853	-0.917969	3.683271
H	1.201782	-0.912265	1.925891
H	-0.950773	-1.942863	4.744024
H	-1.935187	-0.689623	3.987511
H	-2.391608	-2.404457	3.826876
C	-4.909687	-0.467829	0.171876
C	-5.771491	-1.417261	1.024090
C	-4.908214	0.933423	0.807849
C	-5.518344	-0.370095	-1.229598
H	-5.767574	-2.431380	0.610737
H	-5.417939	-1.467346	2.058474
H	-6.805611	-1.057635	1.037867
H	-4.296274	1.628750	0.224309
H	-5.932037	1.320611	0.836539
H	-4.526907	0.917662	1.832957

H	-6.529975	0.039340	-1.151291
H	-4.938514	0.295707	-1.878083
H	-5.593885	-1.350078	-1.712660
O	0.304181	2.788173	1.429623
S	0.393728	3.500836	0.176832
S	1.885819	1.055023	-0.657563
C	-1.227071	3.301749	-0.699060
C	3.177128	1.505827	0.679956
F	-2.155700	3.924076	0.016763
F	-1.537505	2.020191	-0.809869
F	-1.153527	3.847743	-1.902831
F	3.155574	2.809618	0.911619
F	4.355509	1.169950	0.215602
F	2.884485	0.866165	1.788858
O	1.338435	2.734288	-0.850877
O	0.716877	4.903104	0.109310
O	2.482194	0.924859	-1.957097
O	0.689409	0.423067	-0.170683
C	5.134665	-3.848813	-0.379576
H	5.337919	-4.368992	0.560805
H	4.899211	-4.601450	-1.136590
H	6.036186	-3.313301	-0.683127

Vibrational frequencies

-77.8863	14.5593	20.5549
30.4535	38.8338	43.8397
49.4843	56.2825	59.2712
66.7680	70.0852	75.6686
81.5008	83.7512	88.8374
92.1896	99.0976	102.6903
113.1768	122.0712	137.0390
141.3422	145.0711	151.4241
175.7332	180.2091	188.1213
190.8874	219.0333	220.7096
227.9475	236.5952	246.4342
251.5058	255.4675	269.2419
281.9258	284.9758	291.3159
294.4304	299.5537	306.7231
312.8478	317.8291	320.7598
321.2723	331.0761	333.1398
341.9277	353.1560	360.2496
362.9560	365.2859	371.0197
376.7442	380.3038	385.1440
390.5473	392.8629	395.0729

402.3430	422.7743	441.1081
462.2837	468.2140	520.5672
543.7599	550.4533	553.5854
555.3128	564.7525	565.8312
571.9993	573.2927	580.6928
614.8857	638.8879	679.4436
689.1780	711.9611	743.4077
766.1722	777.6751	784.5540
785.3466	785.4817	794.7583
849.2563	851.2570	898.3229
918.3518	924.1876	926.4498
951.4008	951.9058	956.3474
960.0979	962.3812	964.3168
969.5303	970.3108	973.2031
988.1913	1011.5639	1045.0307
1048.4766	1052.4858	1053.8650
1054.3920	1055.7223	1057.3207
1074.1878	1087.1002	1095.8521
1109.9085	1149.8718	1179.9196
1182.3844	1206.2872	1225.1195
1241.3322	1241.9705	1244.1144
1244.5923	1248.0083	1252.5052
1257.4681	1264.3309	1268.6103
1273.8381	1283.5555	1285.1739
1286.6817	1288.3277	1303.2578
1311.4087	1332.9271	1365.2926
1395.6136	1399.8152	1400.3150
1403.2019	1404.3254	1406.8782
1408.4873	1409.6375	1423.2744
1429.3772	1432.8818	1438.8237
1443.1592	1447.3314	1471.9228
1473.0668	1475.7506	1476.2970
1478.3475	1479.6751	1483.8634
1485.3987	1486.3745	1489.2929
1495.1001	1500.4315	1501.6248
1504.1895	1504.4221	1505.2728
1506.6537	1510.9803	1515.9831
1516.7340	1520.7804	1554.5338
1565.4839	1697.1087	1701.7250
3056.1213	3058.2831	3059.3958
3060.0089	3061.8880	3062.1452
3063.9888	3069.2961	3071.1079
3076.1744	3103.8739	3135.3581
3136.7265	3138.0198	3139.8726

3140.4539	3140.9298	3141.6978
3141.8241	3143.2970	3143.7444
3145.8524	3147.3191	3148.5398
3149.4190	3151.1137	3152.0243
3159.3262	3173.9256	3203.2359
3206.4828	3256.8769	3279.2330

20f-ts

Zero-point correction= 0.562098
Thermal correction to Energy= 0.591590
Thermal correction to Enthalpy= 0.592360
Thermal correction to Gibbs Free Energy= 0.505626
Sum of electronic and zero-point Energies= -2863.921215
Sum of electronic and thermal Energies= -2863.891724
Sum of electronic and thermal Enthalpies= -2863.890954
Sum of electronic and thermal Free Energies= -2863.977688

Cartesian coordinates

C	-0.848850	-0.131344	2.072799
N	-1.161411	-0.131385	0.767444
H	2.778986	0.090250	0.502895
N	-0.017197	-0.014332	0.106742
N	0.949500	0.047172	0.972714
N	0.471375	-0.023690	2.218549
C	4.367651	1.327418	0.032308
C	4.459050	-1.062261	0.109781
C	5.794904	-1.021951	-0.248979
C	6.449640	0.194976	-0.477491
C	5.708758	1.367975	-0.328728
H	6.334534	-1.953882	-0.351824
H	6.171602	2.330286	-0.489467
N	3.794605	0.117075	0.233903
C	3.507022	2.569778	0.220589
C	2.347285	2.538962	-0.792074
C	2.981517	2.601924	1.667953
C	4.319965	3.846884	-0.020159
H	1.716418	1.654031	-0.688291
H	1.713026	3.416874	-0.632768
H	2.731357	2.575354	-1.817240
H	3.813989	2.650932	2.378347
H	2.364937	3.496742	1.800944
H	2.364076	1.735859	1.914646
H	3.659972	4.707160	0.124543
H	5.151901	3.944341	0.685353

H	4.712777	3.898798	-1.040882
C	3.690586	-2.349913	0.376513
C	3.164763	-2.331985	1.823236
C	2.534618	-2.467123	-0.633999
C	4.596152	-3.574514	0.211574
H	3.997007	-2.294579	2.534597
H	2.497817	-1.490943	2.023657
H	2.599852	-3.251446	2.007770
H	2.921337	-2.514589	-1.657691
H	1.981512	-3.390810	-0.434571
H	1.826478	-1.638397	-0.568098
H	4.004316	-4.471586	0.415347
H	4.989827	-3.661117	-0.806458
H	5.434440	-3.563338	0.916068
C	7.924947	0.197817	-0.865157
C	8.730055	-0.486360	0.254324
C	8.095216	-0.589987	-2.176287
C	8.464958	1.615891	-1.067262
H	8.602158	0.036350	1.208037
H	8.431068	-1.529851	0.392415
H	9.794371	-0.473255	-0.002718
H	7.522689	-0.130745	-2.988998
H	9.152092	-0.594437	-2.462718
H	7.770298	-1.629480	-2.071695
H	9.520878	1.559604	-1.348268
H	7.936037	2.143030	-1.868487
H	8.396243	2.211451	-0.150901
O	-4.830757	0.253518	-1.209511
S	-6.201450	-0.340458	-0.652979
S	-3.297461	0.268525	-0.323296
C	-7.020941	1.237973	-0.131182
C	-3.019052	-1.609475	-0.547103
F	-6.298458	1.845690	0.793155
F	-8.214965	0.933308	0.360541
F	-7.162493	2.031264	-1.182069
F	-4.006518	-2.140091	-1.253779
F	-2.988390	-2.172394	0.640685
F	-1.894530	-1.786131	-1.202513
O	-5.979089	-1.134221	0.532768
O	-6.954241	-0.835023	-1.778128
O	-3.730871	0.659186	0.990933
O	-2.562494	1.045739	-1.281097
C	-1.819207	-0.240170	3.200163
H	-2.552732	-1.027209	3.012175

H	-1.276452	-0.470421	4.119071
H	-2.364759	0.696577	3.341329

Vibrational frequencies

-97.2026	11.8590	14.4117
17.8884	30.4757	35.4602
40.8100	44.9624	48.9831
54.1443	58.7757	68.0945
76.1437	80.5313	98.9815
105.0582	117.1767	123.3236
124.2127	129.5464	138.7314
142.7165	153.8284	164.2611
166.4967	177.1431	191.9159
193.5732	196.6874	198.1167
237.3203	240.2296	243.0568
246.6772	251.5737	252.5960
254.7480	265.8571	283.5185
293.3568	301.2241	302.4234
306.2771	308.3473	316.0841
319.6529	323.8587	327.9639
348.4108	354.9883	357.6782
360.7326	362.1106	368.7756
372.2677	377.4885	385.5669
391.0209	393.0372	401.4478
404.0184	422.2248	433.8164
461.8554	463.7708	521.2261
542.4006	549.4167	551.1115
554.4726	565.9200	567.8774
568.4906	570.6179	582.0335
614.6576	640.9031	688.2826
694.6664	712.3343	736.6508
773.0297	783.3022	784.4101
784.8747	790.4023	793.0643
839.5643	846.3540	920.5890
924.6049	926.9359	944.3858
951.0334	951.4500	952.9749
955.5936	958.3416	959.4671
962.0350	967.2907	967.5064
1013.6316	1020.7355	1044.2561
1045.8285	1047.0929	1048.5217
1049.7671	1053.1697	1066.1623
1083.2412	1089.1426	1092.8013
1138.2050	1146.3602	1179.9684
1185.4230	1207.0620	1217.8092

1222.6933	1238.9274	1239.4586
1241.4491	1242.5922	1247.5145
1253.7401	1263.5730	1264.6849
1275.6425	1280.3686	1288.4104
1291.8358	1292.6825	1314.0616
1320.8707	1341.5545	1368.4271
1395.1096	1397.5579	1398.4871
1400.4822	1402.6328	1406.1861
1407.0185	1409.5456	1423.5851
1426.6737	1431.6871	1434.8457
1442.8310	1449.6624	1472.6710
1474.1376	1475.1550	1475.5487
1476.6824	1478.7144	1478.8450
1481.0828	1483.2329	1483.7957
1494.1713	1497.9875	1499.5878
1500.3002	1502.0047	1502.5181
1505.8536	1508.9955	1511.4509
1512.1365	1515.5477	1566.3268
1572.4334	1696.6451	1710.9507
2935.2432	3057.2321	3058.0548
3058.8550	3062.0660	3062.2357
3062.3578	3065.3968	3065.7069
3066.5208	3083.5578	3135.5928
3136.0341	3137.3915	3138.1196
3138.6091	3138.8678	3139.0809
3141.9671	3144.7356	3144.9946
3145.7134	3146.9316	3147.3353
3150.1621	3160.0262	3173.9565
3175.1067	3176.7625	3177.1864
3183.9194	3262.7184	3302.8461

27f-ts

Zero-point correction= 0.563547
Thermal correction to Energy= 0.592592
Thermal correction to Enthalpy= 0.593362
Thermal correction to Gibbs Free Energy= 0.510021
Sum of electronic and zero-point Energies= -2863.919536
Sum of electronic and thermal Energies= -2863.890491
Sum of electronic and thermal Enthalpies= -2863.889721
Sum of electronic and thermal Free Energies= -2863.973062

Cartesian coordinates

C	-3.091372	-3.231960	-0.088585
N	-4.305480	-2.803040	-0.455395

H	-0.190618	-2.149019	0.086883
N	-4.185810	-1.487534	-0.598484
N	-2.961667	-1.139126	-0.328794
N	-2.229562	-2.212195	-0.011288
C	1.344209	-1.594663	1.336957
C	1.502025	-1.792680	-1.043985
C	2.782846	-1.270817	-0.998690
C	3.371056	-0.882779	0.211945
C	2.633622	-1.077806	1.380039
H	3.338353	-1.178998	-1.922277
H	3.058590	-0.834270	2.342607
N	0.817673	-1.894603	0.126228
C	0.513101	-1.878842	2.584060
C	-0.656558	-0.884836	2.665140
C	-0.022786	-3.319795	2.512731
C	1.364243	-1.741152	3.850691
H	-1.345722	-1.019470	1.831766
H	-1.205038	-1.060686	3.596915
H	-0.298654	0.149715	2.661868
H	0.796537	-4.044531	2.449853
H	-0.598546	-3.531291	3.419081
H	-0.691969	-3.467938	1.660998
H	0.747338	-2.016393	4.710936
H	2.235641	-2.404611	3.837443
H	1.704606	-0.712682	4.007651
C	0.848464	-2.308814	-2.323265
C	0.294338	-3.719642	-2.062820
C	-0.292651	-1.375470	-2.757095
C	1.873496	-2.390412	-3.460431
H	1.085160	-4.406086	-1.741240
H	-0.493762	-3.707182	-1.306138
H	-0.146421	-4.108224	-2.985950
H	0.067039	-0.350635	-2.896572
H	-0.697217	-1.730561	-3.710572
H	-1.105758	-1.371254	-2.030137
H	1.385841	-2.837024	-4.331704
H	2.236029	-1.401762	-3.759876
H	2.731929	-3.017700	-3.197113
C	4.787154	-0.313310	0.216156
C	5.744309	-1.360328	-0.382812
C	4.814061	0.960833	-0.646664
C	5.265892	0.037158	1.627655
H	5.720895	-2.291330	0.193482
H	5.498573	-1.593287	-1.423262

H	6.767503	-0.971167	-0.359660
H	4.174945	1.738415	-0.217157
H	5.837341	1.347815	-0.690529
H	4.482910	0.768201	-1.671881
H	6.274427	0.457510	1.567899
H	4.621223	0.784088	2.102930
H	5.313659	-0.846901	2.272514
O	-0.342614	2.699435	1.507285
S	-0.393958	3.464830	0.284716
S	-1.895932	1.087836	-0.707597
C	1.234944	3.257529	-0.573746
C	-3.244011	1.472378	0.593463
F	1.501670	1.971649	-0.734904
F	2.171477	3.816011	0.182946
F	1.198548	3.856518	-1.753140
F	-4.403194	1.198519	0.049053
F	-3.203532	2.756874	0.915098
F	-3.022194	0.753123	1.669151
O	-0.691549	4.873527	0.266087
O	-1.334790	2.760146	-0.795412
O	-0.736764	0.410893	-0.193124
O	-2.442737	1.014232	-2.031865
C	-2.780582	-4.657370	0.229756
H	-1.728967	-4.889116	0.048143
H	-2.999937	-4.877752	1.279578
H	-3.395902	-5.316487	-0.386846

Vibrational frequencies

-72.3157	22.4331	30.3644
33.6053	38.7192	44.6510
46.5464	55.3312	56.5381
62.8832	70.0378	71.1943
77.4707	79.5876	93.9833
99.9501	104.4126	114.4160
124.7067	137.2351	141.4492
144.9972	149.8597	177.3885
181.1714	187.5664	191.3539
193.5971	209.1155	233.2695
235.9514	242.0808	248.6668
251.3239	260.9759	270.0148
277.4979	286.5700	291.8540
299.7083	302.3375	306.3385
312.1117	317.2406	319.1331
321.5693	325.2298	333.3932

344.6908 347.7060 354.2189
361.4766 366.5375 370.6008
372.3379 383.4230 384.4575
388.9450 391.4480 395.3075
400.6634 421.3354 437.7234
464.4291 468.8623 522.3325
545.2207 549.2911 554.0205
554.4113 567.6187 568.4277
572.1043 573.7612 581.9684
613.5769 643.3042 682.6631
689.0430 708.4496 743.4425
764.3784 782.1923 784.2711
785.1629 786.1762 795.7881
844.9509 850.8485 908.6734
923.7264 928.2509 929.6402
952.8020 953.5769 955.7154
959.1252 963.5887 965.2413
969.4914 971.9132 977.9753
993.0388 1013.5567 1040.2966
1049.2284 1052.4602 1052.7813
1054.7343 1056.2027 1063.8833
1078.3377 1083.1011 1093.3386
1114.2819 1147.9691 1181.5708
1193.6029 1207.9756 1215.0296
1224.4874 1231.0370 1240.1674
1244.7377 1245.9113 1251.7387
1259.9501 1267.3413 1268.5827
1276.6826 1283.5177 1285.7447
1288.3879 1289.8867 1318.2245
1324.4217 1333.8544 1365.3975
1394.0331 1396.7181 1399.9878
1402.3776 1403.0354 1407.6967
1412.0320 1415.6885 1424.2933
1429.0162 1434.0497 1444.1125
1446.0290 1451.1855 1469.7187
1471.3056 1476.3754 1479.6682
1479.8447 1481.3626 1482.3389
1483.3285 1487.1807 1487.7979
1496.6085 1499.2116 1502.1079
1502.6430 1504.4761 1508.9099
1514.2230 1516.0157 1516.3037
1518.0501 1521.3838 1555.6498
1564.1941 1696.1500 1702.2145
3057.3570 3059.5812 3060.3923

3061.0198	3062.7740	3063.4821
3066.0956	3067.2007	3070.0634
3082.9046	3135.8231	3137.8573
3139.0313	3140.8271	3141.0003
3141.1991	3142.0821	3144.2984
3144.3541	3144.7645	3145.8209
3147.8142	3151.4354	3154.2654
3154.9292	3159.5439	3170.0024
3179.7506	3186.6846	3194.1256
3195.5224	3267.5135	3277.0343

28f-ts

Zero-point correction= 0.562423
Thermal correction to Energy= 0.591977
Thermal correction to Enthalpy= 0.592747
Thermal correction to Gibbs Free Energy= 0.505173
Sum of electronic and zero-point Energies= -2863.916348
Sum of electronic and thermal Energies= -2863.886795
Sum of electronic and thermal Enthalpies= -2863.886025
Sum of electronic and thermal Free Energies= -2863.973599

Cartesian coordinates

C	-0.409267	2.899229	0.866631
N	0.923154	2.903797	0.883247
H	-2.563575	0.782987	0.198307
N	1.263084	1.690238	0.453043
N	0.209087	0.977683	0.188209
N	-0.871941	1.714100	0.437132
C	-4.024797	-0.320638	1.162696
C	-4.018327	0.222965	-1.167732
C	-5.214726	-0.453931	-1.326234
C	-5.849271	-1.075147	-0.243544
C	-5.227114	-0.997519	1.002936
H	-5.661735	-0.497831	-2.309974
H	-5.674204	-1.463971	1.868228
N	-3.468326	0.266756	0.075112
C	-3.298559	-0.201106	2.495879
C	-1.911854	-0.858355	2.371910
C	-3.176284	1.288555	2.863236
C	-4.069261	-0.911065	3.613979
H	-1.291930	-0.398449	1.599951
H	-1.384189	-0.756141	3.325538
H	-2.011522	-1.925890	2.148459
H	-4.166432	1.733203	3.011755

H	-2.610717	1.383909	3.795709
H	-2.650085	1.856574	2.094575
H	-3.509256	-0.793919	4.546227
H	-5.063652	-0.479129	3.767460
H	-4.174296	-1.983843	3.422575
C	-3.281903	0.916930	-2.306052
C	-3.122207	2.410156	-1.969840
C	-1.909301	0.245625	-2.493206
C	-4.063637	0.801235	-3.619007
H	-4.099958	2.884861	-1.833166
H	-2.521607	2.563645	-1.071194
H	-2.611445	2.910428	-2.798522
H	-2.030751	-0.807704	-2.767938
H	-1.372072	0.750581	-3.302479
H	-1.285190	0.300794	-1.598304
H	-3.500595	1.316204	-4.402629
H	-4.190207	-0.240020	-3.932823
H	-5.049548	1.273826	-3.552593
C	-7.171105	-1.804374	-0.462215
C	-8.192435	-0.817343	-1.056192
C	-6.935587	-2.957940	-1.454323
C	-7.737296	-2.376927	0.840008
H	-8.366357	0.024879	-0.378176
H	-7.862439	-0.420704	-2.020928
H	-9.145493	-1.332453	-1.213790
H	-6.203473	-3.671851	-1.062707
H	-7.877749	-3.490099	-1.622314
H	-6.576354	-2.593533	-2.421642
H	-8.686843	-2.877541	0.628227
H	-7.065456	-3.117596	1.286393
H	-7.932886	-1.591917	1.578451
O	4.868583	-0.925127	-1.775699
S	5.701050	-1.027027	-0.600888
S	3.423500	0.433505	0.650637
C	5.527975	-2.746780	0.065805
C	3.793313	1.822117	-0.607205
F	6.097346	-3.575950	-0.799412
F	4.251120	-3.054945	0.206445
F	6.141871	-2.833458	1.235781
F	5.067262	1.772413	-0.973477
F	3.567584	2.973142	-0.021180
F	3.032016	1.648353	-1.662991
O	5.066215	-0.214680	0.618871
O	7.112754	-0.741201	-0.625877

O	3.447861	0.913440	2.002887
O	2.644891	-0.646399	0.116430
C	-1.263571	4.047321	1.289693
H	-2.208998	4.051352	0.740836
H	-1.490780	3.996014	2.359650
H	-0.744361	4.989372	1.100905

Vibrational frequencies

-56.9441	6.8164	11.6350
20.0688	25.0984	35.8395
43.4247	47.0035	48.5249
51.7525	62.0741	64.8166
72.9371	79.0484	95.7551
102.1416	109.3214	115.9936
124.4587	128.0441	138.1760
143.6197	145.3977	153.1518
162.5724	166.5142	186.2566
192.5270	216.0594	230.0170
231.2536	234.6567	244.3920
250.0703	252.1370	256.9788
269.3964	280.1225	287.5946
290.8049	297.3959	301.8352
306.5321	314.9524	320.9054
322.0316	325.6621	327.9897
342.0005	348.2747	352.3874
355.9849	356.5867	359.4519
370.9482	376.4248	383.6593
384.7303	391.4227	393.8728
403.9260	424.3189	438.7533
458.3498	464.0453	520.7467
538.1303	548.6483	553.5539
553.9225	565.9499	566.8002
569.4669	572.8184	579.8781
614.2881	639.9002	689.8125
696.2758	709.7506	747.2124
767.1374	783.4642	784.5122
785.6847	789.1895	794.8218
841.5786	848.9618	919.7566
925.0305	930.3516	939.4772
950.2945	954.6808	954.7808
959.5142	959.9359	962.2395
968.5711	970.1553	970.3782
1010.3891	1019.5551	1046.6109
1048.2069	1049.9712	1052.5728

1054.2510	1056.8390	1061.0404
1072.1229	1084.6191	1094.4152
1123.9921	1147.0524	1178.2865
1182.2986	1204.5366	1227.6680
1228.2669	1232.4474	1238.4648
1242.2580	1244.0405	1248.2810
1256.8630	1264.0591	1266.6634
1275.7886	1280.7356	1286.2509
1290.3243	1290.4429	1310.8153
1329.5335	1335.4915	1369.1035
1396.5827	1399.7263	1400.9631
1402.4520	1402.6010	1404.8845
1410.6378	1412.1960	1425.5109
1426.7086	1433.3788	1442.3682
1448.2332	1451.9233	1472.2128
1473.4931	1476.0512	1478.5636
1479.8017	1481.1885	1482.7049
1484.2034	1486.1285	1486.5447
1494.3926	1499.2240	1501.0640
1501.7906	1504.2476	1506.2234
1507.0285	1509.8550	1512.8586
1514.5712	1518.6890	1560.0465
1571.2049	1697.8085	1708.4877
3020.2770	3058.4153	3058.9719
3060.8365	3062.5323	3066.1090
3066.8063	3067.6403	3068.6921
3070.9081	3072.7217	3136.8624
3137.2524	3139.6725	3140.2134
3140.4681	3141.6542	3142.7473
3144.3579	3144.4905	3145.0747
3147.4913	3148.8458	3150.8340
3151.2256	3154.2671	3164.1722
3176.4725	3178.7472	3185.1503
3188.4702	3265.9215	3279.5073

29f-ts

Zero-point correction= 0.562539
Thermal correction to Energy= 0.591947
Thermal correction to Enthalpy= 0.592717
Thermal correction to Gibbs Free Energy= 0.506011
Sum of electronic and zero-point Energies= -2863.918393
Sum of electronic and thermal Energies= -2863.888985
Sum of electronic and thermal Enthalpies= -2863.888215
Sum of electronic and thermal Free Energies= -2863.974921

Cartesian coordinates

C	0.264143	-0.394749	-0.021117
N	1.239398	-0.716582	0.834328
H	-2.784821	-0.190094	0.234154
N	0.642151	-1.054975	1.977378
N	-0.640990	-0.951327	1.828474
N	-0.918049	-0.538164	0.582373
C	-4.266871	1.255018	0.287485
C	-4.597114	-1.040019	-0.306011
C	-5.945973	-0.794922	-0.494583
C	-6.490389	0.479304	-0.293014
C	-5.621772	1.498362	0.099760
H	-6.583466	-1.612082	-0.802875
H	-5.994403	2.498596	0.262701
N	-3.806428	-0.003424	0.081752
C	-3.272725	2.327177	0.717285
C	-2.681403	1.940467	2.085293
C	-2.168462	2.447119	-0.348484
C	-3.954185	3.692518	0.856744
H	-2.166084	0.978066	2.066656
H	-1.954089	2.700920	2.387308
H	-3.468622	1.899584	2.845625
H	-2.587367	2.773914	-1.306383
H	-1.434187	3.190481	-0.021894
H	-1.640690	1.504537	-0.498554
H	-3.197636	4.425599	1.151588
H	-4.395434	4.031096	-0.086587
H	-4.729012	3.687607	1.630476
C	-3.952088	-2.406156	-0.502114
C	-2.838676	-2.295766	-1.558779
C	-3.383560	-2.886388	0.845415
C	-4.977217	-3.435845	-0.989805
H	-3.243047	-1.954755	-2.517983
H	-2.044250	-1.616128	-1.244685
H	-2.389360	-3.282750	-1.706955
H	-4.184544	-2.994008	1.584520
H	-2.913216	-3.865151	0.706161
H	-2.626875	-2.210613	1.249461
H	-4.466473	-4.393518	-1.125214
H	-5.781850	-3.590867	-0.263699
H	-5.416590	-3.153788	-1.952599
C	-7.983756	0.707937	-0.508341
C	-8.333869	0.362252	-1.966941

C	-8.770393	-0.213696	0.441192
C	-8.390873	2.158537	-0.234735
H	-7.770188	0.988639	-2.666328
H	-8.126390	-0.686552	-2.200356
H	-9.401291	0.538459	-2.134940
H	-8.532053	0.002799	1.487757
H	-9.843643	-0.052841	0.295038
H	-8.561268	-1.270977	0.252466
H	-9.466789	2.264657	-0.402791
H	-8.186377	2.450582	0.800818
H	-7.880776	2.859236	-0.904482
O	5.366279	0.047989	0.732820
S	6.246909	0.029409	-0.596161
S	3.603811	-0.092078	0.790311
C	6.556645	1.847851	-0.773172
C	3.615988	-1.955460	0.371224
F	5.413258	2.495131	-0.916500
F	7.311154	2.029433	-1.849209
F	7.193402	2.295117	0.297871
F	4.862710	-2.382830	0.229120
F	2.969232	-2.133228	-0.760673
F	3.058945	-2.608735	1.363359
O	5.462684	-0.394838	-1.731595
O	7.517593	-0.567772	-0.271463
O	3.206437	0.760099	-0.297997
O	3.462822	0.146992	2.198028
C	0.460337	0.068342	-1.425800
H	0.743966	1.124909	-1.449806
H	1.255404	-0.499319	-1.913575
H	-0.464232	-0.057301	-1.994628

Vibrational frequencies

-89.3668	8.7433	13.2213
20.5107	27.9110	35.5556
38.6570	46.4494	47.3271
57.4063	67.8510	71.0500
77.4286	81.4279	94.3997
97.5579	114.7544	117.5183
128.4404	139.6275	141.5359
147.9286	153.0650	165.5900
168.0623	193.6246	195.3181
204.7541	208.7769	218.7262
229.6149	232.0305	246.8217
249.4118	250.8709	258.4960

262.0051	270.9670	289.2919
291.8746	297.7808	299.5804
306.7888	310.2767	311.6319
314.5969	321.1951	323.2496
336.1464	348.3251	355.0590
359.2698	362.3659	366.8859
371.7840	373.9008	384.3787
389.8278	393.2388	401.9799
407.6153	423.3661	437.6397
460.7808	463.5212	519.8348
540.5041	547.5304	553.0652
553.6337	566.8420	568.0710
568.3632	570.7707	580.5451
614.8343	641.1726	688.0313
696.1219	708.6133	746.4055
767.5328	782.4187	783.5326
783.8717	788.3001	794.8196
837.9362	848.5714	913.8248
924.9689	927.5619	934.4022
950.4810	952.1889	954.9076
959.6065	960.5458	961.0913
962.3376	968.1646	969.1109
1015.9766	1020.8402	1045.0866
1047.1795	1050.7659	1051.1082
1052.8861	1053.9953	1064.6036
1070.2386	1084.8091	1089.1444
1141.8568	1148.1695	1180.3963
1185.2590	1195.4757	1208.1104
1209.9362	1218.9909	1239.3173
1241.8698	1243.4801	1247.4865
1256.2025	1263.1904	1266.9889
1276.1260	1278.0214	1287.4218
1288.5543	1294.0919	1315.5158
1322.8714	1351.0078	1368.1497
1395.5615	1397.0772	1398.9588
1400.4664	1404.1868	1406.0888
1408.0494	1410.6101	1426.0613
1427.6478	1432.7088	1439.4770
1446.7202	1450.4420	1473.1723
1475.3615	1477.2794	1477.5723
1479.2414	1482.5006	1482.5874
1484.0079	1486.4621	1487.1538
1497.5091	1499.7205	1501.0172
1502.2562	1505.3422	1506.0352

1507.0815	1511.1750	1514.8444
1516.4208	1521.2397	1568.2840
1570.8710	1699.5312	1707.1041
2998.1107	3056.2672	3058.7916
3059.6801	3061.0199	3063.8912
3065.2682	3069.8361	3070.6087
3073.2168	3082.2124	3136.1150
3137.8032	3139.5026	3140.9746
3141.4520	3142.1178	3142.5696
3144.0758	3145.6907	3146.2544
3146.4326	3147.7695	3149.9551
3152.6589	3156.4681	3175.4344
3177.6349	3181.5771	3183.8372
3194.1140	3266.4195	3288.9873

25-ts’

Zero-point correction= 0.616142
Thermal correction to Energy= 0.648174
Thermal correction to Enthalpy= 0.648944
Thermal correction to Gibbs Free Energy= 0.555440
Sum of electronic and zero-point Energies= -3055.543394
Sum of electronic and thermal Energies= -3055.511362
Sum of electronic and thermal Enthalpies= -3055.510592
Sum of electronic and thermal Free Energies= -3055.604096

Cartesian coordinates

C	0.451711	2.451293	-0.288563
N	-0.874960	2.591419	-0.221141
H	2.320339	0.001400	0.113423
N	-1.315481	1.401662	0.167854
N	-0.324227	0.572050	0.333011
N	0.812123	1.201480	0.052517
C	1.378486	3.519571	-0.697476
C	2.753828	3.281823	-0.813938
C	0.883085	4.798340	-0.982931
C	3.616687	4.303222	-1.205683
H	3.151762	2.293113	-0.602961
C	1.747249	5.816663	-1.375345
H	-0.183165	4.982971	-0.895568
C	3.117089	5.574139	-1.487900
H	4.680958	4.104049	-1.292006
H	1.349414	6.803298	-1.594030
H	3.789364	6.369800	-1.794758
C	3.565736	-1.192732	-1.031042

C	3.933236	-0.609749	1.263112
C	5.145299	-1.276877	1.234057
C	5.608984	-1.899541	0.069168
C	4.785699	-1.857428	-1.056451
H	5.735902	-1.320082	2.138830
H	5.082112	-2.353785	-1.968422
N	3.202726	-0.564410	0.115203
C	2.601292	-1.179296	-2.212676
C	1.250149	-1.755656	-1.751337
C	2.427214	0.256202	-2.735125
C	3.129192	-2.045144	-3.362486
H	0.785222	-1.163433	-0.959313
H	0.558686	-1.765208	-2.599942
H	1.368252	-2.784481	-1.393907
H	3.388131	0.682601	-3.043389
H	1.765660	0.239775	-3.606937
H	1.971431	0.907088	-1.988782
H	2.389567	-2.030892	-4.168083
H	4.069483	-1.659822	-3.770652
H	3.273352	-3.088338	-3.062183
C	3.363764	0.039210	2.520825
C	3.269785	1.562611	2.329625
C	1.971628	-0.555101	2.802783
C	4.262313	-0.238482	3.731771
H	4.248689	1.991033	2.087527
H	2.558493	1.828596	1.546469
H	2.919788	2.016207	3.262555
H	2.034411	-1.637782	2.957141
H	1.570999	-0.103744	3.716206
H	1.256390	-0.357804	2.000242
H	3.794476	0.203969	4.615692
H	4.381468	-1.310761	3.919786
H	5.253193	0.214365	3.621087
C	6.954033	-2.617827	0.081095
C	8.054997	-1.606289	0.446421
C	6.905874	-3.732652	1.141175
C	7.290283	-3.238876	-1.277067
H	8.098463	-0.791352	-0.283728
H	7.900149	-1.170904	1.438178
H	9.025506	-2.113325	0.450580
H	6.110571	-4.452174	0.920070
H	7.860185	-4.269342	1.149844
H	6.736978	-3.331287	2.145007
H	8.264053	-3.733366	-1.210892

H	6.554330	-3.993345	-1.575255
H	7.354790	-2.481712	-2.065857
O	-5.026814	-1.887040	1.286899
S	-6.025866	-1.247788	0.467302
S	-3.758269	0.535227	-0.233996
C	-6.242546	-2.261696	-1.071183
C	-3.663291	1.017825	1.608279
F	-6.748657	-3.434111	-0.717021
F	-5.074708	-2.436017	-1.662899
F	-7.076142	-1.642213	-1.890096
F	-4.846891	0.813162	2.175516
F	-3.369856	2.294060	1.694421
F	-2.767193	0.262371	2.198817
O	-5.436330	0.089276	-0.207689
O	-7.345168	-0.932623	0.947697
O	-3.852670	1.693818	-1.072080
O	-3.063285	-0.685476	-0.521610

Vibrational frequencies

9.7974	14.9554	17.2517
23.2843	28.1539	32.8010
38.6143	40.6472	43.0784
47.6501	54.3127	63.6180
65.4169	72.2533	77.7859
88.2444	94.9813	106.6730
112.5501	118.0072	125.8998
129.2015	149.8321	152.3025
157.9859	163.8442	167.6428
180.3099	187.3383	196.2573

26’

Zero-point correction= 0.612013

Thermal correction to Energy= 0.643648

Thermal correction to Enthalpy= 0.644418

Thermal correction to Gibbs Free Energy= 0.552461

Sum of electronic and zero-point Energies= -3055.541854

Sum of electronic and thermal Energies= -3055.510219

Sum of electronic and thermal Enthalpies= -3055.509449

Sum of electronic and thermal Free Energies= -3055.601406

Cartesian coordinates

C	0.730622	2.270476	-0.408291
N	-0.571751	2.541186	-0.397199
H	1.915977	0.146181	-0.100171
N	-1.174196	1.367336	-0.205070
N	-0.306731	0.414087	-0.100226
N	0.906488	0.947533	-0.221224
C	1.791048	3.273581	-0.588914
C	3.143492	2.913100	-0.610906
C	1.436313	4.620017	-0.738142
C	4.126162	3.885851	-0.779855
H	3.436138	1.872751	-0.496120
C	2.421316	5.588811	-0.905964
H	0.387232	4.897981	-0.721223
C	3.768396	5.225452	-0.927511
H	5.172213	3.594914	-0.795442
H	2.135863	6.630133	-1.020237
H	4.535355	5.982736	-1.058536
C	3.523691	-1.176240	-1.087896
C	3.575833	-0.753648	1.232089
C	4.834168	-1.336239	1.317275
C	5.479196	-1.839646	0.185335
C	4.784731	-1.769055	-1.018478
H	5.318171	-1.410982	2.281444
H	5.218682	-2.179639	-1.917186
N	2.961345	-0.641883	0.023391
C	2.742465	-1.150725	-2.407615
C	1.347836	-1.760643	-2.185250
C	2.639372	0.286943	-2.944153
C	3.439030	-1.989779	-3.489288
H	0.768141	-1.243045	-1.420696
H	0.780639	-1.715224	-3.120749
H	1.433113	-2.812835	-1.891370
H	3.633897	0.727331	-3.075844
H	2.143415	0.269301	-3.920480
H	2.054548	0.935285	-2.293223
H	2.804650	-1.996192	-4.380713
H	4.408062	-1.571652	-3.781133
H	3.582059	-3.029102	-3.175558
C	2.846888	-0.265871	2.489884
C	2.758176	1.269502	2.500706
C	1.446722	-0.899941	2.548481
C	3.592905	-0.687977	3.764151
H	3.753779	1.719717	2.420757
H	2.137187	1.658282	1.694635

H	2.312022	1.596845	3.445988
H	1.521845	-1.991220	2.610896
H	0.927006	-0.544393	3.444590
H	0.826993	-0.652922	1.686205
H	2.997115	-0.382684	4.629483
H	3.729527	-1.773115	3.819733
H	4.571042	-0.204189	3.853118
C	6.869144	-2.458464	0.312301
C	7.835668	-1.393437	0.860144
C	6.800082	-3.642817	1.292874
C	7.402630	-2.964471	-1.031182
H	7.902042	-0.536916	0.180622
H	7.520218	-1.027377	1.841946
H	8.836986	-1.823949	0.967048
H	6.099788	-4.405581	0.936343
H	7.789789	-4.102600	1.385103
H	6.482420	-3.327067	2.291322
H	8.400956	-3.388701	-0.885536
H	6.766172	-3.751211	-1.450404
H	7.487963	-2.157067	-1.766492
O	-5.067457	-1.622579	1.365343
S	-6.098888	-1.030083	0.552893
S	-3.851839	0.627028	-0.404230
C	-6.394126	-2.128177	-0.916114
C	-3.542079	1.189862	1.388547
F	-6.984065	-3.230082	-0.479097
F	-5.245365	-2.425949	-1.491331
F	-7.182673	-1.502574	-1.772596
F	-4.681671	1.122592	2.066049
F	-3.129594	2.435831	1.369524
F	-2.657796	0.389361	1.937415
O	-5.515405	0.266958	-0.229301
O	-7.388095	-0.651508	1.062814
O	-3.921355	1.763991	-1.273231
O	-3.201820	-0.618629	-0.685307

Vibrational frequencies

-942.7702	7.0126	16.9779
19.6284	22.3643	34.5761
37.9411	44.3867	47.2329
48.8781	51.7528	62.3461
68.7790	69.8198	78.7847
80.4919	87.4899	101.5988
114.1731	116.7951	117.6167

137.8712	146.5281	156.9023
162.6199	163.9457	168.8243
184.5648	190.0781	193.3784

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