

Supporting Information

NHC-Catalyzed Enantioselective Radical Reactions of Pyridinium

Salts: Mechanism and Origin of Regio- and Stereoselectivities

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Part 1: Computational Details

All calculations were carried out by using the Gaussian16 program. All the structures were optimized at M06-2X functional with 6-31G(d, p) basis set in hexafluorobenzene (HFB) solvent using the IEF-PCM solvation model. All reactants, products, and intermediates have no imaginary frequency, and each transition state has only one imaginary frequency. The free energies used in discussion were obtained at the M06-2X/6-311++G(d, p)/IEF-PCM_{HFB}//M06-2X/6-31G(d, p)/IEF-PCM_{HFB} level (denoted as L1 level). The 3D-structures were rendered using the CYLView software.¹ Diagrams of FMO overlap/interaction changes were drawn by Chemcraft.² The Figures 2a and 8a of NCI analysis are generated by analyzing the wave function calculated by DFT by Multiwfn software, and the isovalue of equivalence is set to 0.008.

To ensure that the selected L1 level can be applied to obtain reliable results, we have additionally performed calculations for the relayed-PCET process involving stationary points **M3** and ^o**TS3** by employing other different methods and basis sets, i.e., M06-2X/6-311++G(d, p)/SMD³_{HFB}//M06-2X/6-31G(d, p)/IEF-PCM_{HFB} (L2), M06-2X/def2-TZVP/IEF-PCM_{HFB}//M06-2X/6-31G(d, p)/IEF-PCM_{HFB} (L3), M06-2X/def2-TZVP/SMD_{HFB}//M06-2X/6-31G(d, p)/IEF-PCM_{HFB} (L4), ω B97X-D⁴/6-311++G(d, p)/IEF-PCM_{HFB}// ω B97X-D/6-31G(d, p)/IEF-PCM_{HFB} (L5) and M06-2X/def2-QZVP/IEF-PCM_{HFB}//M06-2X/6-31G(d, p)/IEF-PCM_{HFB} (L6). As summarized in **Tables S1 and S2**, there are small differences between the relative Gibbs free energies for the selected stationary points, so it can be concluded that the computed results and computational level L1 are reliable.

The calculation of ΔG_{gas} uses a reference state of 1 atm and the calculations of ΔG_{s} use a reference state of 1M. Based on the ΔG_{gas} reference state (24.46 L at 298.15 K) from 1 atm to 1M, the Gibbs free energy can be computed by using equation $\Delta G_{\text{gas}}(1\text{M}) = \Delta G_{\text{gas}}(1\text{ atm}) + RT\ln(24.46) = \Delta G_{\text{gas}}(1\text{ atm}) + 1.89\text{ kcal/mol}$.⁵

Since the transition state ^o**TS3** is an open-shell singlet state, spin contamination is inevitable and small in this system, and the calculated spin contamination information is $\langle S^{*2} \rangle = 0.2259$ before annihilation, and $\langle S^{*2} \rangle = 0.0046$ after annihilation by

using M06-2X method, whereas the S**2 value changes from 0.1387 before annihilation to 0.0024 after annihilation by using ω B97X-D method.

Table S1. Comparisons of relative Gibbs free energies (GFE) for selected stationary points at the different levels L1~L5 (unit: kcal/mol).

	L1	L2	L3	L4	L5
M3	0.0	0.0	0.0	0.0	0.0
^{os}TS3	2.3	1.4	2.0	1.1	3.9

Table S2. Comparisons of relative Gibbs free energies (GFE) for selected stationary points at the different levels L1 and L6 (unit: kcal/mol).

	L1	L6
²M6R	0.0	0.0
²TS7R	13.4	12.9

In addition, the extent of enantioselectivity, in terms of enantiomeric ratio (er), was calculated by using the Boltzmann distribution of diastereomeric transition states with the following equation:

$$\frac{[R]}{[S]} = \frac{\exp\left(\frac{-\Delta G_{[R]}^\ddagger}{RT}\right)}{\exp\left(\frac{-\Delta G_{[S]}^\ddagger}{RT}\right)} = \exp\left(\frac{\Delta\Delta G_{[S]-[R]}^\ddagger}{RT}\right) \quad (1)$$

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

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

Part 2: Energy Barriers Involved in Different [1,2]-Proton Transfer Pathways

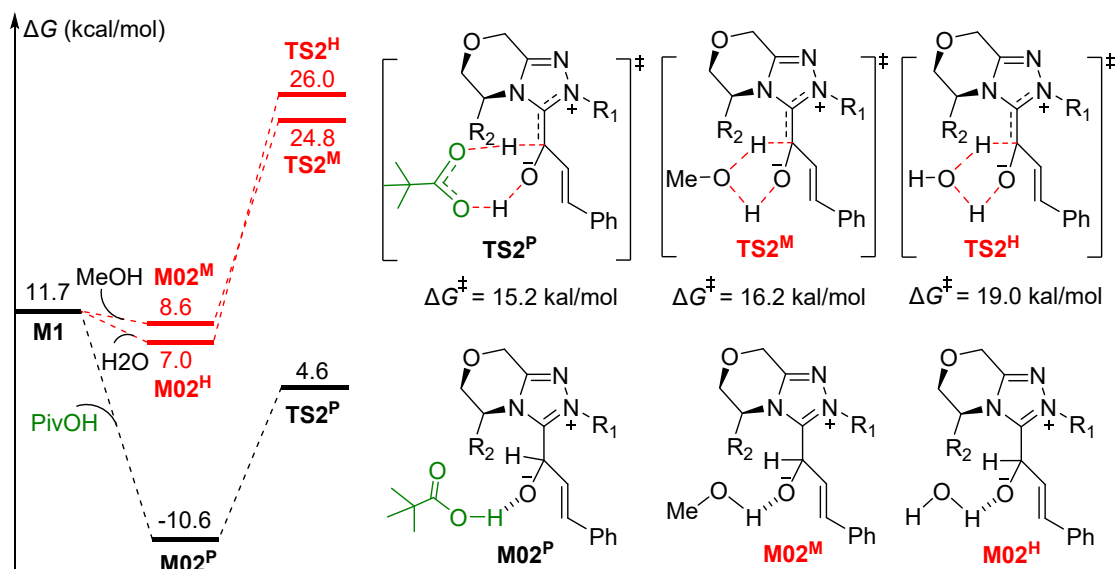


Figure S1 Energy barriers of MeOH- and H₂O-assisted proton transfer.

Part 3: Gibbs Free Energy Changes of the Stepwise PT-SET and SET-PT Pathways

As shown in Figure S2, the Gibbs free energy changes for PT and SET in the PT-SET pathway are 11.7 and 13.0 kcal/mol (ΔG_1 and ΔG_2), respectively, which is an endothermic process. It is worth noting that we have attempted but failed to find the transition state for the PT process, as the proton always automatically returns to the hydroxy oxygen of intermediate **M2**, and the scan curve shown in Figure S3 displays an increasing energy (>8.3 kcal/mol). For the SET-PT pathway, the Gibbs free energy changes for SET and PT are 14.0 and -9.8 kcal/mol (ΔG_3 and ΔG_4), respectively. The Gibbs free energy changes for PT in the PT-SET pathway and SET in the SET-PT pathway are both much higher than the energy barrier of ^{os}**TS3** in the relayed-PCET pathway ($\Delta G^\ddagger = 2.3$ kcal/mol). Therefore, the relayed proton-coupled electron transfer (relayed-PCET) process is the most energetically favored route for the generation of intermediate ²**M4**.

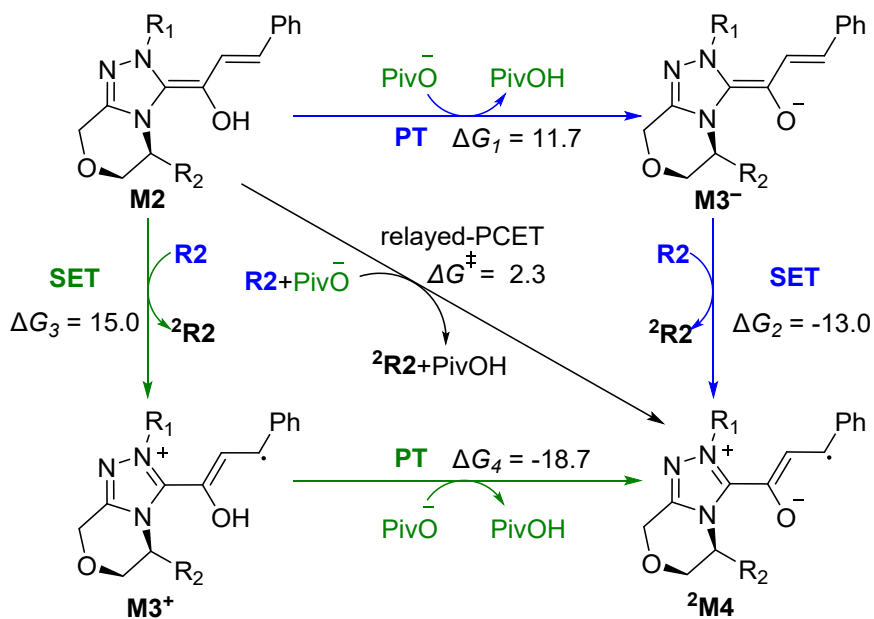


Figure S2. The energy barrier and Gibbs energy changes of the possible pathways (unit: kcal/mol).

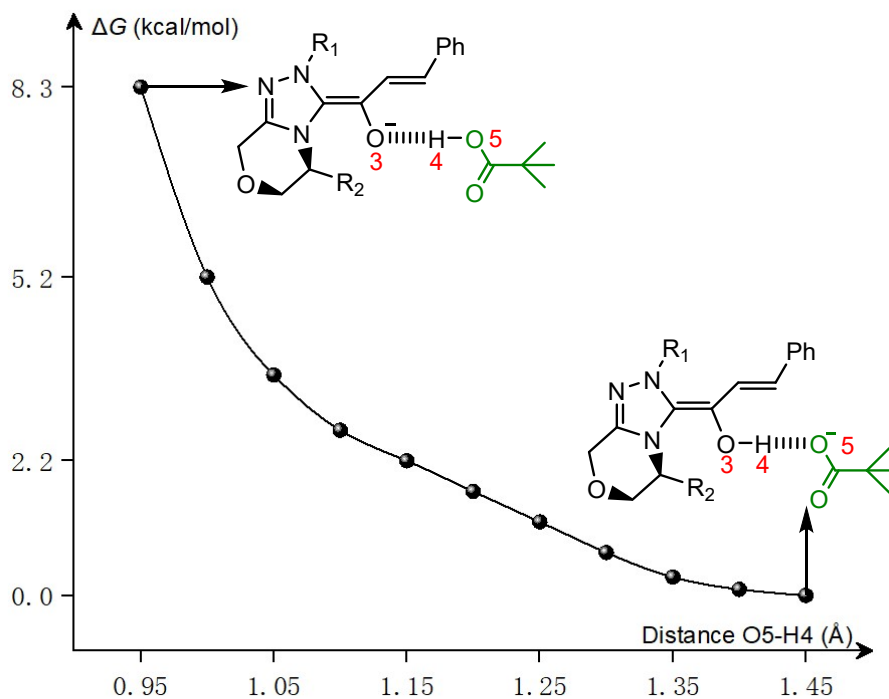
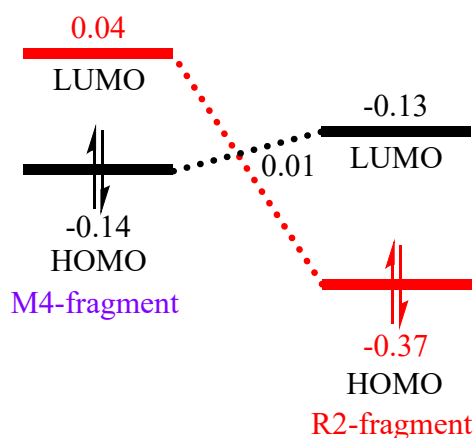


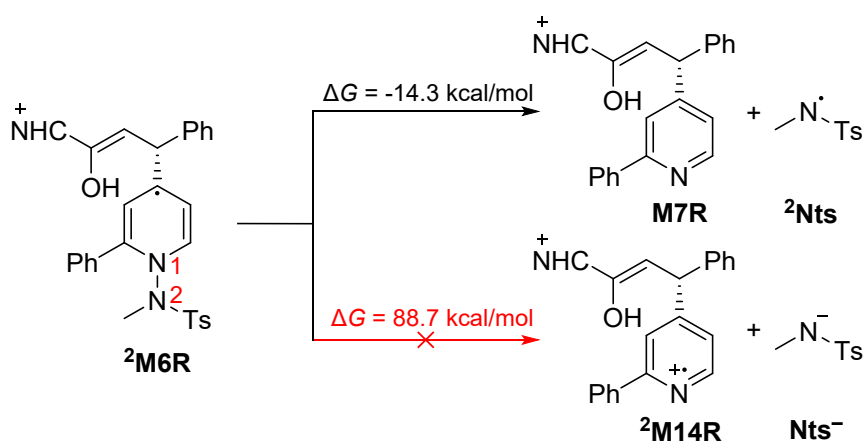
Figure S3. The Gibbs free energy changes by reducing the O5-H4 distance in the first proton transfer process of the stepwise PT-SET pathway.

Part 4: Energy Gap Involved in Relayed-PCET Process of ^{os}TS3



Scheme S1. The energy gap between LUMO (R2-fragment) and HOMO (M4-fragment) involved in the relayed-PCET of ^{os}TS3 (unit: eV).

Part 5: Possible Pathways of N–N Bond Cleavage



Scheme S2. The Gibbs free energy changes of possible pathways of N–N bond cleavage.

Part 6: Comparison of Different Configurations of ²TS5s

For the stereoselectivity-determining step, the nucleophilic addition of ²M4 to pyridinium salt **R2** first undergoes C–C bond formation via four diastereoselective transition states ²TS5RR/RS/SR/SS(²TS5s) to generate intermediates ²M5Rs. Inspired

by the previous studies, conformational searches of $^2\text{TS5s}$ have been performed to ensure the configurations of the optimized diastereoselective transition states associated with the lowest energies, separately.

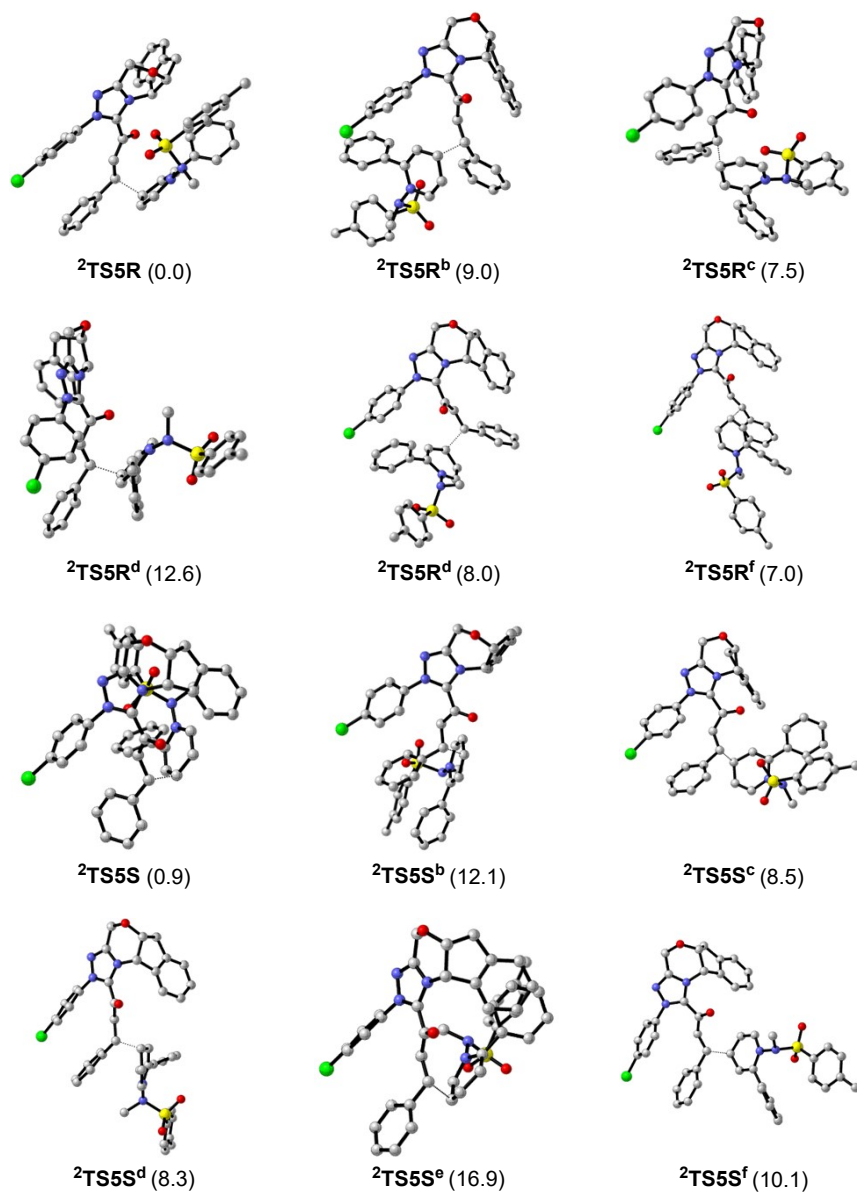


Figure S4. Comparison of relative Gibbs free energies ($\Delta\Delta G^\ddagger$) at L1 level of different configurations of $^2\text{TS5s}$ (unit: kcal/mol).

Part 7: Energy Barriers Involved in Different [1,3]-Proton Transfer

Pathways

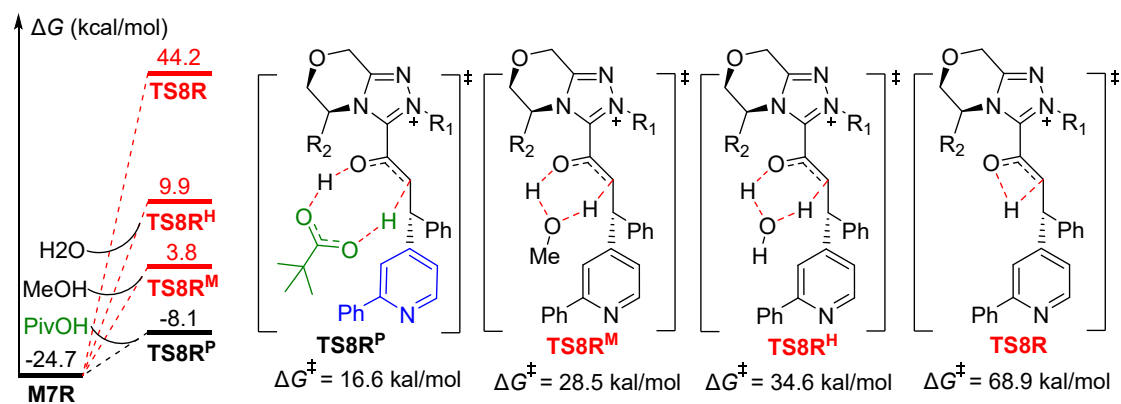


Figure S5. Energy barriers of direct proton transfer and MeOH- and H₂O-assisted proton transfer.

Part 8: Energy Barriers of ²TS4 and ²TS6R¹

The transition state ²TS6R¹ of the intermediate ²M5R through [1,3]-HAT is considered, the energy barrier of this pathway is up to 30.8 kcal/mol, so it can be safely excluded.

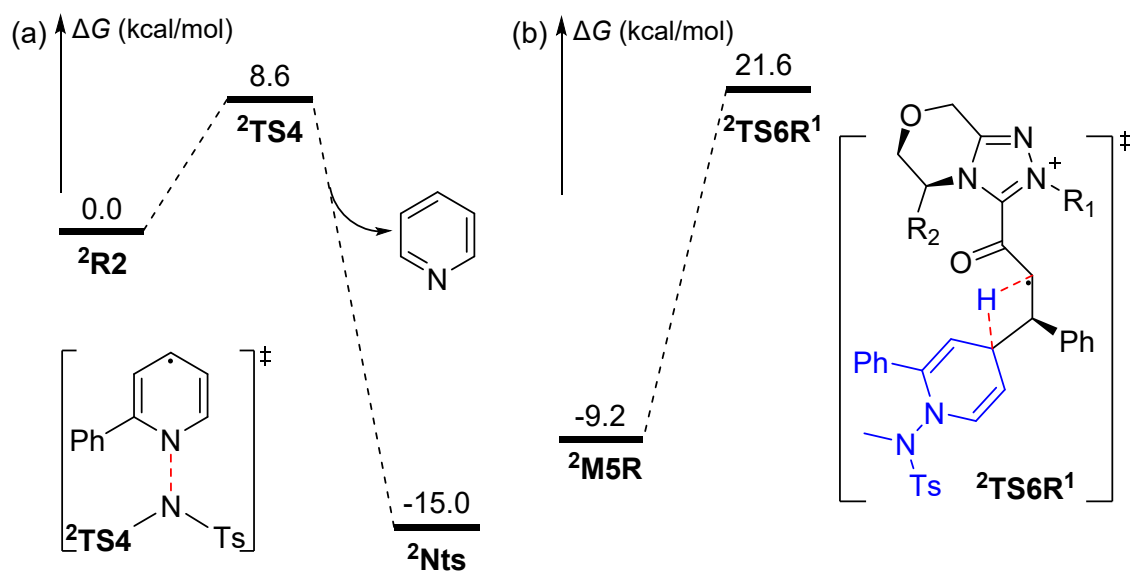


Figure S6. Energy barriers of ²TS4 and ²TS6R¹.

Part 9: Local Reactivity Index Analysis

For disclosing the origin of regioselectivity, we have also performed the local reactivity analysis pioneered by Domingo and coworkers.^{6,7} The nucleophilic (P_k^-) and electrophilic (P_k^+) Parr functions, which allow for the characterization of the nucleophilic and electrophilic sites of a molecule, can be obtained through the analysis of Mulliken atomic spin density (ASD) of the corresponding radical cations (RC) or anions (RA) of the studied molecules, separately. According to Domingo's definition, the Parr functions can be expressed by the following equations:

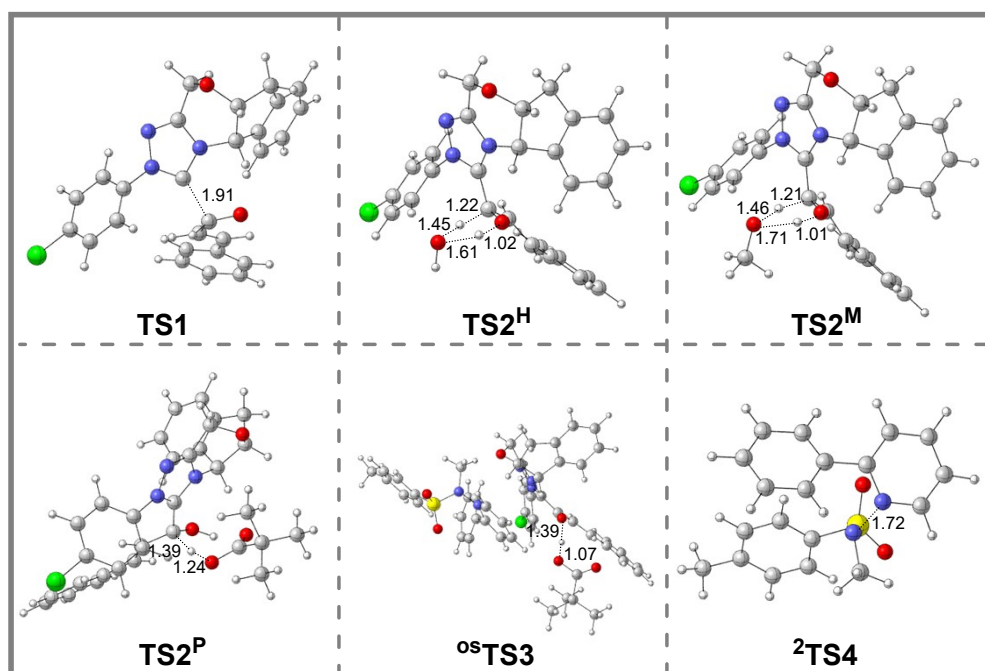
$$P_k^- = \rho_S^{\text{rc}}(r) \text{ for the electrophilic attacks (3)}$$

$$P_k^+ = \rho_S^{\text{ra}}(r) \text{ for the nucleophilic attacks (4)}$$

where $\rho_S^{\text{rc}}(r)$ is the ASD of the radical cation and $\rho_S^{\text{ra}}(r)$ is the ASD of the radical anion. Each ASD condensed at the different atoms of the radical cation and radical anion provides the local nucleophilic P_k^- and electrophilic P_k^+ Parr functions of the neutral system, respectively.

Part 10: Three Dimensional Structures of the Transition States

Involved in Case Study



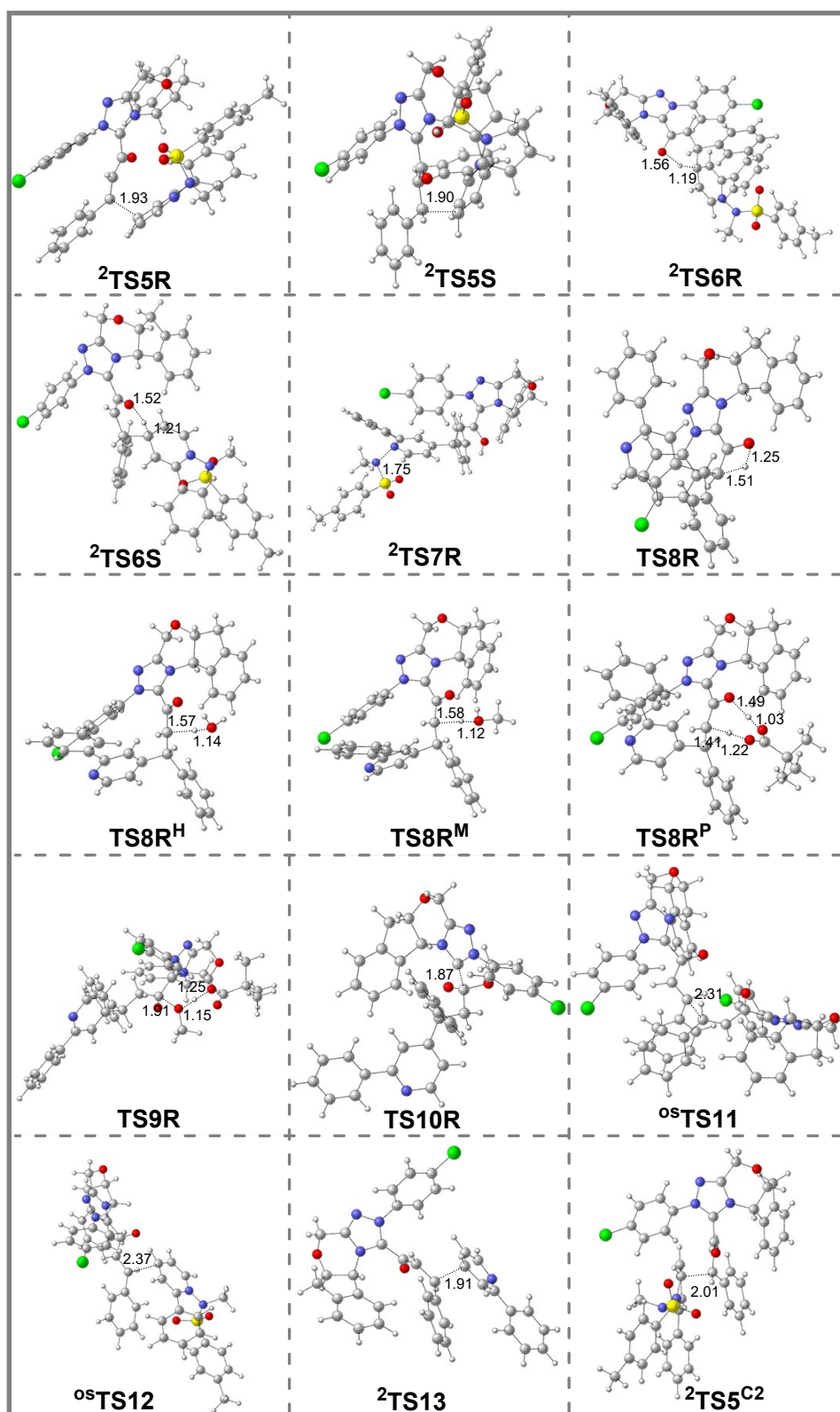


Figure S7. Three dimensional structures of the transition states involved in case study (unit: Å).

Part 11: ELF Analysis for Transition State ²TS7R

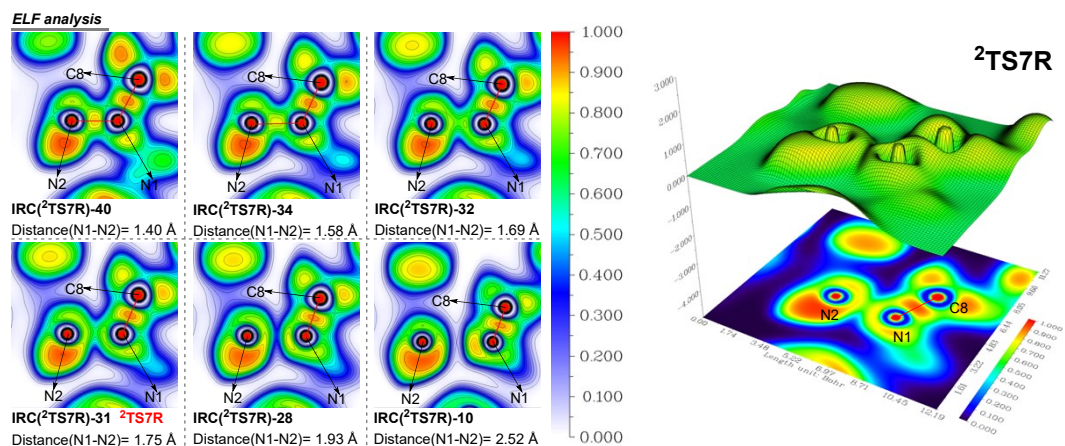


Figure S8. ELF analysis graphs in a selected plane along the IRC results of transition state ²TS7R.

Part 12: The Colorbar Scale of NCI Plots

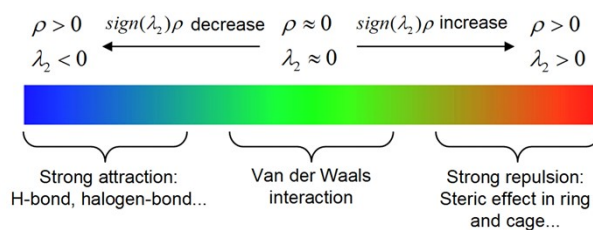


Figure S9. The colorbar scale for the NCI analysis of Figures 2a and 8a. (The symbol ρ , λ_2 and $\text{sign}(\lambda_2)\rho$ represent electron density, the second largest eigenvalue of the electron density Hessian matrix and $\text{sign}(\lambda_2)$ is multiplied by ρ .⁸⁾

It is worth mentioning that the program for mapping non-covalent interactions also has NCIPLOT,⁹⁻¹⁰ which is also very good software. According to the application of Multiwfn and NCIPLOT in NCI analysis by our research group in the past few years, the results obtained by the two methods are almost the same.¹¹⁻¹² Herein, we just used the Multiwfn software to examine the interactions between molecular fragments.

Part 13: Summary of Absolute SPE, GFEC, and GFE of the

Optimized Structures

Table S3. The single-point energies (SPE) at M06-2X/6-311++G(d,p)/IEF-PCM_{HFB} level, Gibbs free energy corrections (GFEC) at M06-2X/6-31G(d,p)/IEF-PCM_{HFB} level, and Gibbs free energies (GFE = SPE + GFEC) of the stationary points involved in the reaction models.

	SPE (a.u.)	GFEC (a.u.)	GFE (a.u.)
Pre-NHC	-1394.277857	0.259122	-1394.018735
PivO ⁻	-346.468105	0.102946	-346.365159
NHC	-1393.841079	0.245152	-1393.595927
R1	-422.902429	0.110316	-422.792113
R2	-1393.154859	0.298728	-1392.856131
PivOH	-346.982608	0.116408	-346.866200
TS1	-1816.739803	0.377056	-1816.362747
M1	-1816.745827	0.379492	-1816.366335
H ₂ O	-76.424142	0.004034	-76.420108
MeOH	-115.70664	0.029539	-115.677101
M02^H	-1893.194118	0.403192	-1892.790926
M02^M	-1932.475516	0.430184	-1932.045332
M02^P	-2163.784426	0.519327	-2163.265099
TS2^H	-1893.160687	0.40009	-1892.760597
TS2^M	-1932.445308	0.425770	-1932.019538
TS2^P	-2163.757446	0.516542	-2163.240904
M2	-1816.769159	0.379668	-1816.389491
M3⁺	-1816.58523	0.380612	-1816.204618
M3⁻	-1816.253747	0.366432	-1815.887315
R2 + PivO⁻	-1739.698496	0.421211	-1739.277285
M3	-3556.508242	0.830684	-3555.677558
^{os} TS3	-3556.500964	0.827084	-3555.673880
² R2	-1393.310169	0.293109	-1393.017060
² TS4	-1393.293537	0.290231	-1393.003306
² Nts	-914.05147	0.130555	-913.920915
Pyd	-479.260191	0.137066	-479.123125
² M4	-1816.167570	0.369056	-1815.798514
² TS5R	-3209.339624	0.69198	-3208.647644
² TS5S	-3209.343458	0.697269	-3208.646189
² M5R	-3209.347807	0.694887	-3208.65292
² M5S	-3209.35095	0.69918	-3208.65177
² TS6R	-3209.318914	0.691592	-3208.627322
² TS6S	-3209.309715	0.686876	-3208.622839
² M6R	-3209.348783	0.693388	-3208.655395
² M6S	-3209.345923	0.691545	-3208.654378

²TS7R	-3209.324535	0.690477	-3208.634058
M7R	-2295.291802	0.535133	-2294.756669
TS8R	-2295.179588	0.532719	-2294.646869
TS8R^H	-2371.674113	0.555526	-2371.118587
TS8R^M	-2410.965646	0.580366	-2410.385280
TS8R^P	-2642.262077	0.668773	-2641.593304
M8R	-2295.291591	0.532263	-2294.759328
MeOH + PivO ⁻	-462.197708	0.150463	-462.047245
M09R	-2757.583440	0.711834	-2756.871606
TS9R	-2757.578414	0.710202	-2756.868212
M9R	-2410.580600	0.577283	-2410.003317
TS10R	-2410.578037	0.575293	-2410.002744
PR	-1016.746557	0.302189	-1016.444368
²M10	-478.984794	0.135747	-478.849047
²M14R	-2294.983562	0.537001	-2294.446561
Nts ⁻	-914.200777	0.133965	-914.066812
^{0s}TS11	-3632.330441	0.765226	-3631.565215
M11	-3632.382087	0.771478	-3631.610609
^{0s}TS12	-3209.47981	0.688998	-3208.790812
M12	-3209.523865	0.694584	-3208.829281
²TS13	-2295.384792	0.528167	-2294.856625
²M13	-2295.392729	0.530547	-2294.862182
²TS5^{C2}	-3209.323658	0.692565	-3208.631093
²M5^{C2}	-3209.331672	0.694327	-3208.637345
²M5^{C3}	-3209.304816	0.692287	-3208.612529
²M5^{C3}	-3209.305456	0.694615	-3208.610841

Part 14: The Cartesian Coordinates, and Frequencies of the

Stationary Points

Pre-NHC

Zero-point correction=0.304941

Thermal correction to Energy=0.321763

Thermal correction to Enthalpy=0.322707

Thermal correction to Gibbs Free Energy=0.259122

Sum of electronic and zero-point Energies=-1393.726910

Sum of electronic and thermal Energies=-1393.710088

Sum of electronic and thermal Enthalpies=-1393.709143

Sum of electronic and thermal Free Energies=-1393.772728

Cartesian coordinate

C	3.74316600	0.67364600	0.61147500
C	3.02387000	0.84520900	-0.57544400
C	2.85548700	2.09755100	-1.15483100
C	3.40850400	3.20196800	-0.50911400
C	4.11841000	3.03974700	0.68162100
C	4.29770100	1.77734900	1.24762000
C	3.80537900	-0.78390000	1.00206900
C	3.46345600	-1.48302600	-0.33247800
C	2.53205000	-0.48827900	-1.06583800
H	2.33320300	2.21514200	-2.10080800
H	3.30107400	4.19036100	-0.94220200
H	4.55141600	3.90829100	1.16657800
H	4.86798700	1.66156000	2.16388500
H	3.06415100	-1.00315100	1.78069400
H	4.37257200	-1.56197600	-0.93246800
H	4.77962600	-1.09447400	1.38379700
H	2.52450500	-0.62089900	-2.14923300
N	1.14775900	-0.76344800	-0.58363700
O	2.93947200	-2.79028100	-0.27852300
C	0.05123300	-0.01287300	-0.72347400
C	0.76408900	-1.88916100	0.09450200
N	-0.93772600	-0.67322600	-0.13962900
N	-0.51091800	-1.85217500	0.37510800
C	1.76215500	-2.94067100	0.47667800
H	1.95051900	-2.87992900	1.55608700
H	1.35509200	-3.92886300	0.25683300
C	-2.31155000	-0.28049700	-0.03515600
C	-2.62305200	1.06223400	0.14453100
C	-3.29003800	-1.26373700	-0.12469700
C	-3.95900800	1.43651100	0.21149300
C	-4.62332300	-0.88622500	-0.04545300
C	-4.94687300	0.45968700	0.11370400
H	-4.23315300	2.47491800	0.35510600
H	-5.40949700	-1.62856900	-0.11600000
H	-3.01009300	-2.30245000	-0.25626200
H	-1.84246100	1.80700300	0.26065300
Cl	-6.61314700	0.92789200	0.19777200
H	-0.02096200	0.93986400	-1.22673200

Variable frequencies

30.9930	46.5084	52.0525
76.4534	91.1057	148.3426
156.4714	175.8098	229.7464
248.3480	266.4864	279.4223

301.6760	321.4962	355.4895
394.3203	415.9579	424.6826
446.8729	459.0259	495.7594
497.3166	533.7432	544.5879
580.0315	605.3866	613.4431
635.6596	646.5850	682.0718
702.8042	722.1904	729.9271
764.8851	787.1066	800.1209
817.1990	844.8450	847.4373
858.1408	885.0873	895.0612
898.8640	919.2387	981.3256
982.2819	995.5994	1004.0969
1006.0465	1033.1077	1038.2087
1045.4499	1052.7970	1063.0725
1095.3798	1120.0210	1134.4434
1141.0807	1150.4552	1166.2764
1183.4185	1187.9032	1203.9952
1214.2300	1230.9798	1239.4306
1255.0409	1268.8044	1277.2470
1306.5628	1317.6404	1326.3559
1332.9397	1342.6638	1356.9267
1360.2926	1375.5328	1383.7085
1420.7604	1443.9965	1468.4461
1493.1119	1499.4575	1508.0616
1522.7255	1536.9859	1553.2386
1611.4237	1663.6391	1681.7838
1685.4098	1690.2725	1704.5051
3076.0221	3086.4798	3150.4659
3153.8656	3162.3976	3173.4418
3199.8199	3210.3339	3224.2180
3231.0152	3236.8994	3242.6325
3246.8194	3251.8137	3321.4419

PivO⁻

Zero-point correction=0.134599

Thermal correction to Energy=0.142515

Thermal correction to Enthalpy=0.143459

Thermal correction to Gibbs Free Energy=0.102946

Sum of electronic and zero-point Energies=-346.216578

Sum of electronic and thermal Energies=-346.208662

Sum of electronic and thermal Enthalpies=-346.207718

Sum of electronic and thermal Free Energies=-346.248231

Cartesian coordinate

C	-0.52298600	0.01396700	-0.00751200
C	-0.98613200	-0.73266000	-1.26027500
H	-2.07765600	-0.85990400	-1.27212300
H	-0.70053300	-0.18494200	-2.16608600
H	-0.50752300	-1.71380200	-1.29386000
C	-1.09755200	1.42640000	0.00686800
H	-2.19617800	1.40492400	0.02820300
H	-0.73517200	1.97563800	0.87932500
H	-0.77750700	1.98297500	-0.87909700
C	-0.98867000	-0.75507700	1.23249800
H	-0.52459900	-1.74454900	1.24027600
H	-0.68774300	-0.23005900	2.14676200
H	-2.08139900	-0.86902500	1.25028600
C	1.05180600	0.02723900	0.01453600
O	1.58467600	-1.10478700	-0.07783900
O	1.60720800	1.14192800	0.13805300

Variable frequencies

74.2984	219.0092	241.8251
245.5994	275.1748	300.9180
342.6178	365.2737	389.2476
530.8478	590.5331	805.2332
810.0972	887.4802	941.4321
953.2214	959.1641	1043.0815
1046.8718	1254.3486	1259.6832
1285.0764	1376.6702	1385.9654
1397.5850	1449.4796	1479.4705
1493.1140	1497.3831	1504.0573
1511.3774	1535.0612	1771.5749
3026.2107	3028.3620	3035.0041
3100.8206	3103.6226	3119.5843
3140.8736	3148.5860	3156.4574

NHC

Zero-point correction=0.291615

Thermal correction to Energy=0.308438

Thermal correction to Enthalpy=0.309382

Thermal correction to Gibbs Free Energy=0.245152

Sum of electronic and zero-point Energies=-1393.294363

Sum of electronic and thermal Energies=-1393.277540

Sum of electronic and thermal Enthalpies=-1393.276596

Sum of electronic and thermal Free Energies=-1393.340827

Cartesian coordinate

C	3.86447000	0.60313700	0.58249200
C	3.01229800	0.88374800	-0.48761400
C	2.75593700	2.19029100	-0.88380200
C	3.38139700	3.22780400	-0.19538800
C	4.24346200	2.95288400	0.86784500
C	4.49027100	1.64003200	1.26604900
C	3.94224900	-0.88297100	0.83095700
C	3.43376700	-1.46103400	-0.50839600
C	2.46309900	-0.39264700	-1.07511000
H	2.07434000	2.39163200	-1.70388300
H	3.19955100	4.25675000	-0.48810900
H	4.72797000	3.77188400	1.39000800
H	5.16049900	1.43211600	2.09487000
H	3.28426800	-1.16009000	1.66356900
H	4.27871600	-1.52570600	-1.19864900
H	4.94555700	-1.24004800	1.07415000
H	2.44262600	-0.39384600	-2.16763300
N	1.10423300	-0.67759900	-0.60379000
O	2.89054500	-2.76335200	-0.47294200
C	0.02221900	0.13787300	-0.78207700
C	0.74532100	-1.84030500	0.03020500
N	-0.93578500	-0.62400900	-0.20149900
N	-0.52183500	-1.83955500	0.29977400
C	1.74785600	-2.90603700	0.34533300
H	2.00913800	-2.87239500	1.41134600
H	1.32372100	-3.88922900	0.13456200
C	-2.30676700	-0.26951100	-0.08755000
C	-2.72681300	0.98394500	-0.53179500
C	-3.21637200	-1.16859800	0.46368600
C	-4.06477100	1.33791800	-0.42522800
C	-4.55635400	-0.81249500	0.57137300
C	-4.96982900	0.43658000	0.12616600
H	-4.40573400	2.30814400	-0.76769900
H	-5.27510700	-1.50306100	0.99741300
H	-2.87173700	-2.13640200	0.80460100
H	-1.99747500	1.66347600	-0.95504300
Cl	-6.65386100	0.88400300	0.25822100

Variable frequencies

25.7704	31.3975	56.3246
60.5252	90.2629	136.0009
155.7083	174.9749	230.3635

243.6445	266.7787	278.6435
308.8710	335.5817	363.0101
383.7320	409.4048	423.8249
446.0971	465.7603	495.0992
527.7833	535.7677	540.6044
579.7609	609.0355	621.2720
642.5454	645.6855	663.0510
691.8784	722.2687	729.9871
759.2128	778.1467	804.8559
826.6590	851.1220	863.5339
871.8260	889.7738	901.5136
913.9998	972.9194	992.0877
993.4662	1006.2658	1009.0199
1020.3680	1027.9058	1033.4273
1056.1537	1067.1721	1095.3693
1109.2814	1131.0245	1134.7757
1138.3669	1164.1249	1182.3005
1192.7365	1196.9672	1201.0453
1235.7387	1246.0870	1262.5196
1273.5825	1280.1234	1308.9565
1322.3209	1323.3412	1343.7899
1345.9681	1352.9726	1371.4157
1373.5408	1386.1693	1422.8612
1432.5877	1474.1504	1482.4395
1493.9239	1513.5504	1522.5892
1541.8309	1560.5856	1677.9797
1682.6515	1695.0748	1703.3545
1707.6525	3066.2202	3078.0850
3119.7872	3128.7027	3141.5156
3161.2849	3203.4363	3210.0319
3224.2186	3235.7538	3241.4494
3248.7558	3264.9741	3265.5408

R1

Zero-point correction=0.144883

Thermal correction to Energy=0.153491

Thermal correction to Enthalpy=0.154435

Thermal correction to Gibbs Free Energy=0.110316

Sum of electronic and zero-point Energies=-422.650967

Sum of electronic and thermal Energies=-422.642360

Sum of electronic and thermal Enthalpies=-422.641416

Sum of electronic and thermal Free Energies=-422.685535

Cartesian coordinate

C	-1.05324700	-0.25667900	-0.00002300
C	-1.97311200	0.72128900	-0.00001300
H	-1.43440900	-1.27793800	-0.00005300
C	-3.41010300	0.38276700	-0.00004400
O	-3.84579100	-0.75013800	-0.00005400
C	0.40412500	-0.11137600	0.00000100
C	1.19374300	-1.26866600	-0.00002500
C	1.04224400	1.13794900	0.00004900
C	2.58188900	-1.18533400	-0.00000400
H	0.70729700	-2.24025700	-0.00006200
C	2.42713700	1.22184400	0.00006900
H	0.45216900	2.04881300	0.00007000
C	3.20158800	0.06069300	0.00004300
H	3.17839200	-2.09160200	-0.00002400
H	2.90810300	2.19461200	0.00010800
H	4.28450700	0.13048300	0.00006000
H	-4.10315000	1.24658700	-0.00000600
H	-1.71216600	1.77548400	0.00001500

Variable frequencies

46.4376	87.0999	127.4388
218.8028	243.7587	286.0069
412.1627	412.6165	501.9407
563.5553	629.1688	704.5747
733.1459	766.4182	859.9312
877.5717	894.7766	949.7843
998.5671	1014.8813	1018.7575
1025.0643	1041.2423	1055.3911
1072.9839	1120.6407	1182.7342
1206.8738	1238.1352	1321.8617
1329.3066	1360.5989	1370.7084
1446.8002	1504.8303	1554.0341
1670.6309	1698.9806	1712.6017
1843.0074	3002.4833	3181.4869
3194.7207	3201.7932	3218.1193
3221.3983	3234.0065	3238.6373

R2

Zero-point correction=0.349430

Thermal correction to Energy=0.370516

Thermal correction to Enthalpy=0.371460

Thermal correction to Gibbs Free Energy=0.298728

Sum of electronic and zero-point Energies=-1392.542902
Sum of electronic and thermal Energies=-1392.521816
Sum of electronic and thermal Enthalpies=-1392.520872
Sum of electronic and thermal Free Energies=-1392.593604

Cartesian coordinate

S	-0.05312800	-1.52734200	-0.67309200
O	0.02206300	-2.97837200	-0.61751800
O	0.58143200	-0.78185700	-1.74421300
N	0.72060100	-0.89937200	0.76381200
N	2.07726500	-0.65686000	0.49303300
C	-2.67822000	-1.92788900	-0.08840200
H	-2.42403800	-2.98102300	-0.03139500
C	-3.97665700	-1.47952600	0.12520400
H	-4.75717900	-2.19695000	0.35799100
C	-1.69975800	-0.98656700	-0.39157400
C	-1.97541600	0.37790600	-0.48715900
H	-1.18942100	1.08652300	-0.73420300
C	-4.29292900	-0.12030400	0.03919500
C	-3.27714500	0.79774600	-0.26490900
H	-3.51418300	1.85554700	-0.33108300
C	-5.70576600	0.35452700	0.24073700
H	-5.72897700	1.30108400	0.78528700
H	-6.29825800	-0.37941400	0.78942700
H	-6.18842000	0.51956500	-0.72773400
C	2.94543000	-1.69771700	0.43879000
H	2.53118600	-2.67236100	0.66735300
C	2.42546100	0.61667400	0.16051700
C	3.74739300	0.84229500	-0.21650700
H	4.03549900	1.85595700	-0.46728900
C	4.25651600	-1.49141400	0.08272000
H	4.93643500	-2.33298600	0.05128700
C	4.66299300	-0.19844200	-0.25247300
H	5.69057400	-0.00770300	-0.54194800
C	0.46095900	-1.66024200	1.99138800
H	-0.61704600	-1.62275500	2.15828000
H	0.77278700	-2.70740400	1.93178200
H	0.96081200	-1.15503700	2.81882300
C	1.41895300	1.69873500	0.17305300
C	0.67296400	2.00105800	1.31757100
C	1.24853800	2.44339400	-0.99683200
C	-0.23891700	3.04785000	1.28547700
H	0.81494800	1.42897900	2.22902900
C	0.32048700	3.48101100	-1.02581900

H	1.81420600	2.18724500	-1.88733000
C	-0.42025300	3.78374300	0.11384400
H	-0.80969000	3.29096000	2.17491000
H	0.17761000	4.04822400	-1.93888700
H	-1.13761900	4.59744400	0.09215900

Variable frequencies

32.0687	37.4839	55.0545
60.9695	63.4359	74.9506
80.3561	92.7415	110.9930
146.9896	175.8362	191.2499
205.6215	240.8499	260.1061
275.9332	290.3793	307.0332
323.6611	331.5994	349.2013
379.9564	412.7072	413.1150
430.8420	456.8223	486.2176
509.7985	519.1793	554.4775
568.0797	581.6865	591.3926
623.4423	640.4338	641.8811
673.1901	700.7210	714.4024
718.2552	757.8334	765.0753
797.0502	802.4005	828.4032
836.7398	852.3540	862.6725
885.7930	907.9486	968.4932
984.4582	992.6215	1002.1772
1014.4725	1016.2473	1017.4331
1033.4139	1038.9712	1052.4786
1056.0796	1064.9794	1080.1368
1085.0437	1110.2481	1118.8041
1125.6066	1145.3298	1150.8648
1168.9933	1183.1924	1188.8475
1192.4378	1213.1706	1213.8023
1218.7740	1255.7075	1270.3581
1312.1775	1319.4897	1334.6482
1344.3997	1350.7194	1362.2801
1363.1916	1388.8712	1424.1774
1458.2724	1461.8269	1481.7256
1497.3040	1498.8579	1502.7451
1508.8863	1521.2747	1538.5780
1548.0926	1570.4295	1653.6374
1667.2024	1671.5910	1686.8551
1692.7341	1707.5237	3077.2115
3083.0440	3150.6177	3171.4344
3172.5230	3201.7487	3210.2919

3211.5244	3215.4756	3217.0230
3223.4431	3226.7747	3239.0748
3241.7492	3246.5025	3247.0313
3260.2346	3264.9380	3271.5789

PivOH

Zero-point correction=0.148507
 Thermal correction to Energy=0.156633
 Thermal correction to Enthalpy=0.157577
 Thermal correction to Gibbs Free Energy=0.116408
 Sum of electronic and zero-point Energies=-346.735308
 Sum of electronic and thermal Energies=-346.727183
 Sum of electronic and thermal Enthalpies=-346.726239
 Sum of electronic and thermal Free Energies=-346.767408

Cartesian coordinate

C	-0.93702200	0.18477000	0.00015200
O	-1.51386800	1.24555200	0.00002500
O	-1.60211000	-0.98777800	0.00005000
H	-2.54780900	-0.77341100	-0.00011600
C	0.57131300	-0.00982300	0.00000200
C	0.96247400	-0.80247600	-1.25675000
H	2.04744500	-0.94261200	-1.27300000
H	0.48403000	-1.78443000	-1.26647600
H	0.67538000	-0.26534500	-2.16580700
C	1.24360000	1.36129100	0.00014700
H	0.95638700	1.93720300	0.88323900
H	2.33033000	1.23705400	0.00004200
H	0.95625300	1.93746300	-0.88273200
C	0.96266900	-0.80282900	1.25646000
H	2.04763400	-0.94304600	1.27243800
H	0.67580400	-0.26591500	2.16571600
H	0.48416300	-1.78475700	1.26603100

Variable frequencies

45.7239	208.5320	257.8120
267.9859	283.2363	301.3971
348.2690	367.0916	378.9746
518.6999	582.0651	603.7414
746.4557	793.4403	890.8875
962.6364	968.2105	970.1887
1056.4194	1056.7937	1182.5233
1256.8835	1262.9183	1292.9393

1393.3261	1403.6970	1423.5717
1445.3876	1490.3021	1498.0399
1499.1481	1513.6195	1515.9769
1535.3544	1881.4491	3064.5755
3066.5731	3077.8904	3145.6687
3146.6994	3159.6586	3159.6763
3162.2802	3171.6079	3828.7872

TS1

Zero-point correction=0.437375

Thermal correction to Energy=0.463363

Thermal correction to Enthalpy=0.464308

Thermal correction to Gibbs Free Energy=0.377056

Sum of electronic and zero-point Energies=-1815.943961

Sum of electronic and thermal Energies=-1815.917972

Sum of electronic and thermal Enthalpies=-1815.917028

Sum of electronic and thermal Free Energies=-1816.004279

Cartesian coordinate

C	-4.74020000	0.29390700	-0.30386100
C	-3.41239500	0.42067100	0.09269000
C	-2.64329300	1.52124100	-0.26584700
C	-3.23158500	2.50460300	-1.05714900
C	-4.56222100	2.38355900	-1.46622600
C	-5.32782800	1.28154900	-1.08975600
C	-5.34505700	-0.97503600	0.24420500
C	-4.14318200	-1.80188900	0.75788500
C	-2.97471100	-0.76453800	0.92146100
H	-1.61676700	1.59932000	0.08070100
H	-2.65334500	3.37317400	-1.35554800
H	-5.00532800	3.15783700	-2.08479000
H	-6.36189800	1.19337200	-1.41000700
H	-5.90506600	-1.55384300	-0.49670900
H	-4.35846000	-2.28325300	1.71267200
H	-6.03072300	-0.75157200	1.06875100
H	-2.80170500	-0.48149100	1.96003600
N	-1.71555100	-1.32445800	0.41406000
O	-3.83574400	-2.88356600	-0.11440100
C	-0.43965300	-1.13617600	0.81379700
C	-1.72255900	-2.11523300	-0.70571300
N	0.25535500	-1.85238000	-0.08850900
N	-0.52079800	-2.46828400	-1.04113400
C	-3.05031900	-2.53761400	-1.24008500

H	-3.51101900	-1.73275900	-1.82927700
H	-2.94554200	-3.42587300	-1.86311300
C	1.66681700	-2.02469900	-0.13411300
C	2.38850700	-2.10239300	1.05342300
C	2.29975800	-2.11162800	-1.36994200
C	3.77100900	-2.23730900	1.00537700
C	3.68010800	-2.26306400	-1.41877100
C	4.40324300	-2.31589600	-0.23114700
H	4.35171800	-2.29187600	1.91875500
H	4.19374900	-2.33264700	-2.37058000
H	1.71130800	-2.06178900	-2.27850500
H	1.87111200	-2.05738300	2.00628000
Cl	6.13561000	-2.49279700	-0.29396400
C	0.78359300	2.28734200	1.14536300
C	0.96390600	0.98172300	1.36181900
H	-0.12305700	2.72740400	1.56047900
C	-0.06298900	0.18928600	2.14111700
O	-1.14689400	0.73767400	2.46946900
C	1.70072100	3.18873700	0.43002300
C	1.52464700	4.57300900	0.54609600
C	2.74726700	2.71713200	-0.37569800
C	2.37608400	5.46160100	-0.10280300
H	0.71189800	4.94989900	1.16130400
C	3.59843600	3.60273500	-1.02398900
H	2.88492100	1.64735800	-0.50784000
C	3.41853200	4.97921900	-0.88883800
H	2.22436100	6.53104400	0.00522100
H	4.40226700	3.21952200	-1.64491300
H	4.08362100	5.66889000	-1.39864800
H	0.43270200	-0.50722700	2.85352800
H	1.86812500	0.46740700	1.04221100

Variable frequencies

-194.4583	10.7331	16.8574
21.6464	28.4854	45.1320
46.2716	51.8831	80.5437
82.8615	97.3781	108.0374
135.4257	138.9004	162.9000
196.0353	215.3400	225.7035
234.7009	248.6713	260.6125
290.1527	297.2927	317.7662
348.1060	373.4523	400.0551
414.5978	416.3099	422.4957
429.5629	443.0764	472.1689

487.8287	501.7771	515.4401
519.4772	527.3750	558.7891
573.5807	598.0428	606.9581
627.5210	630.1149	638.8699
696.3908	708.4700	709.4173
723.6529	726.4574	732.9006
733.5922	761.6805	777.8449
781.4641	807.5585	836.4864
850.6343	854.3936	862.1437
866.3391	872.0355	877.8609
888.8646	894.3145	910.5739
945.6961	949.6811	969.0406
979.2595	979.4647	993.8730
996.9190	1005.1040	1014.6427
1016.3974	1017.5731	1025.5994
1033.7025	1036.6942	1048.7683
1053.6415	1066.2793	1071.3347
1114.0159	1115.9111	1118.2690
1131.0281	1136.2529	1150.2590
1153.5990	1178.3357	1180.2243
1196.4231	1198.1845	1201.2300
1217.0810	1224.6000	1225.2033
1246.9087	1266.1373	1276.8537
1294.5892	1301.0267	1306.3033
1310.7434	1320.6125	1323.9699
1335.8884	1347.3080	1347.6549
1356.0912	1363.4845	1370.2253
1375.2057	1380.2587	1419.8556
1440.8836	1458.9269	1480.8414
1486.3148	1493.4339	1497.4213
1502.0765	1519.7572	1541.1604
1552.3101	1564.7747	1584.5160
1670.3188	1681.2339	1686.7004
1692.9978	1699.8028	1701.6878
1707.8738	1747.9558	2906.0331
3071.9993	3079.5594	3127.7372
3152.1119	3170.0259	3176.9569
3180.3301	3188.9286	3191.7256
3196.0513	3197.0154	3205.2090
3211.0750	3213.2142	3214.6318
3219.8711	3223.0910	3234.9385
3235.0699	3245.7327	3253.8077

M1

Zero-point correction=0.438847
 Thermal correction to Energy=0.464842
 Thermal correction to Enthalpy=0.465787
 Thermal correction to Gibbs Free Energy=0.379492
 Sum of electronic and zero-point Energies=-1815.947028
 Sum of electronic and thermal Energies=-1815.921033
 Sum of electronic and thermal Enthalpies=-1815.920089
 Sum of electronic and thermal Free Energies=-1816.006383

Cartesian coordinate

C	-4.66249500	0.32332800	-0.43760800
C	-3.37411100	0.47349500	0.06538300
C	-2.59313300	1.58394700	-0.23704300
C	-3.12370000	2.54512300	-1.09288100
C	-4.41131200	2.39646800	-1.61705100
C	-5.19250800	1.29108700	-1.28784400
C	-5.31239100	-0.93057200	0.08897400
C	-4.19006700	-1.69383900	0.83741600
C	-2.98592700	-0.68469400	0.95029500
H	-1.60987400	1.68374800	0.21473000
H	-2.53567200	3.42047600	-1.35001700
H	-4.80976600	3.15452600	-2.28416000
H	-6.19629200	1.18616900	-1.68920400
H	-5.73496100	-1.56715500	-0.69583200
H	-4.50676200	-1.99329800	1.83659000
H	-6.12989100	-0.68821800	0.77527000
H	-2.76208300	-0.36107700	1.96714700
N	-1.74003500	-1.31358600	0.46288100
O	-3.86453500	-2.92145300	0.19859700
C	-0.45220600	-1.07039400	0.76683700
C	-1.76484000	-2.25448500	-0.53144600
N	0.23655400	-1.89675300	-0.03578000
N	-0.56893300	-2.64119100	-0.85520200
C	-3.09584200	-2.76166800	-0.97483200
H	-3.56446500	-2.06252800	-1.68209600
H	-2.98879300	-3.73600100	-1.45152700
C	1.65210000	-2.06765000	-0.12597300
C	2.39876300	-2.31334400	1.02058700
C	2.24727400	-1.99760200	-1.38098400
C	3.77629000	-2.46606000	0.91306700
C	3.62167600	-2.16292300	-1.49100900
C	4.37298500	-2.38957800	-0.34134400
H	4.38002600	-2.65554800	1.79276600

H	4.10912200	-2.10906500	-2.45727200
H	1.63572200	-1.81222800	-2.25682100
H	1.91164300	-2.38998900	1.98632000
Cl	6.09666900	-2.58915700	-0.47900100
C	0.85933800	2.22726500	1.13680200
C	1.01890600	0.90487400	1.07522900
H	-0.00802500	2.56711900	1.70316300
C	0.02245700	-0.00162000	1.82295600
O	-1.00674200	0.60131400	2.36940400
C	1.71164600	3.25701500	0.52031200
C	1.26154700	4.58319200	0.50663600
C	2.95665000	2.97542500	-0.06062200
C	2.01778300	5.59442300	-0.07743100
H	0.30191700	4.81523900	0.96120500
C	3.71411300	3.98341600	-0.64361100
H	3.34033700	1.95930100	-0.04507700
C	3.24766800	5.29788900	-0.65743900
H	1.64712600	6.61477000	-0.07727900
H	4.67694900	3.74571700	-1.08563900
H	3.84246800	6.08365300	-1.11209700
H	0.65550300	-0.62281200	2.51542900
H	1.85553800	0.44958000	0.54585300

Variable frequencies

17.3042	22.5113	24.9977
26.3991	35.9389	48.6113
54.8180	83.7041	95.4244
110.6188	120.1234	121.5129
151.4361	179.0140	202.1907
214.4545	224.5543	246.5157
254.9349	271.7233	294.4336
302.0194	323.2418	335.5323
362.7427	380.3634	412.6707
414.4383	420.6078	433.2037
442.1949	452.3316	476.9359
486.3603	511.3728	517.6419
529.0181	549.2476	562.1010
593.9595	611.3118	612.7014
630.4311	644.2898	664.5080
696.8746	709.8582	718.9105
723.2357	730.3109	734.3842
746.1542	770.6413	789.8328
794.9081	815.3964	836.0972
846.4788	858.2155	859.8452

869.6595	874.2910	876.3480
884.3253	900.4642	918.7808
934.7614	948.8905	956.0941
977.9043	991.6087	992.0555
993.3772	1015.6061	1017.6558
1021.5697	1024.8241	1031.9483
1048.6475	1054.6443	1059.5137
1066.6491	1071.2075	1071.7171
1115.7427	1124.0927	1130.7261
1137.3369	1142.3140	1154.5179
1176.8863	1183.4109	1196.4078
1197.9317	1200.4792	1201.3636
1222.1943	1224.1160	1229.7160
1246.4045	1259.3600	1280.5032
1286.7052	1296.0848	1306.7402
1313.8653	1321.9872	1325.5456
1332.2974	1338.9947	1347.0218
1351.8348	1358.7814	1363.2920
1373.3498	1377.9263	1389.0881
1418.6552	1460.6325	1467.5848
1488.7980	1500.9953	1501.3425
1508.8973	1520.6737	1522.0135
1545.8949	1551.6507	1571.3376
1671.5053	1681.0578	1686.1840
1692.2031	1698.3282	1701.5645
1703.7622	1751.4065	2753.5026
3066.7693	3077.8232	3120.0394
3152.3029	3172.2799	3180.0495
3181.6439	3186.5941	3191.5929
3195.0204	3205.4352	3206.0355
3211.7003	3219.9483	3223.0905
3232.3450	3232.7398	3234.5814
3243.1113	3243.8498	3245.5493

H₂O

Zero-point correction=0.021681

Thermal correction to Energy=0.024516

Thermal correction to Enthalpy=0.025460

Thermal correction to Gibbs Free Energy=0.004034

Sum of electronic and zero-point Energies=-76.365252

Sum of electronic and thermal Energies=-76.362417

Sum of electronic and thermal Enthalpies=-76.361473

Sum of electronic and thermal Free Energies=-76.382899

Cartesian coordinate

O	0.00000000	0.00000000	0.11824500
H	-0.00000000	0.75920700	-0.47298200
H	-0.00000000	-0.75920700	-0.47298200

Variable frequencies

1645.2745 3880.8201 3990.7307

MeOH

Zero-point correction=0.052205

Thermal correction to Energy=0.055443

Thermal correction to Enthalpy=0.056387

Thermal correction to Gibbs Free Energy=0.029539

Sum of electronic and zero-point Energies=-115.613194

Sum of electronic and thermal Energies=-115.609956

Sum of electronic and thermal Enthalpies=-115.609012

Sum of electronic and thermal Free Energies=-115.635860

Cartesian coordinate

C	0.65975400	-0.01964700	0.00000200
H	1.08420200	0.98619400	-0.00101200
H	1.02737000	-0.54414500	0.89137000
H	1.02721200	-0.54585500	-0.89041400
O	-0.74561600	0.12259400	0.00000400
H	-1.13238000	-0.75906700	0.00001100

Variable frequencies

392.4070 1081.8704 1131.3074
1186.0351 1392.4293 1500.4623
1510.2404 1530.9443 3037.8864
3096.8737 3153.0584 3901.8767

M02^H

Zero-point correction=0.464974

Thermal correction to Energy=0.493391

Thermal correction to Enthalpy=0.494336

Thermal correction to Gibbs Free Energy=0.403192

Sum of electronic and zero-point Energies=-1892.337680

Sum of electronic and thermal Energies=-1892.309262

Sum of electronic and thermal Enthalpies=-1892.308318

Sum of electronic and thermal Free Energies=-1892.399462

Cartesian coordinate

C	-3.43984800	-1.99486000	-0.76257300
C	-2.69583400	-1.46883800	0.29847000
C	-3.08460700	-0.30068200	0.94036500
C	-4.20811300	0.37277000	0.46315100
C	-4.93625300	-0.13095400	-0.61485700
C	-4.56565600	-1.32736800	-1.22870600
C	-2.86671200	-3.31188900	-1.21497400
C	-2.03132400	-3.72159400	0.01690300
C	-1.54902200	-2.38816900	0.64982000
H	-2.49147100	0.05138700	1.77687500
H	-4.52121700	1.29817700	0.93696600
H	-5.81127500	0.40514900	-0.96950000
H	-5.15190000	-1.73421900	-2.04743200
H	-2.23859100	-3.17386900	-2.10354200
H	-2.69787700	-4.18168700	0.75043700
H	-3.62254400	-4.06119000	-1.46138600
H	-1.32991800	-2.45077800	1.71585500
N	-0.25447500	-2.02428600	0.00911500
O	-1.01430900	-4.67142500	-0.20802400
C	0.53368300	-0.95393200	0.23091500
C	0.47146600	-2.89918300	-0.76171600
N	1.65520100	-1.20369600	-0.44495600
N	1.63824800	-2.41758900	-1.06654400
C	-0.04347600	-4.25362400	-1.13600900
H	-0.43245400	-4.24338800	-2.16238000
H	0.78216500	-4.96539700	-1.09174800
C	2.88147900	-0.46323100	-0.39417800
C	3.32399000	0.21295200	-1.52171900
C	3.61001200	-0.48928400	0.79172400
C	4.53256400	0.89912200	-1.46398100
C	4.81210600	0.20422200	0.85142200
C	5.25798700	0.88878800	-0.27682900
H	4.90702900	1.43870100	-2.32595700
H	5.40315100	0.21321400	1.75959300
H	3.20680300	-1.03995500	1.64030000
H	2.73298000	0.19934000	-2.43103300
Cl	6.76665900	1.75736100	-0.19835400
C	-1.13448800	2.24707400	0.95549500
C	-0.24684700	1.41280800	0.41585600
H	-1.49395300	1.99464800	1.95198900
C	0.30013000	0.22611100	1.20051400
O	-0.40035600	-0.18023200	2.27038400

C	-1.70438300	3.45215800	0.33225500
C	-2.82906600	4.05033100	0.91399800
C	-1.17274000	4.03213900	-0.82805500
C	-3.41819900	5.17698700	0.34809300
H	-3.24201400	3.62116400	1.82353900
C	-1.75807600	5.15702300	-1.39444000
H	-0.28380400	3.60590100	-1.28318900
C	-2.88593600	5.73382000	-0.81108100
H	-4.29105700	5.62218300	0.81530600
H	-1.32942100	5.59214000	-2.29194100
H	-3.33990300	6.61445600	-1.25383900
H	1.34929800	0.51917500	1.43996700
H	0.17289800	1.58496300	-0.57625800
O	1.22237600	-2.11751900	2.58023500
H	0.54632200	-1.35871800	2.65768900
H	1.49200800	-2.33031900	3.47845200

Variable frequencies

9.0049	24.2849	24.8625
38.4778	44.8738	52.3954
58.2835	74.9579	78.6088
96.7137	106.2846	117.6434
138.3406	156.7161	173.0232
179.7772	189.8268	204.6806
213.8218	229.1159	244.9255
248.5823	257.0811	290.6659
293.3097	317.3295	335.4678
345.0626	367.2080	377.6293
407.0730	416.7192	427.3872
431.2075	451.0379	463.0285
469.5307	497.8042	500.3770
524.4838	534.9366	551.4760
565.7292	590.5623	605.2847
613.4482	622.9114	635.5274
642.2437	647.9490	684.6437
705.0667	715.1312	727.4568
736.8628	743.3718	751.5089
767.8884	786.1837	788.6624
815.8159	842.2960	851.0228
853.8313	865.2371	873.1084
880.2619	888.6529	896.4725
915.3500	919.2662	939.4290
982.2459	987.1209	993.2523
993.4996	1009.2502	1013.8984

1017.6124	1028.1553	1031.4865
1036.0616	1039.3814	1043.7316
1055.5192	1066.8747	1075.1660
1078.1751	1088.3872	1100.8129
1124.5635	1126.4276	1128.5074
1135.6355	1154.1114	1160.3565
1171.3256	1191.2749	1194.6286
1199.3018	1202.0352	1210.4489
1226.0355	1235.9178	1247.1431
1250.0601	1260.9172	1277.0283
1294.7900	1303.5435	1307.1691
1322.9019	1324.4027	1328.3036
1339.4889	1342.9791	1349.1839
1354.6184	1357.0727	1373.3422
1376.9200	1378.2607	1384.7041
1421.4543	1456.2281	1465.8433
1488.6259	1506.9877	1510.2120
1513.7639	1520.0015	1532.8763
1539.7057	1561.7936	1584.4197
1676.9246	1677.9346	1678.9991
1688.1089	1696.6156	1705.9817
1706.1962	1728.2410	1764.5003
2802.1553	2889.6635	3064.2255
3077.4364	3134.2551	3145.1857
3164.4161	3167.7498	3180.8305
3182.0396	3192.0678	3194.9276
3196.5399	3197.7599	3204.7908
3205.8258	3213.2870	3219.1135
3222.9735	3231.7906	3239.5532
3246.8190	3254.4263	3937.4106

M02^M

Zero-point correction=0.494105

Thermal correction to Energy=0.524002

Thermal correction to Enthalpy=0.524946

Thermal correction to Gibbs Free Energy=0.430184

Sum of electronic and zero-point Energies=-1931.587359

Sum of electronic and thermal Energies=-1931.557462

Sum of electronic and thermal Enthalpies=-1931.556518

Sum of electronic and thermal Free Energies=-1931.651280

Cartesian coordinate

C	-3.53011300	-1.98160400	-0.75377800
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C	-2.75505800	-1.48416200	0.29859700
C	-3.12372700	-0.33736600	0.98830200
C	-4.25947400	0.35044400	0.56444200
C	-5.01627200	-0.11946600	-0.50904200
C	-4.66620900	-1.29774400	-1.16893600
C	-2.98224200	-3.29809400	-1.24078400
C	-2.13847500	-3.74247600	-0.02565300
C	-1.61865900	-2.42692600	0.61387700
H	-2.50769900	-0.01009300	1.81841400
H	-4.56108000	1.25859300	1.07697100
H	-5.90021500	0.42747300	-0.82223200
H	-5.27872000	-1.67994800	-1.98004400
H	-2.36369700	-3.15338200	-2.13500800
H	-2.80543400	-4.19576700	0.71153900
H	-3.75252900	-4.03138700	-1.48988000
H	-1.39666800	-2.49767800	1.67835500
N	-0.32067300	-2.08902600	-0.04346300
O	-1.14366500	-4.71065200	-0.27171600
C	0.48354400	-1.02121400	0.14251100
C	0.36350000	-2.96579400	-0.85127800
N	1.58391600	-1.28800900	-0.56306200
N	1.52603700	-2.49620300	-1.19221300
C	-0.18379200	-4.31031200	-1.21809700
H	-0.59257900	-4.28780500	-2.23643200
H	0.62814500	-5.03880400	-1.19289500
C	2.80471400	-0.53416900	-0.60803200
C	3.23112300	-0.01346600	-1.82208200
C	3.54303100	-0.39542500	0.56357300
C	4.43323000	0.68364100	-1.86947100
C	4.73871600	0.31245900	0.51458700
C	5.16874900	0.84234900	-0.69910200
H	4.79602100	1.10195800	-2.80075000
H	5.33508100	0.44702600	1.40975600
H	3.16489500	-0.82515600	1.49333100
H	2.63444400	-0.15769100	-2.71640200
Cl	6.66766100	1.72850600	-0.75775500
C	-1.22860000	2.17467600	0.81967600
C	-0.36699000	1.32240900	0.26648000
H	-1.52654600	1.97198500	1.84746800
C	0.25686400	0.18632500	1.06720500
O	-0.37224800	-0.21273200	2.18715900
C	-1.84733900	3.34016900	0.16793300
C	-2.95681900	3.94790600	0.76861600
C	-1.37427700	3.87276900	-1.03970900

C	-3.58869200	5.03687000	0.17546800
H	-3.32326900	3.55757400	1.71487100
C	-2.00238400	4.95986000	-1.63324300
H	-0.49592400	3.44116900	-1.50995100
C	-3.11545700	5.54550000	-1.03067000
H	-4.44869200	5.49069600	0.65791000
H	-1.61836700	5.35885700	-2.56699600
H	-3.60319800	6.39645900	-1.49496100
H	1.30066900	0.53089500	1.24963200
H	-0.01661100	1.45076000	-0.75862500
C	2.25034500	0.17021800	3.81790500
H	2.88098900	0.78442300	3.14975200
H	1.40707900	0.79848800	4.13199800
H	2.84920400	-0.06939600	4.70473200
O	1.80905700	-1.00708400	3.19171000
H	0.85893300	-0.80169200	2.87945000

Variable frequencies

15.9091	24.4524	26.4451
29.2573	32.8364	46.1817
56.1373	59.9117	79.8523
97.4935	100.9035	103.2738
109.9907	117.1266	138.1037
141.6852	172.8493	181.8495
187.4845	200.5880	213.4977
221.6989	242.2084	247.2732
257.9712	291.7424	292.8530
316.5506	341.5540	353.5208
365.9934	367.6424	405.6446
416.2667	426.9833	431.7699
451.8392	463.5512	469.8064
498.1770	502.1446	526.6721
534.9323	549.0221	563.9827
591.0601	606.8901	622.7765
634.9438	642.6989	648.9527
685.9562	705.3874	717.5793
726.2881	734.7757	742.4775
755.2090	767.4342	780.9807
790.2786	813.6183	841.0592
848.3282	851.5276	866.9127
874.1038	878.8542	880.3378
896.3349	910.1908	915.4508
942.9954	977.4841	990.7524
992.6030	997.2638	1008.3070

1016.3899	1017.8657	1026.0157
1027.6687	1037.4028	1044.8926
1053.6113	1060.4874	1069.7087
1074.9018	1078.3160	1098.6611
1122.4523	1123.6422	1128.4693
1138.0892	1140.4951	1156.9670
1161.7902	1167.2856	1175.4807
1185.3815	1190.3140	1195.1006
1201.8349	1205.4846	1210.3435
1224.5201	1234.3754	1235.9565
1247.9770	1253.4666	1262.1924
1277.4870	1294.9496	1304.8567
1306.8566	1324.0611	1329.8424
1330.5584	1338.6380	1343.5701
1352.3364	1353.3410	1356.9102
1371.9251	1377.7108	1382.8163
1388.4670	1422.3332	1452.1810
1468.1608	1487.6697	1490.2582
1502.6994	1508.2628	1511.9774
1518.7492	1521.2557	1523.7027
1537.1652	1540.7124	1560.1732
1580.9979	1582.6542	1673.8056
1679.1832	1680.1939	1684.5387
1693.2279	1703.7409	1705.9124
1765.2181	2751.9918	2918.1336
2984.5723	3067.9405	3069.6164
3079.6077	3112.1829	3136.5255
3147.2132	3155.7960	3166.6578
3168.5955	3178.9857	3184.0395
3198.9229	3200.2900	3203.5794
3208.6198	3213.5376	3220.3843
3221.9079	3225.8420	3228.7741
3234.5685	3241.7472	3254.7428

M02^P

Zero-point correction=0.590112

Thermal correction to Energy=0.625322

Thermal correction to Enthalpy=0.626266

Thermal correction to Gibbs Free Energy=0.519327

Sum of electronic and zero-point Energies=-2162.743183

Sum of electronic and thermal Energies=-2162.707972

Sum of electronic and thermal Enthalpies=-2162.707028

Sum of electronic and thermal Free Energies=-2162.813968

Cartesian coordinate

C	3.09710200	2.89310200	-0.95995800
C	2.50255900	1.68639800	-0.59413100
C	3.10834800	0.46688900	-0.87665900
C	4.34019300	0.47111200	-1.52861400
C	4.94375200	1.67630600	-1.89157600
C	4.32639700	2.89435900	-1.61161000
C	2.24045900	4.06378500	-0.54340300
C	0.87602100	3.44367200	-0.17841400
C	1.19540500	1.94433500	0.12787400
H	2.63449700	-0.46942100	-0.59559100
H	4.83143100	-0.47070800	-1.75126100
H	5.90109000	1.66428900	-2.40284900
H	4.79480100	3.82936200	-1.90455700
H	2.11603600	4.81800200	-1.32550200
H	0.40679900	3.89628500	0.69472700
H	2.67056800	4.56509400	0.33072400
H	1.27043400	1.77705600	1.20128300
N	0.11629200	1.09041200	-0.37554800
O	-0.07716400	3.60977300	-1.22625000
C	-0.47377500	-0.01365700	0.10072500
C	-0.42544100	1.33836900	-1.60892200
N	-1.28256300	-0.42635600	-0.87371700
N	-1.28559600	0.42469700	-1.94399800
C	-0.05389500	2.63538500	-2.25286300
H	0.92943000	2.56853800	-2.73704400
H	-0.80454500	2.91216500	-2.99375300
C	-2.14870300	-1.57036900	-0.86018800
C	-3.30439500	-1.54206700	-0.08687800
C	-1.81112100	-2.66369500	-1.65047600
C	-4.13689800	-2.65673400	-0.09760300
C	-2.64906100	-3.77205900	-1.66485100
C	-3.80147000	-3.75496800	-0.88365900
H	-5.04393900	-2.67118200	0.49516900
H	-2.41333100	-4.63922900	-2.27022200
H	-0.90699900	-2.64197600	-2.24976800
H	-3.52289800	-0.65529000	0.50178900
Cl	-4.85022400	-5.14498200	-0.89464600
C	2.06730900	-1.64959500	1.66699600
C	0.82332800	-1.74900800	1.19600800
H	2.31401400	-0.77128300	2.26033200
C	-0.22170200	-0.68314000	1.44167800
O	0.20799800	0.23875600	2.37501900

C	3.15672600	-2.60130300	1.38888800
C	4.47764900	-2.13620400	1.39198100
C	2.91910000	-3.94940900	1.09221900
C	5.53231300	-2.98874300	1.08125400
H	4.67156500	-1.09285000	1.62720700
C	3.97315500	-4.80232300	0.78653200
H	1.90374800	-4.33367300	1.12610200
C	5.28284700	-4.32433300	0.77582100
H	6.54980100	-2.61091400	1.08241500
H	3.77418000	-5.84641500	0.56646900
H	6.10474800	-4.99275700	0.54065100
H	-1.18096900	-1.14806500	1.71424600
H	0.51722900	-2.58081500	0.56219700
C	-2.16945100	2.16477600	1.51454800
O	-2.58702800	1.00382000	1.30249300
O	-1.03882700	2.42665400	2.03296000
H	-0.38379400	1.08235100	2.33768200
C	-3.09489900	3.33397500	1.12246600
C	-4.32874800	3.25588800	2.03228500
H	-5.05341900	4.03012000	1.75726200
H	-4.80472000	2.27678500	1.93799600
H	-4.05056700	3.40588500	3.08072200
C	-2.40385400	4.68558100	1.28316000
H	-1.58257600	4.78481300	0.56677700
H	-3.11628600	5.49634100	1.09351100
H	-1.99841600	4.80020600	2.29100500
C	-3.52012100	3.13236000	-0.33691400
H	-4.23554500	3.90597300	-0.63744200
H	-2.64894500	3.20010100	-0.99844000
H	-3.98115500	2.15050000	-0.46808400

Variable frequencies

9.6963	11.8378	21.2421
27.3382	32.3233	37.1562
45.2150	55.1559	60.3778
75.2716	80.6210	88.3700
91.8358	105.7652	113.3467
117.1936	128.1800	130.1222
142.2985	156.4025	178.9478
201.9701	216.3172	224.8858
229.1458	254.4866	261.1928
265.8290	273.2168	291.6961
295.2246	300.0872	313.2841
321.0710	335.1760	356.6243

368.9921	376.6669	386.2138
389.0646	401.6892	415.8390
418.0475	421.6112	425.2202
443.7140	458.1494	471.1806
490.4374	511.6091	517.7976
535.9104	542.7347	551.7844
557.0045	596.8113	607.1044
608.6786	625.2421	628.4654
645.6993	689.8699	697.6960
714.3826	723.4395	733.9127
738.2043	743.4467	754.2072
764.2175	788.9245	792.4447
804.8895	817.8083	821.2724
842.5853	854.8408	857.0876
874.3470	877.2024	877.7323
891.2373	894.8579	910.7002
913.2419	928.7777	949.2957
950.5806	957.7883	960.2318
965.5347	983.4866	986.0069
986.7740	1000.1114	1017.3605
1018.7533	1020.0446	1022.9336
1031.2472	1032.9313	1044.2208
1049.9922	1052.6530	1053.2338
1056.0551	1067.1066	1068.7033
1070.2123	1097.5595	1116.1857
1116.6018	1131.3790	1138.8918
1146.2875	1154.1149	1176.7258
1179.7614	1192.5201	1206.2432
1207.7576	1213.1488	1220.8163
1230.9654	1236.0282	1247.9978
1256.2701	1264.0181	1269.6445
1277.1411	1283.7193	1287.2610
1297.7715	1303.4829	1306.7168
1325.6628	1329.2254	1332.4536
1338.0754	1340.8174	1354.8688
1362.8024	1367.0809	1374.6897
1381.8022	1385.1317	1391.3384
1399.6712	1421.2302	1433.7248
1464.7917	1475.2958	1480.8450
1486.4278	1487.7006	1496.6036
1499.3819	1501.0088	1501.1952
1511.9317	1512.2679	1516.1198
1537.9663	1539.7536	1547.8057
1552.8920	1558.8134	1580.4409

1607.6210	1670.3286	1674.6960
1684.2960	1687.8466	1693.4344
1699.1208	1703.6235	1704.7210
1762.5526	2624.8661	3051.7898
3055.3898	3062.9443	3072.0372
3079.8671	3082.2031	3126.6579
3128.8599	3138.4704	3141.6607
3159.2767	3163.1583	3164.8347
3177.6965	3180.1629	3182.5869
3193.1906	3198.1613	3199.8321
3203.0402	3208.3996	3210.7905
3213.8623	3214.6927	3220.6736
3224.4727	3231.0941	3236.2137
3238.8712	3252.9760	3256.1360

TS2^H

Zero-point correction=0.461719

Thermal correction to Energy=0.489438

Thermal correction to Enthalpy=0.490382

Thermal correction to Gibbs Free Energy=0.400090

Sum of electronic and zero-point Energies=-1892.306800

Sum of electronic and thermal Energies=-1892.279081

Sum of electronic and thermal Enthalpies=-1892.278136

Sum of electronic and thermal Free Energies=-1892.368429

Cartesian coordinate

C	-4.10933800	0.06815600	-0.98575500
C	-3.24647000	0.25133000	0.09875100
C	-2.80835800	1.52115800	0.45902400
C	-3.21636100	2.60785500	-0.31258300
C	-4.06624500	2.42738700	-1.40387800
C	-4.52769300	1.15632600	-1.74246400
C	-4.47436500	-1.38287000	-1.15442200
C	-4.08141100	-1.98184700	0.21289000
C	-2.94794900	-1.07397000	0.76750800
H	-2.16215200	1.64730300	1.31916700
H	-2.87002000	3.60411700	-0.05630000
H	-4.37919000	3.28619600	-1.98939400
H	-5.20615100	1.01911300	-2.57921600
H	-3.89973700	-1.82753000	-1.97523400
H	-4.92524400	-1.87816600	0.89849600
H	-5.53154500	-1.54588500	-1.37606500
H	-2.91609400	-1.02170800	1.85471000

N	-1.65049700	-1.65341800	0.33325100
O	-3.76596700	-3.35770000	0.21959600
C	-0.40557500	-1.14552300	0.47890100
C	-1.52964200	-2.81779100	-0.38316500
N	0.39200400	-2.00026500	-0.17534300
N	-0.29711300	-3.04280700	-0.72424000
C	-2.70694600	-3.70894000	-0.63851500
H	-2.99625000	-3.66712300	-1.69564300
H	-2.42889200	-4.73796800	-0.40466400
C	1.82202800	-1.96307800	-0.28542500
C	2.37763700	-1.93713300	-1.55967200
C	2.60604700	-1.99850100	0.86524500
C	3.76001000	-1.93736200	-1.69776600
C	3.98956900	-1.98494900	0.72028100
C	4.55026700	-1.95688500	-0.55258300
H	4.22034300	-1.91892000	-2.67852900
H	4.63019700	-2.00545400	1.59422000
H	2.14596400	-2.01201200	1.85659000
H	1.73223300	-1.92462400	-2.43124100
Cl	6.28527500	-1.95009500	-0.72079700
C	0.47867000	2.40855600	1.04452000
C	0.57123800	1.15508600	0.58640300
H	-0.07230700	2.56562100	1.97035900
C	0.04706600	-0.01979900	1.32763300
O	-0.87834500	0.24133000	2.34981100
C	1.02181100	3.61016800	0.39446200
C	0.55951900	4.86988500	0.79842100
C	1.99106700	3.55785000	-0.61812600
C	1.02919800	6.03516600	0.20119800
H	-0.18207900	4.92903300	1.59120500
C	2.45939000	4.72036700	-1.21724600
H	2.39606700	2.59853700	-0.92674100
C	1.97984800	5.96599000	-0.81330100
H	0.65388200	6.99872200	0.53185800
H	3.21218700	4.65528900	-1.99695500
H	2.35203100	6.87299000	-1.27850700
H	0.87486300	-0.53540300	2.06559900
H	1.09276900	0.93850100	-0.34626000
O	0.94086600	-1.11685000	3.39582800
H	-0.37572200	-0.24210200	3.10109900
H	1.56389600	-0.58551400	3.90544700

Variable frequencies

-899.4819 10.8925 15.9631

19.8630	26.6948	41.7116
53.3308	59.9063	67.0736
87.0258	98.8724	112.0570
126.6970	140.0226	146.0780
169.4124	207.6988	220.2196
233.4538	236.1518	254.2941
266.0032	278.6576	293.8737
322.0363	346.4694	351.6982
360.3273	376.5682	397.4113
414.0248	417.1858	433.7383
443.3387	453.4919	467.6095
476.0873	494.4471	497.2849
514.5336	525.2741	527.6775
537.2753	561.4322	578.2374
595.6804	607.5461	630.1339
633.2024	650.7216	655.9427
697.4606	711.8200	725.3046
731.4754	741.1284	752.6032
761.1145	768.5052	785.0218
807.4392	820.6617	846.5893
850.0161	857.4404	864.8646
872.6804	884.8673	894.7544
901.6195	911.0313	917.0559
940.3015	982.2882	986.6909
994.8386	1002.1301	1006.7392
1012.5871	1015.5087	1020.5264
1030.1473	1033.9750	1034.6622
1056.0271	1068.8144	1071.4241
1077.4211	1082.8149	1097.3076
1115.2083	1121.7253	1131.7358
1133.2205	1146.8635	1163.1729
1174.2805	1178.0183	1182.4681
1202.0067	1203.4828	1207.2273
1222.8926	1227.1960	1242.0558
1250.7234	1262.1551	1271.9572
1277.6428	1303.3283	1316.0679
1327.5994	1331.5280	1336.2638
1342.6788	1342.8190	1350.4882
1351.8837	1363.3257	1365.7560
1375.7966	1384.1068	1418.9487
1461.7975	1465.7908	1483.0817
1492.8967	1501.5276	1507.7843
1517.1853	1522.7263	1537.9307
1551.8799	1555.3141	1569.8739

1588.4818	1668.0786	1676.0267
1682.7022	1685.3723	1693.7967
1699.3009	1703.6615	1749.3516
1981.7525	2826.0886	3077.2429
3090.6768	3134.9529	3144.6951
3146.9312	3168.0690	3172.2070
3179.6644	3188.8480	3192.1643
3198.7712	3199.8178	3208.7556
3210.4706	3217.8918	3228.1710
3228.4291	3231.7608	3247.0367
3253.3397	3254.3572	3896.9863

TS2^M

Zero-point correction=0.490025

Thermal correction to Energy=0.519661

Thermal correction to Enthalpy=0.520605

Thermal correction to Gibbs Free Energy=0.425770

Sum of electronic and zero-point Energies=-1931.561309

Sum of electronic and thermal Energies=-1931.531674

Sum of electronic and thermal Enthalpies=-1931.530730

Sum of electronic and thermal Free Energies=-1931.625565

Cartesian coordinate

C	-4.21242700	0.03427400	-0.94690300
C	-3.31622100	0.21153900	0.11131300
C	-2.88060100	1.48087100	0.47604900
C	-3.32431900	2.57392600	-0.26593100
C	-4.20647400	2.39944800	-1.33234000
C	-4.66605400	1.12844200	-1.67380400
C	-4.56978900	-1.41778000	-1.12293400
C	-4.12389600	-2.03180500	0.22143900
C	-2.98067100	-1.12006400	0.74905600
H	-2.20953600	1.60392600	1.31707000
H	-2.98009800	3.57008700	-0.00658200
H	-4.54651700	3.26291400	-1.89545900
H	-5.37034300	0.99590600	-2.48960200
H	-4.02169000	-1.84621600	-1.97003600
H	-4.94413500	-1.94578800	0.93742700
H	-5.63281800	-1.58713800	-1.30883800
H	-2.91203200	-1.08509300	1.83537800
N	-1.69399200	-1.68006800	0.25966500
O	-3.79403100	-3.40390900	0.19868100
C	-0.44991000	-1.16313000	0.36850400

C	-1.58680700	-2.83363100	-0.47704800
N	0.33352400	-2.00020600	-0.32371700
N	-0.36428000	-3.04136700	-0.86306900
C	-2.76385400	-3.73345900	-0.70202800
H	-3.09174100	-3.68099000	-1.74725900
H	-2.46738500	-4.76245400	-0.49159100
C	1.75888400	-1.93982900	-0.48634100
C	2.26512500	-1.86870900	-1.77931900
C	2.58674600	-1.99164800	0.63272900
C	3.64122700	-1.83806100	-1.96817400
C	3.96358100	-1.94647500	0.43759000
C	4.47471000	-1.87261500	-0.85427200
H	4.06392300	-1.78369600	-2.96440100
H	4.63569200	-1.97710400	1.28724400
H	2.16546200	-2.03832000	1.64006100
H	1.58730800	-1.84415300	-2.62570700
Cl	6.20121700	-1.82711300	-1.08851700
C	0.40751100	2.39672700	0.91830000
C	0.50599300	1.14617100	0.45458400
H	-0.10466700	2.54348000	1.86791800
C	0.03139600	-0.04289900	1.21011800
O	-0.85357700	0.20665400	2.27357100
C	0.89889100	3.60768100	0.24462900
C	0.41270100	4.85724900	0.65150300
C	1.84089700	3.57233200	-0.79381500
C	0.83243700	6.02955300	0.03132800
H	-0.30656200	4.90257100	1.46549400
C	2.25962900	4.74194900	-1.41539300
H	2.26532200	2.62178600	-1.10349400
C	1.75607400	5.97713600	-1.00883200
H	0.44009100	6.98545800	0.36434000
H	2.99263000	4.69126700	-2.21476700
H	2.08950600	6.88968100	-1.49231000
H	0.89891300	-0.55184100	1.88568900
H	0.99134600	0.94108700	-0.49985500
C	2.13068300	-0.25832300	3.78023100
H	3.12747300	-0.41346600	3.31968600
H	1.91704400	0.82360000	3.67482700
H	2.26023600	-0.44443300	4.86099500
O	1.15031300	-1.06783300	3.22467700
H	-0.32927300	-0.23118000	3.01155200

Variable frequencies

-732.4755 12.6514 21.7226

22.6427	30.2790	33.9581
46.5820	51.3950	60.6668
72.8037	81.0758	91.4755
97.9680	118.1792	122.0769
131.9033	143.4810	164.2412
170.7373	206.6391	219.2493
233.5702	237.3002	254.2020
265.8786	281.1464	294.2095
310.2193	325.4328	347.2868
357.8609	366.8839	392.9799
414.5323	417.0755	431.1699
450.6021	455.4804	468.0357
480.0024	495.1514	525.3667
528.1609	534.6370	557.9429
580.9374	595.4060	607.1826
629.7095	632.2491	650.0164
655.6935	697.0172	711.9076
725.8200	730.9218	739.4891
749.3460	760.5275	768.1539
783.0628	808.6290	820.4209
846.8421	851.4377	856.9767
864.8145	871.9350	884.6699
894.3472	894.6322	911.9655
917.8883	940.5339	966.9345
981.1732	987.9916	994.5534
1006.4298	1007.3950	1012.0733
1015.8576	1020.0743	1032.9681
1035.5141	1037.0099	1055.9234
1070.6573	1071.4492	1075.9586
1093.7973	1110.7023	1118.6119
1129.2631	1132.4138	1145.4541
1156.9107	1163.2147	1174.1168
1178.4067	1182.6430	1188.1318
1200.3746	1201.2622	1204.2989
1207.6769	1219.2349	1228.4627
1240.8770	1250.7323	1261.5190
1268.2651	1275.9901	1303.9533
1317.3117	1328.4960	1332.0359
1336.5465	1340.3749	1343.8812
1352.0260	1352.7337	1363.5466
1365.8513	1376.6612	1383.7796
1419.8918	1448.0299	1462.8503
1468.0956	1491.9290	1494.9494
1503.0611	1511.4130	1512.8823

1514.6467	1519.1381	1523.7314
1539.7377	1552.4318	1554.8661
1566.2016	1584.5513	1669.1092
1674.8342	1682.7991	1684.2941
1691.1704	1699.2726	1705.1881
1749.6301	2014.1784	2929.4867
2962.7181	2998.1155	3074.3096
3087.9996	3104.3000	3134.8082
3145.2036	3146.9495	3169.8557
3171.8616	3183.4420	3188.3136
3190.1864	3196.6656	3202.7418
3207.2466	3211.1262	3216.3442
3226.1866	3227.2851	3228.6250
3242.2696	3243.7933	3258.7029

TS2[‡]

Zero-point correction=0.585901

Thermal correction to Energy=0.620922

Thermal correction to Enthalpy=0.621866

Thermal correction to Gibbs Free Energy=0.516542

Sum of electronic and zero-point Energies=-2162.720603

Sum of electronic and thermal Energies=-2162.685582

Sum of electronic and thermal Enthalpies=-2162.684638

Sum of electronic and thermal Free Energies=-2162.789962

Cartesian coordinate

C	-4.21237600	-2.50333200	0.89085300
C	-2.94802300	-2.19730600	0.39610600
C	-1.90995700	-3.12455800	0.41976300
C	-2.15989500	-4.37797800	0.97112100
C	-3.42437800	-4.69146300	1.47708700
C	-4.45950800	-3.76089200	1.43644200
C	-5.16692800	-1.34886600	0.71885500
C	-4.30843800	-0.17505100	0.18276700
C	-2.89527700	-0.78828500	-0.13997400
H	-0.93835100	-2.87556100	-0.00016200
H	-1.36874000	-5.11993700	1.00398400
H	-3.60142800	-5.67349000	1.90423400
H	-5.44206500	-4.01179600	1.82538700
H	-5.66006000	-1.05530600	1.65192700
H	-4.72320700	0.24267000	-0.73493400
H	-5.96047700	-1.59610100	0.00706100
H	-2.71805400	-0.74951200	-1.20879100

N	-1.82355700	-0.01264000	0.50604100
O	-4.27955000	0.92603800	1.07823500
C	-0.49108800	0.06475600	0.24472500
C	-2.04825900	0.64026500	1.69275000
N	-0.00112100	0.81046300	1.26422400
N	-0.96951100	1.16287800	2.17395500
C	-3.44883800	0.71575800	2.19915500
H	-3.71549400	-0.20735300	2.73492100
H	-3.55852500	1.56473200	2.87401800
C	1.32052300	1.32421500	1.44904800
C	1.86507300	2.18131300	0.49746800
C	2.02084300	0.96583100	2.59581000
C	3.15477300	2.66516900	0.68692600
C	3.30440800	1.46112200	2.79176500
C	3.85957400	2.30053900	1.83016800
H	3.60604800	3.32814800	-0.04199500
H	3.87265200	1.19497700	3.67518800
H	1.56355900	0.30230000	3.32149400
H	1.29092500	2.45493200	-0.38348200
Cl	5.47311100	2.91354200	2.06747900
C	2.08568400	-1.88157000	-1.54661100
C	1.57379600	-0.91336800	-0.77382200
H	1.44618900	-2.32421800	-2.30582700
C	0.20875900	-0.37540300	-0.95377300
O	-0.58279400	-1.18604300	-1.78458600
C	3.44921300	-2.41943300	-1.43164200
C	3.74767500	-3.65072600	-2.03044700
C	4.47834500	-1.75185300	-0.74948500
C	5.01745600	-4.21023600	-1.93384500
H	2.96454100	-4.17431300	-2.57239600
C	5.74629000	-2.31110600	-0.64954600
H	4.29142500	-0.77472600	-0.31194300
C	6.02301100	-3.54458000	-1.23809200
H	5.22123700	-5.16738800	-2.40401600
H	6.52827000	-1.77576800	-0.11966200
H	7.01575400	-3.97626500	-1.16188300
H	0.21613900	0.86139400	-1.57779300
H	2.18039300	-0.48541800	0.01862200
C	-1.34940700	2.00996000	-2.24796800
O	-0.07679300	1.98935600	-2.01295700
O	-2.01469700	0.99599300	-2.50666100
H	-1.06076000	-0.56581100	-2.37309200
C	-2.03167300	3.36728600	-2.06946800
C	-3.38080600	3.38073400	-2.78526100

H	-3.88465200	4.33724800	-2.61394000
H	-3.25264800	3.24656900	-3.86343200
H	-4.02044800	2.57433000	-2.42056700
C	-2.24015100	3.51307600	-0.55013200
H	-1.28417400	3.44571400	-0.01793700
H	-2.68877500	4.48636000	-0.32562200
H	-2.91081400	2.73296300	-0.17112900
C	-1.13422700	4.49555500	-2.58346700
H	-1.62355300	5.46143000	-2.42234700
H	-0.17418200	4.49788200	-2.06352500
H	-0.94078200	4.38599100	-3.65492800

Variable frequencies

-1262.0383	16.1746	20.5469
25.1169	35.5138	36.1017
39.9017	41.1800	50.8565
55.1485	56.4328	76.7188
84.9173	90.8388	101.6976
115.1929	127.0458	143.2129
146.6358	157.8166	195.7448
200.8941	208.9657	212.3964
218.0688	233.1155	245.6317
255.3327	262.9094	280.7346
289.6121	294.5756	301.9920
317.6169	328.4778	337.0203
350.6414	364.8025	376.8616
387.2602	394.3353	398.3731
417.4390	424.1780	429.8872
440.9351	448.8903	463.3026
481.0151	487.4751	514.2630
517.3342	528.7897	541.5231
557.4994	575.6497	597.3811
604.3766	611.7896	631.5836
632.8664	648.1932	665.8150
692.8752	710.3340	715.0349
725.4019	737.3328	750.0907
754.6358	759.7308	771.5424
784.1861	791.6684	808.9837
820.3354	828.6469	837.9649
857.1753	869.2799	873.0672
875.6395	880.9680	882.0620
892.8394	902.6629	912.2226
918.3795	946.7618	958.2183
964.5782	966.8064	973.7346

986.1942	989.1193	999.6371
1004.2189	1010.1629	1016.0139
1021.6024	1022.1271	1032.9187
1035.9545	1042.6533	1050.9160
1054.2639	1061.0297	1064.3069
1065.4502	1074.0768	1118.1917
1122.7933	1124.2105	1134.6419
1144.9049	1156.3884	1160.1368
1177.0019	1182.8453	1197.4021
1209.1880	1212.0707	1213.1862
1228.7797	1234.3242	1246.9309
1249.7741	1255.9990	1266.1761
1269.8926	1282.3339	1283.1223
1310.7176	1314.2861	1317.2700
1327.4652	1333.3442	1340.0157
1342.6445	1352.4477	1355.1468
1370.6892	1371.5246	1377.6483
1388.9513	1398.5548	1406.6062
1412.5413	1426.8761	1430.0487
1456.3267	1465.2373	1469.3971
1481.3545	1487.3824	1489.0070
1495.9809	1496.6778	1502.1997
1503.5173	1506.5819	1510.3081
1516.2371	1518.9740	1539.4105
1540.2436	1555.6015	1562.6488
1573.2832	1583.5851	1668.9593
1678.8699	1685.3771	1691.3719
1698.4990	1699.5031	1721.2918
1737.1625	1751.1787	3047.9073
3051.4692	3064.7714	3069.0703
3080.9922	3122.6514	3131.3297
3136.6728	3142.0878	3147.3264
3159.7847	3161.4561	3162.4868
3177.1849	3199.3268	3199.4040
3202.2976	3203.0107	3204.0411
3213.3390	3215.4017	3215.4809
3221.9933	3230.2592	3231.0073
3232.9913	3236.4753	3238.3361
3247.1701	3259.5234	3551.8134

M2

Zero-point correction=0.439339

Thermal correction to Energy=0.465753

Thermal correction to Enthalpy=0.466697
 Thermal correction to Gibbs Free Energy=0.379668
 Sum of electronic and zero-point Energies=-1815.970908
 Sum of electronic and thermal Energies=-1815.944494
 Sum of electronic and thermal Enthalpies=-1815.943550
 Sum of electronic and thermal Free Energies=-1816.030579

Cartesian coordinate

C	-1.67058900	2.24233400	-0.95156600
C	-1.03046600	1.12654700	-0.53878300
C	0.24102600	0.69368100	-1.03754600
O	0.92419900	1.53928300	-1.91599700
H	-1.17880400	2.87913800	-1.68366200
C	-2.98345100	2.69001800	-0.48413100
C	-3.42145900	3.98401700	-0.80471900
C	-3.85261800	1.86944300	0.25542200
C	-4.66447900	4.44950300	-0.39073000
H	-2.76854200	4.63016200	-1.38596400
C	-5.09145400	2.33621700	0.67431200
H	-3.56576400	0.84668400	0.48503600
C	-5.50624100	3.62943600	0.35611900
H	-4.97615200	5.45605600	-0.65273800
H	-5.74454800	1.68218400	1.24420200
H	-6.47731600	3.98861900	0.68070500
H	-1.47915000	0.51013000	0.23487300
C	4.38222200	0.90431400	1.04295200
C	3.37079200	1.26157200	0.14604000
C	2.59217500	2.39430400	0.37927700
C	2.82879400	3.14422500	1.53050600
C	3.83240500	2.78035400	2.42806100
C	4.62171200	1.65935300	2.18505600
C	5.10993700	-0.33258400	0.59323100
C	4.68767100	-0.45716600	-0.88536900
C	3.32404800	0.28486500	-1.01889900
H	1.82778200	2.69674700	-0.32665000
H	2.22750200	4.02628500	1.72587500
H	4.00608700	3.38025800	3.31603500
H	5.41551500	1.38130900	2.87233500
H	4.78951500	-1.19808200	1.18372800
H	5.40778900	0.08164700	-1.50526400
H	6.19538800	-0.25870600	0.69639100
H	3.21412800	0.78151400	-1.98203100
N	2.24649700	-0.71848000	-0.90106200
O	4.66451200	-1.77111400	-1.40160800

C	0.89570900	-0.45875800	-0.67918600
C	2.48351100	-1.99994900	-0.45666700
N	0.43519700	-1.61157900	-0.05903200
N	1.44628300	-2.56549100	0.04943500
C	3.81839000	-2.64613000	-0.69061100
H	4.25827700	-2.97397900	0.25874800
H	3.68183100	-3.52965800	-1.31830600
C	-0.89134100	-2.07922600	0.09664900
C	-1.17716700	-2.88953800	1.19590200
C	-1.88483800	-1.79590500	-0.84254200
C	-2.45580600	-3.40348300	1.36896900
C	-3.16968300	-2.29402800	-0.66223300
C	-3.44503300	-3.09270800	0.44268200
H	-2.68792800	-4.03145100	2.22153700
H	-3.94943500	-2.07569500	-1.38307200
H	-1.65668300	-1.18087800	-1.70521700
H	-0.38876000	-3.11578300	1.90473800
Cl	-5.05878100	-3.72004700	0.66625300
H	0.58041600	1.38354000	-2.80531500

Variable frequencies

15.1685	17.2725	21.0860
28.5078	39.6132	47.7360
63.0995	73.2287	93.3204
119.9712	135.8903	148.0079
176.1728	188.0775	208.1013
223.6397	230.4236	251.7304
254.7003	262.7075	276.2380
293.1490	303.1278	315.3786
348.2621	356.4729	370.9168
400.6517	414.7017	417.8564
424.3141	433.8675	455.0508
471.9439	483.2810	493.7789
517.0750	531.2300	539.0699
562.6642	585.4182	599.3652
607.3471	626.7800	632.6778
638.6680	648.7583	668.8927
693.3027	712.2080	726.4703
728.6345	754.4745	763.2784
772.3400	779.6984	825.1428
846.3757	846.6797	849.8339
858.0505	862.4755	875.0235
880.3417	887.4309	903.9506
915.3486	938.1746	975.1253

978.8689	991.0667	993.4854
994.9855	1003.5144	1005.9104
1014.0676	1015.7180	1022.1144
1032.6234	1038.0367	1047.2193
1072.6215	1073.8710	1091.3797
1106.4935	1121.3805	1129.0814
1134.1754	1142.3504	1164.1763
1176.6917	1183.8666	1184.6978
1190.8166	1200.5542	1204.8632
1211.3360	1228.0352	1235.9742
1241.6762	1249.7772	1257.2044
1271.5231	1302.3941	1308.4715
1324.9106	1325.9301	1330.4819
1334.0522	1341.5695	1344.0298
1348.2891	1352.5850	1368.2829
1370.0440	1378.6487	1382.0676
1417.4714	1451.8812	1471.8929
1483.2166	1495.2188	1506.0454
1515.0477	1516.8230	1536.5517
1554.4680	1556.6877	1661.5253
1667.4551	1676.1166	1679.7842
1692.0659	1701.0194	1707.7837
1709.5562	1738.3631	3080.9202
3094.3548	3131.2960	3144.4771
3150.6711	3174.0500	3184.4198
3193.3834	3195.5411	3197.9394
3207.1580	3207.7983	3211.3855
3215.6451	3220.2465	3229.3276
3231.2555	3232.9037	3238.5770
3246.4895	3252.0623	3837.0728

M3⁺

Zero-point correction=0.440804

Thermal correction to Energy=0.466927

Thermal correction to Enthalpy=0.467871

Thermal correction to Gibbs Free Energy=0.380612

Sum of electronic and zero-point Energies=-1815.794269

Sum of electronic and thermal Energies=-1815.768145

Sum of electronic and thermal Enthalpies=-1815.767201

Sum of electronic and thermal Free Energies=-1815.854461

Cartesian coordinate

C	-1.71510800	1.96420200	-1.08588300
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C	-0.93179300	0.94987300	-0.58886700
C	0.28104400	0.53206400	-1.14384200
O	0.91006800	1.12477400	-2.18463500
H	-1.40264600	2.49971000	-1.98229900
C	-2.97936700	2.40052200	-0.53155400
C	-3.58199700	3.55316100	-1.06559700
C	-3.64070300	1.71277700	0.50482400
C	-4.79148800	4.01899800	-0.57027700
H	-3.08477000	4.08436100	-1.87216100
C	-4.85065100	2.17899000	0.99423200
H	-3.22016300	0.79941200	0.91523500
C	-5.42801200	3.33461200	0.46339200
H	-5.23941300	4.91327000	-0.98956100
H	-5.35337600	1.63862100	1.78911900
H	-6.37478100	3.69465600	0.85145800
H	-1.24973000	0.42003800	0.30206800
C	4.31287900	1.06200500	1.06521600
C	3.38293800	1.30177500	0.04878800
C	2.61949700	2.46653600	0.04998100
C	2.77458200	3.37269600	1.09567200
C	3.69053500	3.12436700	2.11811500
C	4.47223200	1.97167500	2.10441700
C	5.05603200	-0.22711600	0.83986200
C	4.76907200	-0.52073700	-0.64742800
C	3.41459300	0.17662900	-0.96563800
H	1.93116300	2.68333700	-0.75659100
H	2.18804200	4.28496100	1.10672600
H	3.80668700	3.84423200	2.92143500
H	5.20249500	1.79077400	2.88674400
H	4.66576800	-1.01201000	1.49719200
H	5.52505400	-0.02537300	-1.26029200
H	6.12784400	-0.14992300	1.03318000
H	3.33315800	0.49569400	-2.00440800
N	2.33344000	-0.82516700	-0.72984600
O	4.80191900	-1.87520700	-1.03611900
C	0.99230500	-0.62785800	-0.68276900
C	2.55623000	-2.10502900	-0.29613200
N	0.47834800	-1.77715000	-0.20407700
N	1.44785000	-2.69625700	0.04561000
C	3.92973100	-2.70683600	-0.31131000
H	4.27405600	-2.89004600	0.71325300
H	3.88880600	-3.66561100	-0.83168400
C	-0.89706800	-2.12429900	0.00353900
C	-1.28631500	-2.54028800	1.27104000

C	-1.80015200	-2.03063700	-1.05083400
C	-2.62215800	-2.85143900	1.49725000
C	-3.13659400	-2.32769100	-0.81980400
C	-3.53572700	-2.73002800	0.45357100
H	-2.95456300	-3.18021900	2.47473900
H	-3.86411000	-2.25555900	-1.61953800
H	-1.46691600	-1.72131000	-2.03562800
H	-0.55290300	-2.61936000	2.06609700
Cl	-5.20821700	-3.08808000	0.74459200
H	0.51941500	1.98764300	-2.37870400

Variable frequencies

11.4605	18.0257	23.3439
31.4889	36.0605	49.4606
62.4595	72.6162	88.8021
117.4518	134.2845	157.1591
173.3848	192.0611	196.3679
214.2283	235.3918	248.4368
260.2215	264.7828	281.9068
297.7404	327.9495	349.6078
361.9358	373.2510	401.1836
409.5765	421.7554	435.9613
449.9215	461.2770	465.6706
475.3328	491.3771	496.8896
520.4810	536.1364	539.6433
566.0006	586.5688	596.3033
607.1405	629.1748	633.7468
652.6096	658.0831	695.8683
702.6971	725.1448	727.2113
737.7483	759.5388	765.1494
776.0818	782.2626	813.6148
844.0859	848.6544	853.2822
857.6102	863.6510	874.4267
884.3895	893.1865	902.2233
912.6065	954.0821	971.2926
975.7482	985.1625	998.9050
1004.0423	1005.0271	1012.7257
1019.3672	1029.7481	1034.9903
1035.6926	1046.9167	1055.1811
1072.1604	1076.6326	1096.0144
1121.2423	1132.3724	1134.5200
1135.5877	1138.2038	1160.8679
1173.1668	1191.4432	1193.5846
1198.3689	1201.7990	1205.9012

1216.7883	1234.7561	1241.1587
1250.9766	1258.4360	1272.6802
1275.2726	1296.0682	1301.1232
1322.3739	1329.8073	1333.8884
1343.7696	1349.8518	1355.6885
1358.7956	1368.3201	1375.8963
1379.5945	1394.0978	1415.3692
1435.5130	1462.3340	1469.3749
1493.1184	1500.1653	1510.2209
1524.0340	1526.6580	1542.6618
1549.3694	1558.3744	1569.0001
1586.4676	1663.6834	1664.8399
1680.9241	1682.1513	1682.4483
1686.7439	1705.4507	3078.1198
3095.4715	3139.6102	3152.7613
3164.9840	3169.5687	3175.8015
3211.4885	3217.8766	3218.7730
3227.2968	3229.5508	3232.4010
3237.3949	3238.0869	3238.5855
3239.1293	3248.2161	3249.5855
3250.3990	3256.4253	3855.8376

M3-

Zero-point correction=0.425587

Thermal correction to Energy=0.451546

Thermal correction to Enthalpy=0.452490

Thermal correction to Gibbs Free Energy=0.366432

Sum of electronic and zero-point Energies=-1815.456647

Sum of electronic and thermal Energies=-1815.430688

Sum of electronic and thermal Enthalpies=-1815.429743

Sum of electronic and thermal Free Energies=-1815.515802

Cartesian coordinate

C	-1.61393800	2.51144900	-0.78608900
C	-1.08871600	1.34791300	-0.36232700
C	0.18376800	0.83452100	-0.90284700
O	0.86998100	1.53106700	-1.73991700
H	-1.05487100	3.04547300	-1.55188900
C	-2.84838200	3.12577200	-0.29418800
C	-3.10996500	4.47856100	-0.56500600
C	-3.81263500	2.41080000	0.43819000
C	-4.26610900	5.09920800	-0.10450300
H	-2.38217900	5.04492500	-1.14061400

C	-4.96583000	3.03067700	0.90123600
H	-3.66026800	1.35120000	0.62386400
C	-5.20072300	4.38049800	0.63703100
H	-4.43836300	6.14885000	-0.32557800
H	-5.69437500	2.45365400	1.46364600
H	-6.10544500	4.86087000	0.99658600
H	-1.56802200	0.77800300	0.43202600
C	5.01835000	0.59807500	0.06898600
C	3.66120100	0.81922500	-0.16349000
C	3.01354400	1.92743400	0.38024000
C	3.74242500	2.77528200	1.21367400
C	5.09255300	2.53611900	1.47828500
C	5.74459000	1.45207600	0.89395900
C	5.51642200	-0.58839600	-0.71764300
C	4.24070300	-1.29072300	-1.23519700
C	3.07448300	-0.25046000	-1.07054300
H	1.98577000	2.13676500	0.10181100
H	3.25606800	3.64031400	1.65459800
H	5.64276300	3.20807000	2.13080400
H	6.80228600	1.27915800	1.07562000
H	6.11610300	-1.29076000	-0.12897200
H	4.33896100	-1.58900200	-2.28044600
H	6.13910800	-0.25635600	-1.55628500
H	2.77196000	0.19528200	-2.01915300
N	1.90306800	-0.92918600	-0.53941800
O	4.01514900	-2.51582300	-0.54503000
C	0.59210400	-0.38779900	-0.41107700
C	2.04743200	-1.79125900	0.50724200
N	-0.03454600	-1.28062600	0.52022700
N	0.97536200	-2.05993700	1.16566600
C	3.41456200	-2.35558400	0.72598400
H	4.00991300	-1.69289400	1.37221700
H	3.35058900	-3.33958200	1.19280100
C	-1.24361800	-1.94169200	0.32232800
C	-1.63074500	-2.97369900	1.20012400
C	-2.12476700	-1.58486800	-0.71498900
C	-2.85686700	-3.60568600	1.05557300
C	-3.34803200	-2.22485900	-0.85914100
C	-3.71604200	-3.22696700	0.02972100
H	-3.14580100	-4.39822800	1.73812000
H	-4.01264700	-1.94451500	-1.66956700
H	-1.83643400	-0.81056700	-1.41466500
H	-0.95015600	-3.27526300	1.98561900
Cl	-5.27340000	-4.02428200	-0.14232200

Variable frequencies

11.7690	15.0182	29.1398
37.9239	46.3307	54.2958
73.1188	78.5769	94.2321
96.0362	124.9636	138.6604
158.9230	182.5462	199.7910
211.4089	237.2342	254.0877
265.5278	277.6673	293.6748
303.5008	308.3303	347.4125
362.0216	386.2095	396.6567
416.9097	429.0603	430.6918
441.6276	455.1140	478.6546
494.7658	504.1269	519.5090
526.0441	535.7847	561.3266
581.4952	597.6757	604.3294
628.5009	638.9083	647.3703
662.6591	674.4458	707.8291
713.6587	718.8892	727.8673
747.0735	763.4034	774.3037
781.8727	809.8272	833.1344
838.3394	841.3067	852.4774
869.0743	875.8416	886.0870
889.1081	895.6872	908.1388
938.9318	941.3988	962.2118
972.7268	977.1889	989.9305
992.8367	1005.8536	1007.5912
1013.5017	1013.8386	1023.5418
1026.2483	1038.2527	1049.6552
1061.1676	1070.0288	1073.1037
1112.4838	1115.0296	1130.5430
1138.7961	1147.5523	1150.2470
1170.0098	1170.8319	1177.2721
1195.9202	1199.8225	1202.5114
1209.5927	1227.5750	1236.6249
1247.6891	1280.5316	1284.5002
1304.5546	1315.1345	1316.1136
1321.8756	1332.2407	1337.4989
1344.3348	1348.3087	1362.9362
1364.2251	1374.6797	1376.5102
1390.2429	1414.2207	1457.7340
1473.6700	1488.2627	1498.5979
1504.8428	1507.8886	1515.3192
1537.8538	1549.3610	1551.7995

1647.2395	1658.8270	1668.1226
1678.9675	1679.1517	1696.6988
1698.1001	1712.1552	1737.3622
3044.6584	3069.9669	3115.5456
3136.1153	3161.1008	3163.8729
3183.6882	3185.5850	3186.0916
3189.9709	3195.2656	3197.9288
3200.6738	3209.2994	3210.6033
3210.7474	3215.1277	3216.8811
3241.1525	3249.2156	3259.2177

R2 + PivO⁻

Zero-point correction=0.485371

Thermal correction to Energy=0.516098

Thermal correction to Enthalpy=0.517042

Thermal correction to Gibbs Free Energy=0.421211

Sum of electronic and zero-point Energies=-1738.844939

Sum of electronic and thermal Energies=-1738.814212

Sum of electronic and thermal Enthalpies=-1738.813267

Sum of electronic and thermal Free Energies=-1738.909098

Cartesian coordinate

S	-0.75287500	-0.63670900	-1.20167100
O	0.28593300	-1.54911600	-1.64217900
O	-1.17333800	0.48219300	-2.02943500
N	-0.29938300	0.10110200	0.30191300
N	0.34089000	1.33219200	0.06617100
C	-2.03897600	-2.94583500	-0.52433400
H	-1.10225700	-3.43867100	-0.76391600
C	-3.14779000	-3.66051300	-0.08488000
H	-3.07907400	-4.73856800	0.02535000
C	-2.15177200	-1.56564900	-0.65610700
C	-3.33338200	-0.88699800	-0.36775300
H	-3.39348900	0.19056900	-0.49010100
C	-4.34959500	-3.01277800	0.21619800
C	-4.42551800	-1.62190600	0.07084100
H	-5.35394600	-1.10802600	0.30340100
C	-5.55280800	-3.80106600	0.65981900
H	-6.19739300	-3.20618500	1.31036400
H	-5.25814500	-4.70636200	1.19459200
H	-6.14731900	-4.10602900	-0.20739400
C	1.66635300	1.36008400	-0.20517900
H	2.25051200	0.40932800	-0.14955000

C	-0.45700400	2.44193300	0.05534500
C	0.13194800	3.65061100	-0.27437700
H	-0.49283800	4.53547400	-0.27862900
C	2.27068500	2.57053000	-0.50173600
H	3.34126100	2.52813200	-0.67213100
C	1.49551800	3.72008400	-0.55678600
H	1.94494200	4.67631600	-0.80388300
C	0.40672300	-0.78937300	1.24220200
H	-0.25748900	-1.63895500	1.41316900
H	1.38234300	-1.12602300	0.87855900
H	0.51662500	-0.24380500	2.18152300
C	-1.89514500	2.34318400	0.39713900
C	-2.31684300	1.81126800	1.61990900
C	-2.83416700	2.84689900	-0.50552800
C	-3.67034700	1.78307600	1.93218500
H	-1.58519300	1.42335000	2.32167500
C	-4.19075300	2.80874400	-0.19116000
H	-2.50017500	3.23384200	-1.46320100
C	-4.60901800	2.27861100	1.02666400
H	-3.99442400	1.37321000	2.88282800
H	-4.91744400	3.18972500	-0.90056600
H	-5.66564600	2.25211900	1.27261900
C	5.75528200	-1.14107800	0.43161200
C	6.60981600	-1.15669600	-0.84144000
H	7.55733700	-1.67971700	-0.66596000
H	6.08556200	-1.66691600	-1.65661600
H	6.82222700	-0.13304800	-1.15854600
C	5.41349200	-2.56701200	0.85476300
H	6.32887000	-3.13348800	1.06457800
H	4.78997300	-2.56611500	1.75301100
H	4.85451500	-3.08073700	0.06854800
C	6.52712600	-0.42484200	1.54521500
H	6.72357900	0.60909900	1.25237900
H	5.94965400	-0.41366200	2.47654800
H	7.48014000	-0.92926300	1.74412200
C	4.47656900	-0.31454700	0.12943200
O	4.64918100	0.88366000	-0.19121000
O	3.36201900	-0.90570000	0.22346300

Variable frequencies

17.0472	22.1813	28.0471
36.6103	45.7012	49.3294
60.1974	64.7113	71.4978
79.9130	80.0718	93.0648

99.2884	113.6105	119.8189
136.8504	147.9954	162.4340
175.2704	213.6176	217.7754
231.1947	248.8107	254.1880
279.5076	287.7161	291.1683
296.9356	305.2529	311.1374
324.1971	334.1872	352.0665
366.8145	376.7584	380.8921
383.1406	412.6141	417.9953
438.1484	459.5709	489.6347
511.4163	520.9156	540.9522
564.1004	570.9044	580.1197
593.4629	601.3982	626.7376
637.2083	642.8859	672.7547
704.5132	719.5592	720.7272
758.2539	774.8546	800.2430
804.0405	814.4943	830.7414
840.0816	843.7589	859.7988
870.9716	885.6884	907.8927
958.4701	960.6327	963.1120
966.7045	975.9818	988.2878
1005.5995	1011.2829	1015.3751
1016.7423	1033.6739	1034.4584
1044.6356	1053.0585	1055.9861
1056.1980	1068.2591	1073.2171
1082.6633	1103.9244	1120.6243
1124.2521	1127.1897	1144.8997
1149.8735	1165.7360	1184.6142
1187.2713	1192.7046	1211.6277
1213.3581	1229.3803	1253.7884
1257.2165	1264.6281	1265.4498
1285.1016	1318.4995	1330.6761
1334.3721	1340.8098	1357.2730
1361.1680	1366.8061	1390.7752
1393.8575	1400.4200	1418.1046
1426.1849	1455.6058	1462.6444
1472.5879	1477.5673	1486.1582
1494.7156	1500.4679	1501.8726
1502.1843	1505.1468	1508.7442
1510.1617	1514.8110	1526.1262
1537.5551	1546.4861	1551.0149
1582.2224	1651.3898	1669.4109
1669.9820	1690.7995	1692.7362
1702.8923	1713.0127	2717.2610

3047.2243	3051.6235	3057.4549
3074.9707	3079.6591	3118.9941
3127.4236	3136.8096	3151.9145
3156.8189	3160.4624	3161.2445
3174.2563	3174.4813	3179.8900
3203.8047	3216.5002	3218.2251
3227.0768	3227.1793	3230.9015
3232.6986	3236.8920	3239.7716
3246.7596	3248.5053	3267.7079

M3

Zero-point correction=0.927188

Thermal correction to Energy=0.984850

Thermal correction to Enthalpy=0.985794

Thermal correction to Gibbs Free Energy=0.830684

Sum of electronic and zero-point Energies=-3554.855818

Sum of electronic and thermal Energies=-3554.798156

Sum of electronic and thermal Enthalpies=-3554.797211

Sum of electronic and thermal Free Energies=-3554.952322

Cartesian coordinate

C	4.66194000	-0.51056600	-0.28233200
C	3.45123300	-0.19075700	-0.77762800
C	2.62265900	0.84458800	-0.18878900
O	3.11668200	1.58477900	0.84198800
H	5.01252400	-0.00060100	0.61121600
C	5.55129000	-1.55566800	-0.79830900
C	6.57978600	-2.01631700	0.03959100
C	5.41299700	-2.13571700	-2.06856400
C	7.43070900	-3.03567900	-0.37534600
H	6.67668000	-1.57163900	1.02811300
C	6.26586100	-3.15225200	-2.48037100
H	4.64068500	-1.77855500	-2.74403400
C	7.27781600	-3.60900500	-1.63600700
H	8.21592000	-3.38388200	0.28913500
H	6.14559900	-3.58792100	-3.46781600
H	7.94294600	-4.40262800	-1.96173300
H	3.06754300	-0.69602200	-1.65966300
C	1.77997400	5.76610600	-0.72679700
C	2.19870000	4.44027300	-0.63660100
C	3.36207600	4.00567300	-1.26779600
C	4.08196900	4.92410500	-2.02838500
C	3.65444700	6.24911500	-2.13991500

C	2.50580800	6.68266900	-1.48232200
C	0.54036200	6.00635300	0.09886600
C	0.06054900	4.60097800	0.52793200
C	1.25156600	3.62227300	0.21551000
H	3.70594900	2.98285400	-1.15075300
H	4.98968500	4.60858700	-2.53240700
H	4.22965700	6.94983800	-2.73690600
H	2.18361200	7.71739400	-1.55659000
H	-0.25748500	6.52418000	-0.44384000
H	-0.18921800	4.57186400	1.59098100
H	0.77357500	6.61321700	0.97985500
H	1.74735000	3.28852200	1.12618800
N	0.74326000	2.42742700	-0.45915700
O	-1.15600100	4.23351900	-0.12377900
C	1.42475900	1.22010300	-0.72348900
C	-0.19242500	2.56795900	-1.44834200
N	0.65759600	0.64108400	-1.76283800
N	-0.32300000	1.54326000	-2.21371500
C	-0.95613300	3.85132400	-1.47377400
H	-0.39778800	4.62005200	-2.02627700
H	-1.93008200	3.72368100	-1.94819400
C	0.41237100	-0.71622800	-2.02481000
C	-0.27735800	-1.05670200	-3.19803100
C	0.80973000	-1.73386800	-1.14816600
C	-0.58821300	-2.38147200	-3.47026400
C	0.48653900	-3.05842200	-1.41697800
C	-0.21657300	-3.37650300	-2.57234400
H	-1.12358200	-2.64220000	-4.37689100
H	0.78586600	-3.83990900	-0.72614300
H	1.37797500	-1.48902500	-0.25924700
H	-0.57573700	-0.27153600	-3.88178600
Cl	-0.64433400	-5.03880200	-2.89976700
S	-4.52659400	0.81034000	1.79344900
O	-4.83367300	2.19095900	2.13353300
O	-4.00720000	-0.11051200	2.78812600
N	-3.32796400	0.79643400	0.54586000
N	-2.04576200	0.61909500	1.07864700
C	-6.97015200	0.89942600	0.58766500
H	-6.98236100	1.94551600	0.87536700
C	-8.02976100	0.32050300	-0.10470700
H	-8.89070000	0.92669100	-0.36813500
C	-5.88217000	0.09995100	0.91782400
C	-5.82280500	-1.25346800	0.58229900
H	-4.96377000	-1.85696200	0.86196300

C	-8.00285200	-1.02901400	-0.46342300
C	-6.88826900	-1.80436500	-0.11122200
H	-6.85758000	-2.85533200	-0.38494800
C	-1.42339500	1.65899700	1.69051600
H	-1.93653900	2.61244500	1.63793100
C	-1.54246600	-0.65161200	1.08709900
C	-0.33124800	-0.85497200	1.72987700
H	0.08047400	-1.85778700	1.72598400
C	-0.20869300	1.47134300	2.30438000
H	0.28468200	2.31322800	2.77424800
C	0.36778300	0.19846800	2.30986000
H	1.35969200	0.02640500	2.73591300
C	-3.44815600	1.84364700	-0.47112400
H	-2.74228200	1.60717400	-1.27112800
H	-4.46524400	1.78827400	-0.86448200
H	-3.26112600	2.84967100	-0.08035100
C	-2.26835600	-1.74910400	0.42102800
C	-2.70726300	-1.63141700	-0.90119200
C	-2.45481500	-2.94642000	1.11720300
C	-3.33531100	-2.70557400	-1.51717800
H	-2.52442600	-0.71507900	-1.45349800
C	-3.09454600	-4.01636700	0.49682800
H	-2.12195400	-3.02769800	2.14759500
C	-3.53438800	-3.89625500	-0.81924100
H	-3.65587900	-2.61847600	-2.55013900
H	-3.24549200	-4.94213000	1.04121300
H	-4.01886300	-4.73514200	-1.30792000
C	4.28605500	-0.83679800	2.90284300
O	5.46752800	-0.49724300	2.79779600
O	3.26895900	-0.08516100	2.66642100
H	3.30602700	0.94032800	1.64325100
C	3.92456100	-2.28813700	3.29695300
C	3.21092600	-2.91429300	2.09009800
H	2.88763100	-3.93701800	2.31755300
H	2.33550600	-2.31149700	1.82421700
H	3.87322500	-2.94474000	1.21783200
C	5.18463600	-3.08344900	3.62767900
H	5.73507700	-2.61171000	4.44589800
H	4.92453900	-4.10710500	3.92042900
H	5.84985800	-3.12577800	2.76129500
C	2.97659100	-2.27067500	4.50074400
H	2.69536000	-3.29262600	4.77991700
H	3.45172500	-1.80112500	5.36825800
H	2.06612900	-1.71063700	4.26909300

C	-9.14653200	-1.65463500	-1.21528500
H	-8.80514900	-2.05239000	-2.17528600
H	-9.57076100	-2.48830700	-0.64863500
H	-9.94044400	-0.93092100	-1.40643300

Variable frequencies

11.8299	16.1373	19.8415
22.1160	24.3542	27.7838
31.3637	31.9702	37.4827
37.7865	41.3268	44.6995
53.3980	55.3277	60.0303
63.2255	67.6412	69.9720
75.6507	78.2043	85.2328
86.7467	91.1439	99.4394
103.7302	112.5740	118.2101
128.5106	134.5235	139.7984
145.3281	151.4611	154.6318
160.3827	170.8096	181.8938
189.8188	202.4790	206.8547
214.1595	218.5276	230.4119
232.3652	237.6992	249.4499
263.1676	268.1358	269.3954
271.7096	272.6245	275.9902
282.0439	296.0595	298.5675
299.6027	304.1367	312.6193
315.8176	323.7909	335.3313
340.4922	352.4701	356.5445
360.9835	366.0111	379.3551
384.8726	389.5728	400.6779
416.6147	418.4413	419.0226
420.9440	430.9901	433.4459
436.8210	446.4289	457.3338
465.0198	484.2775	487.7692
491.7825	504.8630	507.1590
517.7819	521.7022	532.3917
542.8318	554.0283	557.6997
559.2509	564.1700	584.7240
585.7833	587.8049	597.8453
602.0203	607.0423	626.1074
626.8840	632.1783	637.3594
643.1500	643.2629	661.7785
674.1255	681.4726	703.0603
711.7142	715.9024	717.5910
720.4486	721.6331	725.9569

743.2303	752.5879	763.9479
770.5954	774.0134	781.0114
788.9291	802.9997	804.6088
814.8419	818.5535	833.8159
837.7690	844.7223	847.2666
860.3773	862.4706	866.8618
869.6283	875.5313	876.0277
880.9783	887.1303	892.2929
898.5989	902.0067	910.2249
912.8985	949.5771	952.5099
954.0141	954.7567	956.2916
963.1773	973.5663	980.3250
993.6237	994.4440	996.2008
999.7825	1004.4283	1005.6143
1012.8856	1015.2867	1015.6069
1015.9528	1017.8961	1023.9713
1027.5739	1029.0165	1032.4952
1035.7322	1045.8697	1049.3585
1052.0330	1053.3472	1053.8464
1058.0816	1068.0561	1069.4690
1076.1853	1079.1900	1085.0691
1086.9791	1095.2662	1114.7437
1118.3082	1121.6173	1122.9880
1126.6212	1133.9271	1143.7858
1150.1082	1151.6142	1159.4797
1166.6831	1169.4658	1176.5438
1178.7790	1181.6027	1185.9471
1186.1463	1189.1169	1200.8696
1204.6122	1213.5003	1217.6419
1218.4118	1219.6684	1226.5493
1234.4915	1241.9737	1252.7587
1254.2380	1255.6987	1261.3369
1261.9771	1277.3284	1277.4529
1287.4443	1291.3698	1309.4398
1315.4615	1320.9179	1321.7759
1327.1560	1334.6242	1336.4212
1337.7048	1341.6866	1347.1380
1349.4603	1356.2137	1358.6280
1360.2190	1363.0801	1369.2911
1372.1070	1375.1217	1376.4103
1380.2281	1388.7997	1390.0690
1395.9103	1416.8627	1421.3508
1423.1644	1431.9853	1447.2766
1458.6567	1468.1258	1469.7917

1483.0964	1484.5725	1486.0560
1492.5397	1495.0848	1495.7494
1497.5641	1502.9593	1503.9365
1504.7227	1505.1323	1507.1069
1510.5794	1512.3036	1513.6669
1518.1710	1528.9896	1530.3510
1538.6932	1542.5423	1551.2247
1552.5517	1558.2251	1579.2025
1642.9675	1659.2702	1665.2754
1667.3414	1674.8767	1681.8879
1683.5550	1689.5800	1689.9385
1694.1804	1698.3012	1699.6259
1712.8922	1719.9457	1741.7835
1755.5601	2386.6269	3047.8084
3054.6253	3062.6737	3071.1809
3071.9341	3076.0737	3087.9218
3127.1876	3129.2214	3129.9816
3136.5929	3138.9992	3142.6903
3144.2552	3147.5492	3147.8241
3162.7025	3165.0155	3165.7145
3174.4893	3177.4845	3180.6228
3193.1012	3195.9767	3197.8693
3203.6640	3208.1926	3208.6303
3209.3830	3211.6185	3214.6930
3217.0330	3217.3997	3217.8840
3221.9844	3222.4028	3224.5611
3226.7322	3227.6657	3233.1838
3234.4119	3235.8731	3240.4024
3243.1793	3243.2294	3252.0415
3255.0535	3258.5511	3266.3713

^{os}TS3

Zero-point correction=0.923437

Thermal correction to Energy=0.980861

Thermal correction to Enthalpy=0.981805

Thermal correction to Gibbs Free Energy=0.827084

Sum of electronic and zero-point Energies=-3554.854888

Sum of electronic and thermal Energies=-3554.797463

Sum of electronic and thermal Enthalpies=-3554.796519

Sum of electronic and thermal Free Energies=-3554.951241

Cartesian coordinate

C	-4.54497300	0.32683600	-0.28067400
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C	-3.27228300	0.22338200	-0.71678000
C	-2.39664300	-0.80942300	-0.17882700
O	-2.84267500	-1.62888500	0.73966100
H	-4.88339100	-0.39403000	0.45831100
C	-5.53797700	1.32568600	-0.67307200
C	-6.76805400	1.31907200	0.00556800
C	-5.32201200	2.30825300	-1.65310100
C	-7.74969000	2.25950300	-0.28550500
H	-6.92715100	0.57149600	0.77968600
C	-6.30617700	3.24356200	-1.94518200
H	-4.37651600	2.34277200	-2.18768700
C	-7.52419300	3.22477200	-1.26430200
H	-8.69167700	2.23959500	0.25401500
H	-6.12426600	3.99533900	-2.70718300
H	-8.28851700	3.96051500	-1.49362200
H	-2.90254400	0.86982400	-1.50451200
C	-1.41685900	-5.65960200	-1.04434400
C	-1.86184800	-4.34550100	-0.92180300
C	-3.00868900	-3.90484800	-1.57664800
C	-3.68758600	-4.80538500	-2.39407100
C	-3.23492000	-6.11918200	-2.53688700
C	-2.10182300	-6.55894100	-1.85649000
C	-0.20344600	-5.90680400	-0.18247900
C	0.24094700	-4.50787700	0.30381200
C	-0.96827800	-3.54955300	0.00417500
H	-3.37248500	-2.89207600	-1.43272100
H	-4.58281200	-4.48642800	-2.91792100
H	-3.77836300	-6.80672000	-3.17742200
H	-1.76015100	-7.58509900	-1.95721000
H	0.62043200	-6.39712900	-0.71119600
H	0.46808100	-4.50510100	1.37186600
H	-0.45965300	-6.54174100	0.67208700
H	-1.50410800	-3.27944700	0.91167400
N	-0.48777300	-2.30281400	-0.59590100
O	1.46123300	-4.09898200	-0.31121200
C	-1.14406200	-1.07575900	-0.74752300
C	0.50996000	-2.34496100	-1.52111200
N	-0.32680900	-0.39964400	-1.67091500
N	0.67164900	-1.23686800	-2.16106000
C	1.28267100	-3.61747200	-1.62998100
H	0.73728600	-4.34296900	-2.25057400
H	2.26372900	-3.44815200	-2.07443100
C	-0.26495800	0.94610300	-2.07385300
C	0.39613200	1.25316300	-3.27090600

C	-0.78067200	1.98759700	-1.29327000
C	0.58477900	2.57538400	-3.64925800
C	-0.58320200	3.30890800	-1.66807800
C	0.10921700	3.59858200	-2.83948100
H	1.10763700	2.81025200	-4.56979300
H	-0.96229200	4.11254100	-1.04636300
H	-1.31692100	1.76247600	-0.38137400
H	0.78300900	0.44971500	-3.88438300
Cl	0.38167600	5.26241200	-3.29589400
S	4.53681400	-0.56192900	1.89590700
O	4.84665100	-1.90379100	2.37276500
O	3.90091000	0.41050800	2.76807100
N	3.48862400	-0.65781600	0.53276900
N	2.15116800	-0.49005200	0.88083000
C	7.12282700	-0.64743600	1.02166600
H	7.13279200	-1.65999800	1.41138600
C	8.24284800	-0.08854000	0.41227900
H	9.15142800	-0.67613700	0.32242900
C	5.97352900	0.12558400	1.13037500
C	5.91175400	1.43427700	0.65045600
H	5.00153100	2.01845400	0.75348100
C	8.21583900	1.21671500	-0.08323800
C	7.03788300	1.96644900	0.04267000
H	7.00363200	2.98175600	-0.34244000
C	1.49441700	-1.49029800	1.55974200
H	2.02739500	-2.43203500	1.62393600
C	1.63608300	0.79808700	0.81962200
C	0.41391200	1.03059700	1.40820900
H	0.02023600	2.03832600	1.35821800
C	0.25467900	-1.27304900	2.08924200
H	-0.25697600	-2.08331500	2.59449100
C	-0.34609900	-0.00392500	1.96141100
H	-1.33296200	0.18155600	2.37155500
C	3.76798500	-1.73889200	-0.41086900
H	3.22106900	-1.51456000	-1.32890400
H	4.83934900	-1.72228400	-0.62118000
H	3.48408000	-2.72655400	-0.03096000
C	2.37936400	1.85517700	0.11557700
C	2.89679800	1.64525300	-1.16789900
C	2.51610800	3.11056300	0.71867200
C	3.54225900	2.67898700	-1.83495100
H	2.75708500	0.68230800	-1.65136800
C	3.17022100	4.14066000	0.04913500
H	2.13431600	3.26338500	1.72363000

C	3.68492300	3.92638200	-1.22774100
H	3.92554000	2.51453100	-2.83696000
H	3.28035200	5.10867100	0.52641100
H	4.18831300	4.73172100	-1.75272700
C	-4.69047700	0.00473900	2.96546400
O	-5.62879300	-0.67270500	2.57939300
O	-3.43280400	-0.23071000	2.65571900
H	-3.29238700	-0.92544300	1.84776600
C	-4.86616800	1.25529700	3.83011600
C	-4.37843800	2.45427200	3.00190300
H	-4.50715400	3.37917000	3.57411300
H	-3.32125700	2.34231400	2.74645800
H	-4.95033900	2.54237600	2.07145800
C	-6.34075200	1.42888400	4.18472200
H	-6.71938200	0.55419000	4.71971000
H	-6.47092500	2.31289600	4.81743400
H	-6.94316700	1.55444900	3.28069900
C	-4.01719900	1.12052100	5.10025500
H	-4.11016400	2.02669300	5.70797200
H	-4.34691100	0.27015200	5.70567400
H	-2.96379900	0.97537700	4.84880500
C	9.43035100	1.82509300	-0.73208000
H	9.17828000	2.25540600	-1.70513100
H	9.83197100	2.63216000	-0.11192300
H	10.21824100	1.08383000	-0.87607000

Variable frequencies

-697.2700	11.7503	15.1448
20.2047	23.1894	25.5231
27.3659	31.1147	33.9275
34.6026	41.2256	42.6492
47.6685	48.0491	51.5191
55.6801	61.7728	66.9713
72.0805	73.9836	78.7678
83.9261	87.6703	94.5810
102.0867	103.7626	117.3321
119.3807	129.1616	130.5772
135.5288	146.0169	151.2276
154.7352	163.1834	180.5367
185.6163	190.8430	200.5800
205.6767	208.5102	219.7917
226.9943	235.6766	242.0873
250.7482	263.6837	263.9615
269.5605	273.6302	275.5952

282.3700	288.0418	295.5848
303.8655	304.4830	310.9254
319.1500	323.5037	329.7752
338.4523	345.4626	354.7656
360.6128	364.0730	375.9597
380.4755	386.3347	387.4956
401.2273	415.3553	419.6101
421.2225	426.8576	440.4067
445.5295	448.1517	448.5134
465.2541	477.9903	484.3668
492.7567	498.8963	507.1423
513.3307	520.3320	525.2148
531.7602	542.6812	552.8699
561.1404	566.2983	577.3085
582.3064	587.9065	590.8193
600.3478	608.4767	618.0972
627.7735	630.6753	634.4944
642.3725	643.6216	644.5592
667.6429	674.2296	692.3747
708.7613	712.2473	715.4861
718.8368	722.0897	725.6968
726.7088	737.6094	755.2606
767.8087	775.3127	779.1426
785.0077	791.9821	795.7635
797.7117	809.2915	817.7722
830.0482	838.9782	840.5032
842.1318	855.3007	862.5394
871.8702	872.6701	875.0086
876.1625	878.8393	892.5719
894.9410	901.9965	904.7385
910.7592	939.3066	946.9607
952.2090	955.1349	958.3959
961.7874	968.8709	971.9359
976.3727	981.7194	991.2198
1001.8433	1004.4088	1004.9547
1008.5119	1011.5322	1014.3216
1016.0578	1016.1777	1016.6169
1022.0615	1025.2485	1027.0752
1031.3716	1034.1443	1043.4381
1050.5050	1053.3473	1054.9361
1055.0611	1057.8593	1064.6664
1068.8254	1070.6873	1072.6185
1074.7316	1083.5752	1104.4756
1106.7068	1118.8945	1120.3517

1122.2763	1124.2991	1138.3368
1141.3480	1146.3099	1148.3770
1151.9671	1172.8683	1176.7066
1179.1080	1183.0331	1184.4887
1185.1949	1186.5418	1188.7181
1200.9473	1205.0084	1209.5074
1211.8950	1216.0440	1223.6600
1235.1803	1240.2670	1249.2229
1253.9513	1254.0242	1256.6611
1256.9936	1269.2343	1277.6185
1278.4864	1290.6415	1295.2958
1310.0481	1313.0918	1320.0608
1321.4991	1325.2182	1327.8872
1332.2954	1336.5726	1341.5433
1350.6581	1351.8090	1359.3797
1360.2696	1363.2446	1371.2113
1373.4533	1374.7628	1376.9404
1380.5926	1382.2187	1394.2180
1398.7393	1401.0999	1419.8109
1420.3571	1422.2250	1436.6594
1454.4799	1457.0171	1461.2943
1472.2293	1482.3792	1484.3070
1486.4170	1494.0071	1495.3882
1498.6065	1499.6639	1501.7510
1503.0668	1504.7320	1505.4564
1506.3851	1509.4547	1513.6038
1516.6883	1518.7319	1529.6797
1534.3985	1535.7583	1539.3983
1548.3849	1553.9202	1556.3918
1561.1204	1578.1167	1661.4848
1661.6128	1668.0513	1669.0546
1683.2270	1685.8603	1687.4927
1691.1645	1692.6792	1696.9635
1699.6726	1701.1840	1733.2671
1777.2296	2051.7270	3051.1781
3058.0680	3062.8758	3066.7919
3072.0740	3073.3380	3086.2736
3129.1956	3131.4292	3136.2299
3140.7394	3142.4754	3143.3415
3146.2163	3154.1218	3156.7083
3163.2274	3176.4860	3178.4636
3183.5609	3186.7681	3191.2548
3195.8166	3196.6766	3203.1119
3208.3075	3209.1985	3210.5471

3211.6410	3215.8321	3215.9147
3221.6486	3222.7647	3224.2089
3225.4488	3225.9394	3226.2895
3226.7216	3230.7423	3231.0553
3232.2690	3237.3330	3239.6118
3245.7822	3248.0479	3248.4826
3253.7899	3262.1995	3270.4965

²R2

Zero-point correction=0.345326

Thermal correction to Energy=0.366841

Thermal correction to Enthalpy=0.367785

Thermal correction to Gibbs Free Energy=0.293109

Sum of electronic and zero-point Energies=-1392.692544

Sum of electronic and thermal Energies=-1392.671029

Sum of electronic and thermal Enthalpies=-1392.670085

Sum of electronic and thermal Free Energies=-1392.744761

Cartesian coordinate

S	0.06899600	-1.63964300	-0.51007400
O	0.08349500	-3.08879000	-0.32703200
O	0.70961200	-1.03504500	-1.66655500
N	0.76384700	-0.85359300	0.85095100
N	2.10724900	-0.51001100	0.69230100
C	-2.61511400	-2.00028200	-0.12405800
H	-2.36951300	-3.05276000	-0.02856100
C	-3.92487100	-1.54290000	-0.00883600
H	-4.72494500	-2.25262800	0.17959300
C	-1.60599900	-1.07694400	-0.36767900
C	-1.87046000	0.28670800	-0.49647000
H	-1.06482700	0.99069100	-0.68546700
C	-4.22462700	-0.18433600	-0.13003700
C	-3.18179200	0.72007800	-0.37151900
H	-3.40049900	1.78072800	-0.46095800
C	-5.64344900	0.30873500	-0.02371200
H	-5.69761200	1.22040700	0.57668300
H	-6.29370700	-0.44279300	0.42809700
H	-6.04198800	0.54529000	-1.01545400
C	3.03850000	-1.55700000	0.56733400
H	2.74064300	-2.49078100	1.02725500
C	2.37431500	0.72911200	0.06059400
C	3.57644100	0.89136000	-0.58831500
H	3.77599100	1.86689500	-1.02005200

C	4.22242900	-1.37324400	-0.07040500
H	4.91805200	-2.20391800	-0.11291800
C	4.53498600	-0.12772100	-0.66781800
H	5.47737700	0.02989600	-1.17468600
C	0.44017700	-1.47608100	2.13276700
H	0.79935800	-0.81466100	2.92209500
H	-0.64646400	-1.56022500	2.20592300
H	0.87968600	-2.47226500	2.25272100
C	1.35804000	1.78488400	0.15266100
C	0.63407700	2.01172700	1.33347700
C	1.07793000	2.57958900	-0.96748800
C	-0.34055500	2.99849900	1.38905500
H	0.84876100	1.40957500	2.21067400
C	0.10341600	3.57217900	-0.90822300
H	1.59949700	2.38205500	-1.89897400
C	-0.61468300	3.78176800	0.26677000
H	-0.88915600	3.16001500	2.31169700
H	-0.10836000	4.16909100	-1.78969900
H	-1.38133000	4.54878700	0.31056400

Variable frequencies

25.1953	29.0650	38.7133
62.2502	65.5521	72.4397
90.1869	101.3316	107.2561
140.7328	174.2607	186.7797
193.9908	229.2096	253.2115
267.9310	283.6621	307.1943
313.0881	328.5680	350.9527
376.8329	402.2375	417.1889
419.1100	439.9711	486.0333
493.8667	509.1563	536.3824
557.6261	569.2689	576.0181
623.8449	629.1659	643.0322
653.5342	662.9341	691.5953
703.3783	717.3502	721.9111
746.2817	758.3574	783.1406
820.1249	836.5743	841.4874
872.6628	876.9864	934.2456
948.4429	953.6573	989.9742
999.4185	1003.9137	1012.2898
1013.6368	1017.6089	1032.6911
1034.8181	1042.5017	1067.0244
1068.6655	1086.6533	1110.3743
1113.5192	1119.5271	1130.7731

1143.4409	1152.5257	1171.2882
1177.1222	1199.8000	1211.0672
1217.0567	1254.0374	1268.9653
1273.9546	1316.2909	1329.3950
1334.9860	1349.3503	1354.5738
1356.0293	1369.6875	1396.7440
1423.3015	1448.8254	1450.9946
1454.7511	1494.7580	1497.0460
1499.6130	1504.0088	1515.7823
1540.2645	1550.6798	1566.8357
1658.9701	1668.8290	1680.2098
1693.0034	1694.3893	3071.3791
3075.0294	3143.7153	3157.7488
3166.8848	3184.8889	3198.6330
3200.7198	3208.1789	3208.8099
3214.2222	3220.2339	3222.4431
3224.4998	3228.8776	3231.2735
3232.1787	3249.0865	3255.7047

²TS4

Zero-point correction=0.343433

Thermal correction to Energy=0.364986

Thermal correction to Enthalpy=0.365930

Thermal correction to Gibbs Free Energy=0.290231

Sum of electronic and zero-point Energies=-1392.678076

Sum of electronic and thermal Energies=-1392.656523

Sum of electronic and thermal Enthalpies=-1392.655579

Sum of electronic and thermal Free Energies=-1392.731278

Cartesian coordinate

S	-0.04820600	-1.61767300	-0.27061100
O	-0.07750000	-3.05673000	-0.00395500
O	0.62457300	-1.12991100	-1.46923400
N	0.58558600	-0.74952900	1.01089700
N	2.26845200	-0.43533900	0.81449900
C	-2.77264600	-1.92218600	-0.17253500
H	-2.56207100	-2.98488400	-0.11389400
C	-4.07696200	-1.43329900	-0.17167600
H	-4.90948300	-2.12855800	-0.11322900
C	-1.72135400	-1.01843400	-0.24827400
C	-1.94106700	0.35839900	-0.31127200
H	-1.09891800	1.04506200	-0.34690200
C	-4.33120700	-0.06248600	-0.24127000

C	-3.24719400	0.82378000	-0.30611000
H	-3.43273700	1.89370200	-0.34811800
C	3.01986000	-1.57283800	0.69498200
H	2.84001200	-2.33408100	1.44688900
C	2.46095500	0.58420800	-0.08588900
C	3.40983400	0.46067900	-1.09155000
H	3.57544500	1.30366300	-1.75360500
C	3.94368300	-1.73995200	-0.30918600
H	4.51429900	-2.66055300	-0.35460600
C	4.15337100	-0.70640100	-1.22914800
H	4.88505700	-0.80740000	-2.02169300
C	0.38279600	-1.35292400	2.31926700
H	0.87430100	-0.71152400	3.05327900
H	-0.69027000	-1.37387600	2.53735100
H	0.76773700	-2.37653500	2.39649300
C	1.60212200	1.77388400	0.06361700
C	1.14708500	2.17207900	1.32674000
C	1.18123100	2.48619900	-1.06464800
C	0.29658700	3.26141800	1.45841700
H	1.46471300	1.61042100	2.19988800
C	0.32935700	3.57943300	-0.93126800
H	1.48476300	2.15247300	-2.05201000
C	-0.11691900	3.96888600	0.32902400
H	-0.04874900	3.56004400	2.44302100
H	0.00189500	4.11642300	-1.81572600
H	-0.78689300	4.81652500	0.43208100
C	-5.74258500	0.46292400	-0.26518300
H	-5.83488800	1.36998400	0.33748400
H	-6.04016000	0.71665300	-1.28777900
H	-6.44926800	-0.27777800	0.11438300

Variable frequencies

-651.7624	18.9938	22.2593
35.6681	58.9717	65.6415
72.4722	82.0251	83.7194
117.8436	130.1788	163.2851
176.9670	183.9507	213.2020
239.9095	264.8683	268.6531
300.8155	311.5049	325.2316
354.1570	381.9524	411.7990
417.8932	418.5795	440.9791
486.6035	488.5927	500.5619
545.0591	558.7314	567.1727
585.7956	627.1161	637.0306

642.4648	659.6305	695.3932
715.0877	721.1094	738.0474
761.9283	767.8648	799.6425
831.2175	837.8878	870.1075
874.8040	877.2935	937.7651
949.3899	959.9268	984.8292
989.4317	1001.3901	1002.0932
1014.4002	1014.6712	1022.1864
1034.2214	1042.9476	1065.2938
1073.4575	1088.8170	1108.6682
1116.8145	1118.4528	1135.7567
1139.5486	1147.5479	1165.4426
1173.0164	1177.6058	1185.0097
1206.6447	1208.0952	1252.6924
1279.6011	1299.1779	1326.5087
1335.3440	1343.6521	1345.6651
1358.8174	1361.6768	1423.5120
1435.4577	1452.9255	1453.3221
1482.3425	1498.6725	1501.1668
1503.0648	1505.0363	1513.0152
1549.6469	1553.9167	1594.0220
1655.1057	1669.4228	1672.3132
1693.0950	1697.6063	3050.6244
3072.9243	3123.3940	3142.7899
3162.6928	3169.6282	3196.1170
3200.2746	3203.2645	3209.5922
3213.6626	3215.0825	3218.6056
3224.8818	3225.9499	3229.7786
3231.3187	3238.5385	3249.4785

Pyd

Zero-point correction=0.171616

Thermal correction to Energy=0.180303

Thermal correction to Enthalpy=0.181247

Thermal correction to Gibbs Free Energy=0.137066

Sum of electronic and zero-point Energies=-478.978417

Sum of electronic and thermal Energies=-478.969730

Sum of electronic and thermal Enthalpies=-478.968786

Sum of electronic and thermal Free Energies=-479.012968

Cartesian coordinate

N	1.36333200	-1.14935800	-0.25238800
C	2.69447500	-1.18972800	-0.26038500

H	3.14015500	-2.16048000	-0.46716700
C	0.76338100	0.02351800	-0.00207600
C	1.49590600	1.18619500	0.26793800
H	0.98656400	2.11147900	0.51148200
C	3.50470600	-0.08260600	-0.02545500
H	4.58434400	-0.17599900	-0.04940500
C	2.88315500	1.13005500	0.25071000
H	3.46932800	2.01910600	0.46093800
C	-0.72458800	0.02214200	-0.00535200
C	-1.41408100	-1.17170800	0.23262100
C	-1.45761200	1.18832800	-0.24809300
C	-2.80362100	-1.19406800	0.24484400
H	-0.84082100	-2.07550200	0.40711200
C	-2.84873500	1.16431500	-0.23963800
H	-0.94326800	2.11756300	-0.47304100
C	-3.52632200	-0.02580800	0.01126700
H	-3.32498400	-2.12624000	0.43824300
H	-3.40320600	2.07583200	-0.43867600
H	-4.61142300	-0.04407200	0.01894500

Variable frequencies

55.3954	97.7107	152.2187
254.3991	330.6363	397.1953
417.5807	419.9412	482.8059
567.2655	620.7928	632.6677
649.8538	715.4530	764.3670
773.1995	777.2685	829.5707
877.4674	921.1929	956.4216
1000.5241	1003.8063	1014.2327
1020.7493	1025.7219	1029.8435
1058.1949	1083.2166	1102.7896
1124.0947	1134.6121	1178.2690
1183.6279	1214.7370	1304.5668
1317.8893	1341.8974	1354.4744
1367.7303	1477.2105	1507.4395
1530.8374	1565.2573	1661.1741
1683.1164	1689.7305	1703.2953
3193.5111	3198.1916	3205.1156
3213.5114	3216.9477	3223.7350
3232.6686	3234.5246	3240.1810

²M4

Zero-point correction=0.428418

Thermal correction to Energy=0.454158
 Thermal correction to Enthalpy=0.455102
 Thermal correction to Gibbs Free Energy=0.369056
 Sum of electronic and zero-point Energies=-1815.381817
 Sum of electronic and thermal Energies=-1815.356078
 Sum of electronic and thermal Enthalpies=-1815.355133
 Sum of electronic and thermal Free Energies=-1815.441179

Cartesian coordinate

C	-1.68554900	2.13742800	-0.94048900
C	-1.00298100	1.08241600	-0.45817200
C	0.28768900	0.69095000	-1.02541300
O	0.90982500	1.39384600	-1.87088000
H	-1.22603900	2.69330500	-1.75578100
C	-2.99185000	2.60164000	-0.46839900
C	-3.45992000	3.86019200	-0.87161400
C	-3.81641600	1.82094400	0.35861600
C	-4.69601900	4.33542500	-0.44744400
H	-2.83810800	4.46931100	-1.52218100
C	-5.05039800	2.29540000	0.78257000
H	-3.49836700	0.82413800	0.65195200
C	-5.49543900	3.55636800	0.38515700
H	-5.03681700	5.31428800	-0.76976800
H	-5.67482000	1.67466300	1.41760600
H	-6.46185400	3.92296300	0.71560400
H	-1.38746200	0.51034100	0.38130500
C	4.63899000	0.90404100	0.85118800
C	3.53582300	1.19209600	0.04332700
C	2.80958100	2.36716700	0.23238800
C	3.19175800	3.22992700	1.25830700
C	4.28550800	2.93484000	2.07286500
C	5.02159200	1.77116000	1.86841500
C	5.29447900	-0.39112100	0.45933500
C	4.68518100	-0.68387300	-0.92794700
C	3.34183600	0.10790300	-1.00495500
H	1.97706400	2.60543400	-0.41951700
H	2.63618000	4.14845800	1.41781200
H	4.57157900	3.62244700	2.86269600
H	5.88501100	1.54551500	2.48759200
H	5.05683800	-1.17624500	1.18534900
H	5.34022300	-0.26958300	-1.69710200
H	6.38408400	-0.32468200	0.40909400
H	3.13680800	0.51438800	-1.99444400
N	2.23709100	-0.82014000	-0.69005500

O	4.56198200	-2.05419200	-1.25328100
C	0.89681900	-0.52651300	-0.57109900
C	2.40939000	-2.10232300	-0.25203900
N	0.35443200	-1.66542900	-0.03156000
N	1.30678600	-2.64427300	0.15775500
C	3.74116100	-2.77901000	-0.36764300
H	4.19995600	-2.90505300	0.62020100
H	3.59737400	-3.77061400	-0.80006900
C	-1.00957200	-2.03707800	0.10054100
C	-1.40899800	-2.69077500	1.26320700
C	-1.91884800	-1.78407200	-0.92655300
C	-2.73454700	-3.08031600	1.41330000
C	-3.24710100	-2.15846400	-0.77196300
C	-3.64290800	-2.80106100	0.39816000
H	-3.06323200	-3.58724000	2.31316100
H	-3.96928600	-1.96392500	-1.55639000
H	-1.59071100	-1.28964200	-1.83434000
H	-0.67945500	-2.88901200	2.04034000
Cl	-5.31159600	-3.27043000	0.59207700

Variable frequencies

14.7689	18.9252	25.6271
39.3537	43.0760	51.4413
60.4459	71.9658	91.9293
116.9891	132.3672	150.7559
175.1881	185.8431	204.4395
218.8535	226.4439	255.4715
260.5994	269.4046	290.0460
298.5226	334.5299	356.5729
357.4811	382.3202	410.0971
415.9311	424.1503	427.0368
453.6797	463.8988	478.5900
496.3378	501.7010	519.1102
534.6202	550.4934	576.5679
587.8541	604.4022	609.2784
632.4584	635.9283	648.8329
649.0853	676.7807	691.0340
713.1028	727.8509	730.4313
758.3990	772.8716	778.7104
787.0681	821.2466	844.6481
847.5852	852.2836	859.2270
870.0496	882.0993	891.1854
899.5511	908.0602	921.3210
946.2515	977.5076	987.0544

992.0817	998.2099	1008.5430
1012.4216	1014.9436	1018.2067
1024.3394	1033.9158	1037.3684
1044.6871	1056.0784	1073.4677
1075.3682	1095.2182	1122.8435
1123.9130	1131.0439	1135.2389
1140.0609	1157.3162	1174.9278
1183.4570	1187.7248	1196.9958
1200.0947	1204.0484	1213.6381
1233.6280	1238.6485	1242.6063
1258.8433	1284.9827	1302.1169
1312.2473	1320.7762	1327.5713
1333.6326	1341.2911	1342.7118
1346.3491	1353.5521	1364.3127
1371.1254	1375.8031	1386.9374
1421.1865	1445.8328	1470.0947
1490.5003	1491.9419	1499.2190
1505.3115	1519.9250	1524.1704
1538.2659	1555.3517	1559.2403
1627.0009	1664.1188	1674.3467
1680.1303	1685.3650	1694.4974
1697.8657	1702.5747	1703.9408
3080.0586	3095.6234	3132.3063
3144.6954	3171.0494	3183.4737
3193.0515	3196.6399	3197.3172
3204.0138	3205.6373	3210.9777
3218.7011	3220.1621	3225.7582
3229.3691	3232.6245	3238.4417
3241.0217	3244.7118	3246.1752

²TS5R

Zero-point correction=0.778664

Thermal correction to Energy=0.826393

Thermal correction to Enthalpy=0.827337

Thermal correction to Gibbs Free Energy=0.691980

Sum of electronic and zero-point Energies=-3207.941420

Sum of electronic and thermal Energies=-3207.893691

Sum of electronic and thermal Enthalpies=-3207.892747

Sum of electronic and thermal Free Energies=-3208.028104

Cartesian coordinate

N	0.16065300	-2.88888900	-0.81176900
N	1.21617800	-3.05730400	0.07608200

C	1.42868400	-4.42779300	0.55740800
C	-1.10630900	-3.34290200	-0.47959400
C	-2.17017700	-3.08469700	-1.26439800
C	-2.04541700	-2.16621500	-2.38315700
C	-0.68278500	-1.87663300	-2.77742500
C	0.38412800	-2.18753900	-1.99227700
C	-2.90488900	-0.51833100	-1.86464000
C	-2.22316500	0.03281600	-0.75434600
C	-1.16341500	0.93655500	-0.93102900
O	-0.60073100	1.23436000	-2.00408300
S	1.22476500	-1.85308200	1.30070400
O	0.91961100	-0.61463500	0.59075500
C	2.92633300	-1.89855200	1.75584000
O	0.39524600	-2.25537100	2.42927200
C	3.27616200	-2.19177400	3.06720300
C	4.62770200	-2.20944400	3.40180500
C	5.61116000	-1.94594400	2.44590300
C	5.21929700	-1.65858700	1.12925300
C	3.88070000	-1.63051800	0.77258700
H	1.42925700	-5.08539100	-0.31254900
H	2.41060700	-4.46713600	1.03229200
H	0.67107300	-4.75612900	1.27587400
H	-3.13564200	-3.50298600	-1.00560500
H	-2.74876100	-2.31817200	-3.20058900
H	-0.48901000	-1.37609700	-3.71902900
H	-2.69644400	0.00891600	-2.79707200
H	2.50568600	-2.40137400	3.80170700
H	4.92093700	-2.43575300	4.42203900
H	5.97674100	-1.46124300	0.37557500
H	3.57328300	-1.41535300	-0.24810900
C	-4.33212000	-0.92462900	-1.70987900
C	-4.89636000	-1.25237900	-0.47054300
C	-5.14184500	-0.98946000	-2.84992500
C	-6.23439700	-1.62250400	-0.37654300
H	-4.29921500	-1.21417300	0.43638300
C	-6.47930800	-1.35979000	-2.75706300
H	-4.71797900	-0.73210600	-3.81812700
C	-7.03107600	-1.67683400	-1.51844700
H	-6.65648500	-1.86308100	0.59408200
H	-7.09171700	-1.39404500	-3.65212400
H	-8.07505900	-1.96168900	-1.44238400
H	-2.50249200	-0.24396800	0.25441000
C	3.26601600	3.79337300	-0.97687500
C	1.97684200	3.30209400	-1.16921600

C	1.07813800	3.93114500	-2.02622900
C	1.49333000	5.08345100	-2.68705800
C	2.78389600	5.58448600	-2.49707400
C	3.67964700	4.94234000	-1.64625300
C	4.05090200	2.92780000	-0.02531800
C	3.03306500	1.91311400	0.54637300
C	1.74889000	2.04994400	-0.35506000
H	0.08748700	3.51529300	-2.17952400
H	0.81216900	5.59453100	-3.35926200
H	3.09128500	6.48399500	-3.02059200
H	4.68168700	5.33522500	-1.50332800
H	4.51466200	3.49091500	0.79098200
H	3.39993900	0.88907300	0.48363200
H	4.85667200	2.40173500	-0.54787000
H	1.61802300	1.15896700	-0.96685000
N	0.54776500	2.15265600	0.48205400
O	2.79414300	2.10784800	1.93121700
C	-0.68870200	1.67115900	0.29788000
C	0.57998700	2.73337900	1.71591500
N	-1.36590700	2.01485000	1.40087900
N	-0.57865700	2.66033600	2.30542000
C	1.91135000	3.17258200	2.22666100
H	2.22365800	4.11388000	1.75395200
H	1.87845000	3.30256700	3.30784000
C	-2.74261300	1.76541200	1.71992500
C	-3.74235700	2.20044100	0.85651100
C	-3.02708400	1.05398500	2.87841900
C	-5.06381400	1.88606000	1.14513600
C	-4.35231800	0.75390600	3.17544200
C	-5.35444900	1.16262300	2.30010300
H	-5.86290200	2.19555800	0.48197500
H	-4.60517600	0.19780800	4.07039800
H	-2.22053900	0.73135800	3.52766600
H	-3.49106700	2.76070000	-0.03738800
Cl	-7.00592200	0.75507600	2.64998900
H	-1.15950600	-3.94407400	0.41953100
C	1.77572600	-1.84864600	-2.37269900
C	2.79438200	-2.80833600	-2.37782400
C	2.06261700	-0.53864100	-2.76658600
C	4.08698000	-2.45322800	-2.74550000
H	2.57283500	-3.83421000	-2.10085700
C	3.36491400	-0.18004300	-3.11153100
H	1.25877200	0.19366200	-2.78756100
C	4.37905300	-1.13430900	-3.09628300

H	4.86909000	-3.20529700	-2.75594400
H	3.57948800	0.84475000	-3.39960800
H	5.39166000	-0.85817700	-3.37200300
C	7.07126000	-1.96608200	2.80815400
H	7.61953500	-2.66461500	2.17003500
H	7.51564600	-0.97674100	2.66637200
H	7.22002900	-2.26038000	3.84811400

Variable frequencies

-250.6379	11.2310	15.3080
16.9308	20.8077	24.6332
27.9683	33.0296	37.0383
40.4422	45.5013	49.4374
57.3830	59.8282	64.9450
70.1664	73.9618	78.8108
82.8093	86.5703	95.6228
107.6475	114.9635	119.5292
136.3088	139.7770	146.3601
153.5604	169.3436	178.9685
184.7843	198.2233	199.0363
213.0339	220.1155	223.1746
232.4133	247.2286	256.1250
263.6447	271.9691	276.0684
289.1996	307.3347	310.8436
315.3852	331.5285	345.1417
356.5636	358.4385	364.7210
371.8740	388.8088	404.1412
412.3669	417.5191	418.4428
421.6785	423.9160	426.2728
441.9723	448.3664	453.6439
477.5866	486.2986	488.4664
498.1780	500.1669	518.0422
526.8618	529.3399	533.9653
554.9871	566.4765	574.9392
583.4168	593.6550	598.3803
601.2658	604.9560	623.9306
625.5107	631.3035	633.7363
641.2107	649.7799	664.1891
672.5246	683.0942	710.5050
712.8765	719.8402	720.8872
722.3842	725.4407	730.6007
732.3198	755.6291	762.7827
769.0444	774.6567	780.2519
785.0375	793.2673	798.5863

820.7399	824.8523	828.6671
837.1933	844.6025	849.8141
854.8469	866.5798	871.4978
874.7139	877.4304	878.1183
881.0322	886.1063	897.2040
911.2235	921.3542	948.3550
952.2166	959.3530	972.3646
974.1303	984.3917	995.2618
996.1678	1002.3184	1004.5412
1010.5671	1013.4371	1013.7596
1015.9139	1016.5861	1025.1770
1027.9615	1028.3111	1033.2489
1034.9918	1039.4236	1043.7659
1059.1905	1061.4327	1063.2853
1068.2914	1068.6575	1071.9766
1078.4329	1083.2291	1100.7617
1115.9666	1119.1307	1121.1464
1121.9881	1122.9128	1131.7901
1140.1241	1146.3456	1147.7584
1151.4551	1158.3997	1162.6711
1171.9670	1177.7568	1179.3330
1180.8910	1181.8410	1187.4648
1198.1051	1200.3858	1206.1209
1209.6278	1213.2710	1214.2876
1216.5787	1232.8380	1238.7212
1250.4670	1252.5999	1271.3898
1277.6403	1282.6018	1290.9775
1297.5283	1307.6774	1310.5883
1319.2923	1323.3656	1324.8776
1331.9947	1333.1646	1339.6952
1342.1974	1344.8262	1349.9500
1358.5439	1360.3444	1362.7943
1368.6961	1370.2615	1373.4059
1381.8146	1383.1481	1418.4633
1426.1462	1451.9325	1454.5125
1456.0538	1462.5473	1473.9984
1489.1978	1489.7738	1494.9811
1498.9896	1501.4761	1503.3559
1506.2087	1506.5255	1517.4921
1527.9509	1534.9423	1538.8055
1542.0573	1546.9739	1549.8075
1550.3727	1577.7383	1584.9945
1624.6164	1643.1718	1666.2921
1668.5374	1673.8045	1679.5635

1683.0346	1683.4699	1686.7726
1693.0908	1694.4882	1695.7973
1701.7691	1720.7783	3077.1399
3077.2113	3080.3347	3090.5945
3132.9028	3149.2111	3151.1554
3162.0764	3166.5946	3170.8801
3170.9258	3182.7283	3189.4089
3192.8350	3195.2325	3202.9400
3203.3847	3207.9584	3208.1541
3210.5407	3217.1699	3217.7384
3218.8874	3221.6508	3223.0353
3224.3303	3227.1380	3228.7924
3232.4423	3234.1493	3234.9371
3237.1599	3237.3622	3238.2913
3241.0849	3242.5758	3249.2347
3253.3163	3255.8924	3274.7930

²TS5R^b

Zero-point correction=0.778512

Thermal correction to Energy=0.825968

Thermal correction to Enthalpy=0.826913

Thermal correction to Gibbs Free Energy=0.694871

Sum of electronic and zero-point Energies=-3207.928667

Sum of electronic and thermal Energies=-3207.881211

Sum of electronic and thermal Enthalpies=-3207.880267

Sum of electronic and thermal Free Energies=-3208.012309

Cartesian coordinate

C	-5.39325700	-1.99696600	1.92128300
C	-5.28476400	-1.64255600	0.57295200
C	-4.63636300	-2.46349400	-0.34469700
C	-4.04827000	-3.63816400	0.12083300
C	-4.13418500	-3.98448500	1.47025400
C	-4.81701100	-3.17589900	2.37839100
C	-6.18635600	-0.96814500	2.68971400
C	-6.92636800	-0.22716900	1.55469600
C	-5.97364100	-0.32185400	0.33820200
H	-4.58653400	-2.19254100	-1.39563500
H	-3.51831600	-4.28637800	-0.56923200
H	-3.67362400	-4.90477900	1.81440000
H	-4.90085600	-3.46665100	3.42088100
H	-5.51457700	-0.29850000	3.24101500
H	-7.82659500	-0.78753200	1.29401900

H	-6.88103700	-1.39948400	3.41280900
H	-6.47691800	-0.22132000	-0.62520600
N	-5.02893700	0.82726700	0.45081000
O	-7.36913400	1.08595100	1.81759500
C	-3.88986600	1.03122800	-0.22405200
C	-5.19417000	1.90500300	1.28403700
N	-3.41977800	2.20002400	0.19995800
N	-4.21768500	2.75915100	1.14946500
C	-6.36713300	1.99133600	2.21382900
H	-6.03032600	1.81215000	3.24285300
H	-6.79608800	2.99355400	2.16541700
C	-1.44787700	-1.39070200	-1.85239600
C	-2.16059900	-0.59244800	-0.90982400
C	-3.27934700	0.15986400	-1.30080200
O	-3.84653800	0.18622100	-2.40763900
H	-1.81447600	-0.51883400	0.11879500
C	-2.27268800	2.88168800	-0.32526400
C	-2.20193100	3.08326600	-1.70162200
C	-1.26531700	3.29882000	0.53642400
C	-1.07933400	3.70666000	-2.23075900
H	-3.00726800	2.74554400	-2.34660500
C	-0.14130600	3.92153600	0.00315400
H	-1.34798900	3.12329400	1.60363200
C	-0.06043200	4.11663600	-1.37340500
H	-0.99390500	3.87484500	-3.29785700
H	0.67700600	4.22926000	0.64624700
Cl	1.34807100	4.88057900	-2.04198200
S	3.97064300	-1.68858100	0.04285900
O	4.30643600	-2.95510700	-0.59504800
O	2.75418600	-1.55395800	0.82962200
N	3.85478500	-0.44106100	-1.14190900
N	2.57254000	-0.33647900	-1.66714400
C	6.54488600	-1.82352900	0.94290800
H	6.61224100	-2.73922300	0.36458600
C	7.62230500	-1.34548000	1.68239300
H	8.55615400	-1.89893100	1.68489700
C	5.35716000	-1.10236900	0.96383100
C	5.21416400	0.07552600	1.69739500
H	4.26862500	0.61195100	1.70042200
C	7.51887700	-0.16590300	2.42364600
C	6.30390900	0.53430300	2.42107200
H	6.21434100	1.44972500	2.99938800
C	8.69284900	0.36203800	3.20317000
H	8.37863100	0.72525400	4.18456600

H	9.15608900	1.20146100	2.67495600
H	9.45436500	-0.40661000	3.34524100
C	2.13604100	-1.16961000	-2.67845900
H	2.88169400	-1.84708400	-3.07604800
C	1.68979200	0.55486300	-1.07233500
C	0.40909900	0.60936200	-1.50596500
H	-0.24190500	1.32912700	-1.02431300
C	0.87920600	-1.09804500	-3.17083200
H	0.61512800	-1.74169100	-4.00210900
C	-0.13797900	-0.25930200	-2.54579700
C	4.93982500	-0.41880700	-2.12712000
H	5.87966300	-0.31135700	-1.58273800
H	4.98615800	-1.32445400	-2.74017300
H	4.79462900	0.45828500	-2.75914600
C	2.17873700	1.44139200	0.01468200
C	3.16282400	2.40559900	-0.21736500
C	1.59599500	1.34013900	1.28023200
C	3.55145200	3.26598300	0.80548300
H	3.61367600	2.48842500	-1.20184200
C	1.99403300	2.19265700	2.30706400
H	0.84652600	0.57403200	1.45699900
C	2.97088500	3.15908600	2.06978100
H	4.30825400	4.02008100	0.61664400
H	1.54841400	2.09732600	3.29193400
H	3.28154600	3.82566100	2.86786800
C	-0.77675800	-2.63365000	-1.37436100
C	0.09849300	-2.63213500	-0.28647900
C	-0.99357600	-3.82632800	-2.07089500
C	0.73607600	-3.80518800	0.10449200
H	0.31959900	-1.70762400	0.24047600
C	-0.37044200	-5.00470000	-1.66856800
H	-1.65896600	-3.82987900	-2.93097900
C	0.49647600	-4.99567700	-0.57909700
H	1.43444700	-3.77658900	0.93356600
H	-0.55437300	-5.92534900	-2.21320600
H	0.99497400	-5.90903400	-0.27159800
H	-2.02583900	-1.55402200	-2.76447300
H	-0.83082300	0.24188700	-3.22593900

Variable frequencies

-232.9392	14.3372	21.8776
23.3678	28.9183	32.6072
36.7811	43.1355	45.1868
51.4144	52.8108	57.4893

64.2496	68.6342	74.6481
75.4582	84.5756	90.2816
91.2254	96.3379	100.1583
104.2460	110.9278	117.3150
131.2446	145.0401	149.4943
154.8340	171.2658	180.8512
186.0076	189.9419	209.6195
212.7835	219.0772	230.2425
239.1504	251.5899	254.7879
261.1442	271.9129	280.8223
287.3914	309.2020	311.6389
314.9592	328.3401	338.6017
343.1985	351.0690	354.0152
366.3975	382.9072	385.3191
405.7395	415.9140	416.8350
422.0137	425.9280	427.4821
444.5211	451.0562	460.8445
468.1492	484.3632	487.6114
496.0746	497.7158	524.7820
534.7491	538.7338	539.8968
555.0197	563.2591	569.7195
573.0160	583.1767	589.3913
604.4143	614.3692	620.0646
628.2113	637.8647	640.2714
641.8889	644.4217	653.1794
665.5825	685.5791	691.2714
708.4556	713.9442	720.5670
721.9088	723.7241	727.5449
731.5944	751.7429	760.3911
768.2109	777.6455	782.4520
788.1833	795.1831	803.9394
809.3344	820.9634	828.7454
835.9685	844.2098	846.4715
851.4913	854.7991	870.6393
870.8120	881.8417	885.4244
886.8073	893.1759	900.5273
911.4288	917.3672	947.7917
951.0352	960.0052	971.8326
984.6882	985.5480	987.9669
1006.2011	1006.5149	1007.4615
1007.8442	1008.6747	1016.6944
1017.2821	1021.2970	1026.3700
1027.9522	1031.7780	1032.1311
1034.4993	1035.2051	1044.0901

1054.5862	1065.0283	1066.3025
1068.8598	1071.4694	1075.1367
1085.3348	1098.8749	1103.1464
1114.3797	1119.1053	1122.1158
1129.3589	1134.3120	1135.4379
1139.3224	1143.3673	1145.8512
1153.9416	1163.1009	1169.0332
1179.7132	1180.9355	1182.1672
1183.3219	1186.3314	1187.7265
1201.1153	1201.9732	1205.3360
1209.1172	1209.9753	1211.4643
1218.7100	1230.1594	1243.5985
1250.1934	1254.9791	1255.6103
1267.1072	1279.6831	1297.4816
1305.5644	1310.5336	1314.1139
1319.3285	1322.2179	1325.9097
1328.5912	1338.4609	1344.1549
1346.7495	1356.0344	1358.1269
1358.7634	1360.2392	1361.8308
1370.4554	1373.9421	1376.6374
1377.9540	1385.3153	1422.5098
1428.5530	1448.5208	1449.1365
1454.6587	1459.4310	1464.9671
1484.1719	1493.7911	1494.2937
1497.8295	1498.3063	1500.7736
1505.6558	1508.4477	1520.1765
1522.1790	1524.9454	1535.8018
1539.9606	1547.7360	1548.5399
1550.4735	1567.7116	1593.0002
1643.6873	1644.4906	1665.1534
1667.2152	1669.8332	1678.5490
1678.9505	1681.0994	1686.6965
1690.6603	1695.2077	1696.8286
1703.3348	1728.7948	3073.0476
3077.2376	3078.3160	3086.4396
3113.6646	3138.7437	3147.0447
3147.2946	3157.8000	3161.6576
3164.8359	3169.8514	3181.8805
3188.3816	3193.8701	3196.5611
3204.7245	3205.6502	3206.7936
3209.1997	3209.7363	3212.2084
3214.5398	3217.0915	3221.3179
3221.5077	3221.7071	3222.3142
3223.6012	3225.4579	3230.3512

3234.3465	3235.0391	3235.5260
3236.5152	3236.5912	3240.0774
3245.4449	3252.2262	3266.7356

²TS5R^c

Zero-point correction=0.779158
 Thermal correction to Energy=0.826612
 Thermal correction to Enthalpy=0.827556
 Thermal correction to Gibbs Free Energy=0.693779
 Sum of electronic and zero-point Energies=-3207.931682
 Sum of electronic and thermal Energies=-3207.884228
 Sum of electronic and thermal Enthalpies=-3207.883284
 Sum of electronic and thermal Free Energies=-3208.017061

Cartesian coordinate

N	2.10668700	1.38046200	-1.73997700
N	3.14838000	0.47866700	-1.91926500
C	3.55610500	0.22932900	-3.30381400
C	0.90222000	1.20121900	-2.39496800
C	-0.21915700	1.80756000	-1.95675200
C	-0.21352100	2.46526500	-0.65528000
C	1.11481600	2.93713200	-0.26428200
C	2.23789600	2.33550900	-0.73073700
C	-0.62978600	1.16527400	0.58888900
C	-1.92653500	0.62118800	0.33333600
C	-2.09974300	-0.39022200	-0.62243300
O	-1.26345000	-0.84731800	-1.42685500
S	2.94648000	-0.94458400	-0.96606200
O	2.32206700	-0.47481500	0.26639800
C	4.63654000	-1.36382800	-0.68016300
O	2.30837300	-1.99414100	-1.74982800
C	5.13432100	-2.55402700	-1.19678100
C	6.46919500	-2.87064800	-0.96228100
C	7.29484900	-2.01210200	-0.23271300
C	6.75717200	-0.81903700	0.27176400
C	5.42983900	-0.48314600	0.05677700
C	8.74452000	-2.34341800	-0.00147300
H	3.69899300	1.19672900	-3.78701700
H	4.51192200	-0.29789000	-3.27723200
H	2.83454700	-0.37197700	-3.86574700
H	-1.13837400	1.67930600	-2.51376000
H	-1.02111000	3.17297900	-0.47617400
H	1.21611800	3.72055400	0.47733600

H	0.17331400	0.47219500	0.32544200
H	4.48456700	-3.21153400	-1.76463500
H	6.87416000	-3.79898200	-1.35289600
H	7.38995700	-0.14533000	0.84265500
H	5.01588700	0.44074800	0.45193500
H	8.95724400	-3.38736600	-0.23729100
H	9.38423400	-1.71743200	-0.63129200
H	9.02639700	-2.15776500	1.03792900
C	-0.42682700	1.81547300	1.91827400
C	-1.31820900	2.77201700	2.41289100
C	0.70729400	1.48928800	2.66697000
C	-1.08442800	3.38588600	3.63947300
H	-2.19658700	3.04626300	1.83200400
C	0.93855300	2.10117300	3.89696400
H	1.40559600	0.75440800	2.27258700
C	0.04487000	3.05140400	4.38502200
H	-1.78172800	4.12858500	4.01325500
H	1.81862500	1.83466500	4.47417300
H	0.22600500	3.53036700	5.34150300
H	-2.78583300	0.95155000	0.91082000
C	-2.02015800	-3.95192400	1.86508500
C	-1.53037100	-3.23163900	0.76966700
C	-0.34481700	-2.50547000	0.85764900
C	0.31345700	-2.46123600	2.08483000
C	-0.19506600	-3.14446500	3.19028900
C	-1.35740800	-3.90732200	3.08563300
C	-3.24528800	-4.74691500	1.48630900
C	-3.11140800	-4.80270900	-0.05107500
C	-2.41905100	-3.47031200	-0.43060100
H	0.06776700	-1.99348400	-0.00572900
H	1.23928200	-1.90040100	2.16273500
H	0.33286800	-3.10128400	4.13761300
H	-1.72817200	-4.46886300	3.93768700
H	-4.15765100	-4.22199100	1.79636600
H	-2.41995100	-5.60467900	-0.31815800
H	-3.27545600	-5.74399100	1.93012400
H	-1.90264300	-3.49008700	-1.39050700
N	-3.51529300	-2.45758500	-0.55050300
O	-4.28385900	-5.05706400	-0.79335200
C	-3.41523600	-1.11894100	-0.60520200
C	-4.85305000	-2.75433700	-0.57847100
N	-4.66449000	-0.66211600	-0.66110800
N	-5.57683800	-1.67188800	-0.64023700
C	-5.34499500	-4.17005400	-0.54000500

H	-5.82678600	-4.36434700	0.42630600
H	-6.08806100	-4.31494700	-1.32602600
C	-5.09296900	0.70034200	-0.75786600
C	-6.10956700	1.13779300	0.08208100
C	-4.48560800	1.54349700	-1.68278800
C	-6.51880900	2.46343500	0.00788800
C	-4.88866200	2.87099700	-1.74784500
C	-5.89806300	3.31887200	-0.89835700
H	-7.30746600	2.83381200	0.65204800
H	-4.43898100	3.55106500	-2.46171900
H	-3.72442300	1.16212300	-2.35571500
H	-6.56999900	0.44914200	0.78152100
Cl	-6.39851400	4.97907400	-0.97770700
H	0.93063600	0.55764000	-3.26515500
C	3.59617600	2.65153200	-0.23551300
C	4.67719900	2.81594700	-1.10987800
C	3.80179300	2.78414500	1.14033500
C	5.94340400	3.09550800	-0.61350300
H	4.52169800	2.72844300	-2.18056100
C	5.07347100	3.06423500	1.63623000
H	2.96661900	2.64317100	1.81977300
C	6.14629700	3.21333200	0.76221500
H	6.77400200	3.22329700	-1.29957700
H	5.22449300	3.15810100	2.70656700
H	7.13766400	3.42659900	1.14877500

Variable frequencies

-168.8841	12.1921	14.3803
21.0365	22.6775	26.5849
29.6208	34.3014	38.8755
49.9418	55.8335	56.6687
59.8979	61.8703	65.8739
71.1897	75.4010	78.0491
82.9777	93.0246	98.9058
105.5061	113.0235	127.1609
142.2373	145.7898	156.1125
173.7103	181.2485	188.8302
197.3303	205.4379	217.5137
219.0250	224.9195	232.6413
238.3090	250.4339	256.2353
262.2089	276.8861	282.1174
292.3572	296.3716	310.1548
312.7962	319.8377	339.8800
346.7627	350.4169	364.2806

368.7261	386.9776	390.3426
400.5009	416.4771	417.8431
425.2714	425.4832	434.4473
443.8911	452.4566	461.3415
462.0446	481.8590	494.7621
497.0530	500.1229	515.7650
529.4038	542.3193	545.5091
550.3484	559.6480	567.3115
578.0851	584.8615	592.1677
605.9748	607.8665	623.2476
627.9951	632.9929	635.4923
642.5820	642.9540	654.8233
666.9911	681.0323	686.7188
708.4335	714.2781	717.8449
725.6354	728.7175	729.1901
731.3180	756.1573	757.6217
767.4456	782.8201	786.0646
788.2780	791.7399	798.1830
810.2272	822.4749	828.6452
840.1069	843.5632	846.7450
854.7603	856.8694	867.4970
873.5375	878.7609	886.9165
888.6540	893.0781	900.5288
917.3789	920.8694	952.7905
957.6495	966.2480	983.2353
987.4297	988.5335	992.0625
1000.4452	1005.2173	1006.8334
1007.1235	1013.9526	1015.4721
1015.8804	1017.6680	1028.5140
1028.7984	1032.8682	1034.1523
1036.3583	1040.9980	1043.5651
1059.7539	1068.0252	1068.6263
1072.5420	1073.8830	1077.3276
1090.4107	1095.9563	1113.9010
1118.6818	1119.8098	1123.8057
1129.9103	1135.8596	1137.3293
1142.3898	1148.7236	1150.0713
1156.5677	1160.6378	1165.6545
1172.9444	1177.8304	1180.7905
1183.1605	1185.3672	1189.6596
1203.5355	1204.9094	1207.2913
1207.4241	1211.8572	1215.4763
1218.1996	1227.4270	1234.6780
1246.0966	1256.4437	1257.5095

1265.3487	1282.4932	1288.2576
1299.8914	1308.8683	1314.0696
1320.6781	1321.3185	1326.7617
1335.4040	1337.9611	1341.0694
1344.4585	1351.2647	1354.9210
1361.3664	1362.0472	1366.9970
1369.2897	1369.9289	1376.1827
1378.4093	1385.2850	1423.5402
1425.5390	1443.7463	1453.0820
1456.0316	1458.5222	1467.9104
1481.2965	1491.6617	1497.0118
1499.5682	1500.9125	1504.4558
1506.6275	1512.7353	1518.3701
1520.7203	1522.6123	1532.9387
1544.4151	1548.8880	1551.8612
1552.9391	1567.1744	1594.8765
1624.3362	1639.7731	1665.9404
1667.8327	1671.6034	1678.3266
1678.7799	1687.0297	1689.7630
1690.7997	1696.9180	1698.5357
1701.0323	1719.1767	3074.1774
3076.9396	3081.3911	3087.9486
3140.2609	3142.7053	3152.8214
3153.1248	3161.8769	3165.3240
3165.8508	3171.7510	3178.5671
3192.8905	3199.2525	3203.2494
3204.8865	3209.8444	3210.8548
3211.2365	3214.4889	3215.4917
3216.4946	3221.5062	3223.8545
3225.5146	3227.4135	3231.2582
3232.1619	3232.3960	3235.4904
3235.5217	3236.7033	3241.1148
3242.3376	3244.6220	3250.4312
3251.8272	3254.1261	3270.3703

²TS5R^d

Zero-point correction=0.778749

Thermal correction to Energy=0.826215

Thermal correction to Enthalpy=0.827159

Thermal correction to Gibbs Free Energy=0.693115

Sum of electronic and zero-point Energies=-3207.923273

Sum of electronic and thermal Energies=-3207.875807

Sum of electronic and thermal Enthalpies=-3207.874863

Sum of electronic and thermal Free Energies=-3208.008907

Cartesian coordinate

N	-1.68602900	-0.60844800	-1.17054600
N	-2.69353900	-1.46577600	-0.73566700
C	-2.22393900	-2.67345700	-0.05728700
C	-1.82831200	0.75613800	-0.91484700
C	-1.00888300	1.63748100	-1.54771100
C	0.00949700	1.22932200	-2.50469600
C	-0.01995600	-0.18375200	-2.82937700
C	-0.82821200	-1.03743300	-2.16489700
C	1.77044100	1.68626800	-1.94224100
C	2.10510200	1.08591300	-0.69411900
C	2.31174300	-0.29016600	-0.57997600
O	2.24074900	-1.14129400	-1.49652300
S	-3.89662500	-1.73168300	-1.95116500
O	-3.96204000	-0.46664700	-2.66212600
C	-5.32855700	-1.95533200	-0.94343800
O	-3.59802300	-2.97597200	-2.64828300
C	-5.87791900	-3.22591900	-0.80894100
C	-7.00078500	-3.37901000	-0.00246200
C	-7.56750700	-2.28532900	0.65817300
C	-6.98577100	-1.02012800	0.49937400
C	-5.86885100	-0.84129500	-0.30255300
C	-2.90388400	1.19552500	0.00761900
C	-3.70269300	2.28184500	-0.36326800
C	-4.70277900	2.74407200	0.48971400
C	-4.91462100	2.12505300	1.71858100
C	-4.12349800	1.03936400	2.09370700
C	-3.12896800	0.57334900	1.24282100
C	-8.80114700	-2.45317800	1.50330100
H	-1.60541500	-2.36660400	0.78858000
H	-3.10000500	-3.20314700	0.32283900
H	-1.65912600	-3.34657700	-0.71071100
H	-1.13499800	2.69297300	-1.33130500
H	0.11113600	1.89769300	-3.36071100
H	0.61711900	-0.57889100	-3.61035300
H	-0.88399100	-2.09422600	-2.39774500
H	2.23512100	1.19252800	-2.79902700
H	-5.43422100	-4.06627500	-1.33264000
H	-7.44639500	-4.36230800	0.11294600
H	-7.41765700	-0.16358200	1.00935400
H	-5.42433400	0.14107100	-0.43581500
H	-3.55947300	2.74186100	-1.33572700

H	-5.32028100	3.58283200	0.18697700
H	-5.69354600	2.48490900	2.38263600
H	-4.28373400	0.55284000	3.04990500
H	-2.52188100	-0.27491700	1.54293800
H	-8.77239000	-1.80018300	2.37843500
H	-9.69361200	-2.19128200	0.92618900
H	-8.91394500	-3.48472700	1.84193200
C	1.78904200	3.17519500	-2.01270700
C	2.19739700	3.81098900	-3.18918200
C	1.35359100	3.96043000	-0.93807300
C	2.19328700	5.19908500	-3.28399300
H	2.52993000	3.21101100	-4.03273700
C	1.34773700	5.34813200	-1.03293400
H	1.00640200	3.48434700	-0.02279300
C	1.77025100	5.97155800	-2.20521200
H	2.52270500	5.67728700	-4.20063200
H	1.01042900	5.94324300	-0.19039400
H	1.76627200	7.05386600	-2.27832000
H	2.17890900	1.70636200	0.19062400
C	6.51676600	-2.14204400	-0.11497300
C	5.28888800	-1.90101500	-0.74053800
C	5.20717800	-1.05607200	-1.84596800
C	6.36853700	-0.42830100	-2.29072600
C	7.58884600	-0.64939900	-1.65170000
C	7.67316900	-1.51638600	-0.56482200
C	6.37605300	-3.13486900	1.00786300
C	5.02473300	-3.80187400	0.68031800
C	4.20136900	-2.72889800	-0.08578900
H	4.26303900	-0.90509400	-2.35582700
H	6.32530200	0.22971200	-3.15210300
H	8.48402700	-0.15617800	-2.01636700
H	8.62755500	-1.70928800	-0.08479200
H	6.35645200	-2.61735700	1.97387700
H	5.19484300	-4.62024600	-0.02237900
H	7.18666100	-3.86524700	1.04917600
H	3.47233000	-3.14345100	-0.77944600
N	3.42242200	-1.96014900	0.93602700
O	4.32776800	-4.37801800	1.76391500
C	2.67839100	-0.84863100	0.77143900
C	3.42212500	-2.24490500	2.27520800
N	2.29091300	-0.49288400	2.00242800
N	2.74914100	-1.35534700	2.94807200
C	4.06473100	-3.48596700	2.81793700
H	4.96525800	-3.23046200	3.38838500

H	3.36349700	-3.97718600	3.49491200
C	1.55079100	0.66364900	2.42449400
C	2.12681400	1.48424900	3.38742000
C	0.31385400	0.95100000	1.85950500
C	1.45915600	2.63836500	3.77928100
C	-0.34421800	2.11611500	2.23664800
C	0.23806900	2.94953600	3.18896300
H	1.88669000	3.29766100	4.52522400
H	-1.30348900	2.37344500	1.80135800
H	-0.11606200	0.29180600	1.11144100
H	3.08719600	1.22391600	3.81831400
Cl	-0.58415600	4.40722500	3.65145600

Variable frequencies

-236.0521	12.2228	16.8625
19.0635	21.7686	25.1344
27.4079	31.2535	36.4341
47.2187	50.4870	52.0321
58.5486	63.0867	65.3509
70.0373	76.2887	85.7081
88.7907	94.4637	108.9174
113.1225	120.6986	126.7373
148.6681	152.3876	158.6726
170.2797	178.0255	180.6341
183.3171	193.9472	198.8467
214.0139	225.4040	240.1964
249.9000	251.1399	257.5027
260.5509	262.7382	277.9979
286.7583	300.0183	309.0928
313.5038	328.1269	343.8460
349.1075	361.9622	368.2781
370.8190	384.3182	384.9674
405.4138	417.0358	419.5610
420.9162	425.5691	431.9037
442.8140	449.4826	456.9999
466.4452	490.8285	492.1913
495.7644	508.4863	512.9272
527.5469	538.0186	542.5425
555.3065	567.2802	568.2275
585.1035	590.0203	600.6594
606.2020	609.8210	625.6977
628.4471	631.7310	640.7387
643.7918	645.1690	653.7074
660.2300	676.9195	694.3971

709.6286	711.1555	719.0584
720.7034	721.5216	726.8321
730.3255	753.7202	756.8695
767.1177	776.6547	785.0633
789.0916	791.3579	797.0003
813.0814	826.6633	839.4262
844.3906	844.6150	849.6880
851.8855	853.9399	864.5062
875.4914	881.1788	883.4937
886.4369	896.0104	899.0053
913.2671	925.1935	940.8256
952.3748	960.5287	965.0380
979.9155	988.4703	996.9288
1000.7389	1004.0786	1008.9972
1011.9054	1014.6377	1015.9525
1016.9847	1018.9324	1028.1511
1028.9308	1030.4896	1034.6042
1035.1052	1038.2469	1044.8852
1055.6450	1066.4474	1067.5873
1069.7984	1072.6916	1079.4093
1081.7084	1095.9119	1100.4006
1118.0628	1119.8130	1125.2538
1130.2454	1131.6978	1134.3176
1137.1577	1146.1255	1148.2829
1157.0831	1159.4600	1167.8414
1177.2004	1180.2438	1182.4616
1184.7935	1187.7650	1190.8372
1199.1049	1201.7574	1203.2437
1211.2512	1213.8396	1216.5994
1218.3435	1219.5565	1236.2303
1242.3017	1255.8403	1259.6199
1261.6904	1274.5968	1289.1823
1297.4750	1300.9393	1316.7926
1317.8431	1320.9472	1325.3950
1334.1183	1336.6036	1343.9468
1344.0126	1351.4727	1354.3764
1359.7159	1362.8426	1365.5089
1368.0074	1371.8239	1374.2817
1380.5811	1381.2091	1420.7515
1426.0391	1446.7641	1456.0362
1457.1748	1458.4486	1461.2597
1487.4565	1491.8670	1496.6267
1497.9492	1500.4016	1503.2097
1505.1080	1505.7428	1506.8413

1511.5072	1523.7753	1532.9521
1537.2590	1544.3535	1550.6696
1554.8352	1569.1025	1572.4054
1619.6277	1636.2383	1668.5340
1669.1823	1671.4576	1674.6990
1679.5944	1681.1057	1686.5246
1691.0373	1696.4297	1699.8570
1703.1843	1721.7825	3073.1260
3074.0077	3078.2978	3089.5665
3126.3809	3135.1564	3141.4107
3151.0082	3152.1787	3159.1274
3167.1079	3170.0767	3179.9832
3184.6649	3196.8624	3197.5283
3206.4825	3208.9147	3213.3873
3215.6121	3221.5043	3222.4702
3224.7677	3225.0669	3226.9261
3230.3335	3230.8676	3232.9324
3233.6155	3234.7212	3239.1011
3240.3376	3241.0607	3242.8594
3246.1132	3247.0629	3248.6637
3250.3813	3253.6101	3255.2168

²TS5R^e

Zero-point correction=0.778086

Thermal correction to Energy=0.825822

Thermal correction to Enthalpy=0.826766

Thermal correction to Gibbs Free Energy=0.691752

Sum of electronic and zero-point Energies=-3207.928844

Sum of electronic and thermal Energies=-3207.881108

Sum of electronic and thermal Enthalpies=-3207.880164

Sum of electronic and thermal Free Energies=-3208.015177

Cartesian coordinate

N	-2.34067100	1.47181600	0.45211100
N	-3.45435900	1.51325200	-0.38154800
C	-3.27942100	2.37648800	-1.55488800
C	-1.76108600	0.24431300	0.72555200
C	-0.63901500	0.20582800	1.49159700
C	0.00733700	1.41641300	1.94571800
C	-0.83249700	2.59596300	1.90285800
C	-1.93470400	2.61075500	1.12053600
C	1.43109400	1.80248800	0.65031300
C	2.27710600	0.66785500	0.56354900

C	2.04808300	-0.30479900	-0.41749200
O	1.12468400	-0.36328000	-1.25573500
S	-4.91063800	1.77772700	0.50333400
O	-4.75419100	0.97003600	1.70171900
C	-6.07934000	1.08347500	-0.62275600
O	-5.16237800	3.20971600	0.62083900
C	-7.21352900	1.82567300	-0.93275700
C	-8.16376900	1.26317200	-1.77890300
C	-7.98603100	-0.01580800	-2.31218000
C	-6.82407100	-0.72958700	-1.98740000
C	-5.86570500	-0.19434800	-1.14047800
C	-2.41165300	-0.97692200	0.18116800
C	-3.32547500	-1.68644500	0.96444100
C	-3.91633600	-2.84397000	0.45903500
C	-3.59666800	-3.28960500	-0.82281100
C	-2.67630300	-2.58343300	-1.59915800
C	-2.07926700	-1.42862200	-1.09824200
C	-9.02537000	-0.63229200	-3.20887000
H	-2.42801800	1.99471300	-2.11996200
H	-4.17823600	2.29570200	-2.16848100
H	-3.12074400	3.42634100	-1.28720100
H	-0.19377700	-0.76145400	1.69665900
H	0.66977700	1.32677900	2.80303100
H	-0.54977000	3.49362700	2.43806900
H	-2.57977100	3.47421700	0.99896200
H	0.76630800	1.90169100	-0.20936600
H	-7.33832400	2.82130300	-0.52090600
H	-9.05494300	1.82931900	-2.03128500
H	-6.66999800	-1.71989400	-2.40669300
H	-4.96159500	-0.74415500	-0.89858500
H	-3.58276700	-1.31885400	1.95179900
H	-4.62471600	-3.39560600	1.06793400
H	-4.05605500	-4.19148900	-1.21422000
H	-2.41918500	-2.93593300	-2.59272500
H	-1.33973300	-0.88381400	-1.67926200
H	-8.56019700	-1.13559300	-4.06001300
H	-9.60324900	-1.38229100	-2.65968000
H	-9.72185200	0.11780400	-3.58688100
C	1.99394300	3.08883600	1.13055900
C	1.59486200	4.27914600	0.51225600
C	2.92340900	3.15023900	2.17519800
C	2.13773800	5.50024300	0.90361500
H	0.86527500	4.24005400	-0.29287700
C	3.46464500	4.36894000	2.56758100

H	3.23338400	2.23947900	2.68120000
C	3.07951300	5.54728300	1.92881600
H	1.82720100	6.41323600	0.40590900
H	4.18939500	4.40153000	3.37467200
H	3.50506900	6.49695800	2.23556400
H	3.15683600	0.57536400	1.19344300
C	6.43315000	0.96094800	-1.13505900
C	5.08486900	0.93538500	-1.50670900
C	4.26865700	2.04780100	-1.32577900
C	4.80666000	3.17370100	-0.70468100
C	6.14135900	3.18534400	-0.29681000
C	6.96928000	2.08686000	-0.52189300
C	7.12977000	-0.31176200	-1.54182300
C	6.16878900	-0.85865400	-2.61971900
C	4.76058400	-0.37991600	-2.17428100
H	3.23590700	2.04403800	-1.66178700
H	4.18403400	4.04735500	-0.53651900
H	6.54328900	4.07199800	0.18295700
H	8.01661700	2.11535200	-0.23744000
H	7.21985200	-0.99522800	-0.68903800
H	6.37984200	-0.35658400	-3.56639200
H	8.13360300	-0.15241600	-1.94014100
H	4.04685800	-0.30984000	-2.99797500
N	4.22332500	-1.41934400	-1.24275200
O	6.24102300	-2.23636900	-2.90215500
C	3.09250000	-1.40463000	-0.51262400
C	4.78156400	-2.66391800	-1.07680800
N	3.01587100	-2.60355700	0.05624100
N	4.06400200	-3.40075800	-0.27893800
C	6.03648200	-3.06937300	-1.78708600
H	6.88505700	-3.04910500	-1.09250700
H	5.92228900	-4.08952800	-2.15634900
C	1.94066100	-3.11890500	0.85229300
C	2.22849500	-3.70527300	2.07917800
C	0.65015600	-3.06340800	0.33857600
C	1.18452000	-4.23453000	2.82715600
C	-0.39134000	-3.59924600	1.08645500
C	-0.11351300	-4.17284200	2.32318600
H	1.37114800	-4.69367000	3.79081700
H	-1.40527900	-3.58203600	0.70371900
H	0.46281900	-2.60464000	-0.62709600
H	3.25084100	-3.74822600	2.43817800
Cl	-1.42224000	-4.83435100	3.25655300

Variable frequencies

-157.2548	8.2147	17.2292
18.2855	20.7684	23.7495
29.7882	33.7065	40.2857
46.8031	51.6375	57.6378
60.1010	63.7618	66.4919
76.5518	79.1035	82.0816
87.9279	100.6016	102.3875
104.5269	109.4181	120.1171
126.6937	138.8254	149.4195
157.0996	161.5941	183.6367
184.4406	188.3464	199.1752
210.8472	229.4503	235.6558
244.5936	251.0306	251.3334
258.2122	261.1670	273.6124
280.2733	285.1934	311.1865
312.7020	326.9946	340.0978
346.3184	349.5493	359.6254
376.7967	379.0544	383.5471
403.7522	411.7572	415.8564
416.1195	417.7735	431.4853
438.6183	453.6488	459.0345
460.4360	484.1195	498.0660
499.6575	507.7396	522.8917
526.7816	538.5143	540.4900
558.1024	561.3841	573.4564
584.4170	590.8521	592.9905
605.3814	606.8873	615.6854
626.9094	627.9445	638.9824
640.3906	642.8012	652.2809
668.0193	693.0303	699.6984
711.2408	716.9124	717.4283
720.9428	723.4905	726.4387
728.0823	758.6441	763.3855
768.9306	774.6789	778.3546
788.7911	798.8775	802.5614
806.0027	814.2739	831.1002
841.9864	842.1328	852.1141
854.2747	859.7958	869.1550
871.9230	872.5000	878.7091
882.6741	887.7439	900.2873
911.0738	912.9168	943.0112
958.0614	975.6375	981.4362
989.5273	992.1495	992.8244

997.5284	1003.4166	1005.4851
1006.9479	1009.9854	1015.9249
1016.8096	1018.4885	1020.3099
1024.0055	1026.7093	1027.8760
1036.4426	1037.1867	1044.1520
1054.3869	1066.0735	1066.7946
1069.5290	1072.8201	1073.6565
1086.2548	1094.8808	1098.9850
1112.4537	1115.6979	1116.7653
1123.4669	1124.5848	1130.2534
1134.1402	1139.7158	1151.0355
1151.1835	1153.5278	1161.9541
1174.8537	1177.0454	1180.5521
1183.2689	1183.8824	1187.4054
1200.2114	1202.1905	1205.6061
1206.7824	1207.7583	1216.7429
1220.5404	1221.6002	1237.8358
1247.2070	1253.6299	1257.3996
1267.3816	1278.7180	1288.3338
1300.6050	1302.5549	1315.6098
1322.1356	1324.1717	1326.1450
1335.3564	1339.2000	1339.8003
1344.5851	1356.2224	1358.2157
1358.3971	1360.3175	1360.8744
1362.1751	1368.5074	1375.4638
1376.2757	1383.5732	1423.5138
1426.8278	1449.3469	1453.4982
1457.4134	1459.0982	1468.0665
1493.3011	1495.1495	1495.9541
1497.7027	1498.4393	1498.8955
1503.4391	1504.1734	1506.5651
1514.1147	1519.2145	1536.0459
1538.6376	1543.7785	1545.5687
1553.6229	1567.9101	1587.8161
1626.0089	1646.7949	1668.6976
1669.0793	1669.3774	1673.2452
1676.7229	1685.1695	1689.2805
1691.5691	1691.7847	1694.6080
1705.2221	1721.2762	3072.2301
3076.4873	3079.6618	3088.5776
3143.5574	3147.9031	3148.5195
3149.1593	3157.2559	3162.6370
3168.2020	3178.1199	3184.7202
3190.2618	3190.8749	3192.3968

3202.7751	3205.7024	3206.3455
3210.4860	3211.1952	3214.5541
3217.1454	3219.1304	3219.3659
3222.8386	3227.7710	3228.8282
3229.9234	3230.4096	3234.2250
3235.2387	3237.2401	3242.7085
3243.3400	3243.7119	3252.1865
3252.6894	3254.3180	3258.3373

²TS5R^f

Zero-point correction=0.778710

Thermal correction to Energy=0.826159

Thermal correction to Enthalpy=0.827103

Thermal correction to Gibbs Free Energy=0.693481

Sum of electronic and zero-point Energies=-3207.932064

Sum of electronic and thermal Energies=-3207.884614

Sum of electronic and thermal Enthalpies=-3207.883670

Sum of electronic and thermal Free Energies=-3208.017293

Cartesian coordinate

N	2.59645800	0.21469500	0.01088300
N	3.88371700	0.33951800	0.51881500
C	3.95365200	0.45558000	1.97697700
C	2.33032500	-0.82087800	-0.87102400
C	1.09885900	-0.88907500	-1.44665700
C	0.01868900	0.00657600	-1.07517500
C	0.47676300	1.21288200	-0.40521800
C	1.70779900	1.26412700	0.14337000
C	-1.05761100	-0.93654700	0.10748100
C	-2.26803700	-0.19147800	0.25723400
C	-3.17990600	-0.18097100	-0.80381100
O	-3.05598900	-0.73874400	-1.91569000
S	4.81958600	1.49434500	-0.35856900
O	4.36540300	1.34891800	-1.73133600
C	6.43427900	0.81548000	-0.15437900
O	4.74841400	2.78309500	0.31997700
C	7.36265700	1.47712200	0.64459000
C	8.62871200	0.92152100	0.78268900
C	8.96668900	-0.27422700	0.13867700
C	8.00810100	-0.90910800	-0.65868000
C	6.73681200	-0.37290300	-0.81371900
C	3.40301500	-1.79799500	-1.17160300
C	3.78752500	-1.99292700	-2.49952800

C	4.78046600	-2.92075100	-2.80849900
C	5.38808800	-3.65525400	-1.79366100
C	4.99995400	-3.46559700	-0.46687700
C	4.01146800	-2.54043300	-0.15428000
C	10.33790500	-0.86780200	0.32081900
H	3.46135400	-0.41975500	2.40460100
H	5.00809100	0.45134700	2.26062100
H	3.48466500	1.37034600	2.35561000
H	0.90379900	-1.70932800	-2.12895700
H	-0.74338600	0.13706000	-1.84443300
H	-0.19609300	2.05131500	-0.26614200
H	2.08813100	2.12278900	0.68586500
H	-1.19938900	-1.79609700	-0.55240600
H	7.09250900	2.40762700	1.13303900
H	9.37042400	1.42562400	1.39520400
H	8.26003500	-1.83380100	-1.16951000
H	5.99614600	-0.85833300	-1.44249700
H	3.32737000	-1.39570900	-3.28045500
H	5.08266100	-3.06139800	-3.84084400
H	6.16284500	-4.37626300	-2.03388300
H	5.47128200	-4.03874900	0.32466800
H	3.70217000	-2.38989300	0.87633100
H	10.43684800	-1.30017100	1.32157600
H	10.52980300	-1.65666800	-0.40818100
H	11.11208300	-0.10362300	0.21755300
C	-0.23672900	-1.25402600	1.30746900
C	0.48096000	-2.45427200	1.35198100
C	-0.11415400	-0.35978400	2.37787900
C	1.28179200	-2.76642400	2.44739300
H	0.40897600	-3.15014900	0.51958400
C	0.68509700	-0.66889500	3.47362900
H	-0.64231900	0.58969700	2.35464700
C	1.38326300	-1.87512300	3.51362900
H	1.82008000	-3.70883700	2.46969500
H	0.76255900	0.03187300	4.29878400
H	1.99988200	-2.11996700	4.37261600
H	-2.47545300	0.39508500	1.14668800
C	-6.47325300	-2.82600900	0.69856000
C	-5.46731400	-2.46930400	-0.20445900
C	-4.21010600	-3.06495100	-0.15580100
C	-3.96036000	-4.00142900	0.84530100
C	-4.95439800	-4.34178200	1.76352800
C	-6.22136000	-3.76530600	1.69120100
C	-7.75847600	-2.09837400	0.39757200

C	-7.53169800	-1.64140100	-1.05952900
C	-5.99732100	-1.45492900	-1.19066900
H	-3.45312800	-2.81336300	-0.89183300
H	-2.98733700	-4.47785200	0.90535300
H	-4.74470000	-5.07809700	2.53258900
H	-7.00058600	-4.05447600	2.38953800
H	-7.88622300	-1.24857400	1.07877700
H	-7.80587800	-2.45721100	-1.73169300
H	-8.64769100	-2.72505400	0.49029400
H	-5.61972900	-1.56690600	-2.20789400
N	-5.69818800	-0.05060500	-0.78642100
O	-8.27503200	-0.52771500	-1.50323600
C	-4.49750100	0.51630000	-0.58927100
C	-6.63826300	0.92323200	-0.57366700
N	-4.74495600	1.78551500	-0.27234100
N	-6.07897300	2.05573800	-0.25156500
C	-8.10064900	0.64041700	-0.73880900
H	-8.58028600	0.57020800	0.24520400
H	-8.56559200	1.46207800	-1.28582600
C	-3.79382100	2.84091300	-0.09175800
C	-3.92152500	3.68623500	1.00308100
C	-2.79515300	3.01277600	-1.04523600
C	-3.01019400	4.72366100	1.15950100
C	-1.88352900	4.04927600	-0.88526500
C	-1.99629000	4.89108500	0.21900600
H	-3.08288500	5.39814100	2.00450300
H	-1.10007000	4.21177000	-1.61685100
H	-2.74437600	2.36170500	-1.91281700
H	-4.72323500	3.53579400	1.71735600
Cl	-0.85510900	6.18202600	0.42196100

Variable frequencies

-69.0962	14.1757	15.1974
19.2710	23.3114	26.4843
29.4668	36.2096	42.7981
47.3475	57.1977	60.1402
61.3937	64.5640	70.0797
74.8254	77.6379	81.8799
85.5018	89.5114	95.3458
107.2532	114.9816	124.1991
140.1067	144.7430	150.3807
158.9874	173.1596	179.6331
181.8902	197.8413	214.3713
219.4475	229.4908	241.7171

247.6219	255.0098	256.3361
265.6747	268.0699	275.3744
283.6748	294.4301	309.8842
319.8167	328.3827	342.6181
346.2122	355.9565	366.7022
376.0925	381.2606	389.0517
404.1475	416.5077	417.1238
421.1475	424.4227	428.3952
444.9347	450.6810	462.1731
467.4170	489.0232	492.8398
498.0567	505.6484	519.5233
533.2905	539.8299	546.4705
557.6996	560.6069	576.5591
583.1916	585.8806	593.7610
606.6640	616.4309	625.0119
629.6420	633.9935	641.6306
643.1837	644.5409	654.8397
666.2195	688.2665	698.5238
708.1678	714.3074	719.4858
720.8769	722.5087	728.3812
730.6104	754.6684	763.2940
771.1417	775.3137	784.0348
785.7794	792.4869	802.6153
809.9421	818.1458	829.7479
832.7774	843.6090	850.1106
854.3111	856.6660	864.6630
869.0989	875.7254	877.5880
879.4141	888.4753	901.7702
915.5501	920.8368	944.1711
956.0916	964.4575	970.8043
984.2314	987.6597	988.3842
994.1574	1002.1152	1003.7927
1009.8458	1010.1087	1016.0938
1016.4781	1018.6520	1022.5468
1026.1044	1028.3660	1031.7945
1034.5127	1034.7347	1047.8561
1054.2265	1067.2297	1069.4726
1071.3717	1073.1923	1079.4904
1086.7123	1099.0829	1103.4388
1114.7492	1119.8258	1120.4170
1122.2348	1133.4974	1136.7412
1140.4429	1146.0832	1151.2393
1162.4102	1163.6498	1170.6009
1179.7717	1181.4588	1183.3284

1188.6190	1189.3741	1196.8517
1201.7718	1205.2379	1209.6843
1211.0897	1212.8912	1214.1983
1220.3561	1222.5765	1241.4681
1249.5898	1250.9129	1252.9787
1265.3941	1282.8183	1289.2206
1303.4690	1306.8362	1320.6897
1325.7966	1327.8734	1329.5520
1332.5499	1340.3225	1341.3426
1346.2967	1357.4888	1358.8946
1360.6431	1360.9853	1367.4337
1370.7376	1372.9810	1375.7676
1378.4031	1384.9306	1420.0683
1427.2642	1453.0954	1454.1244
1459.2028	1460.6003	1471.0621
1492.1988	1494.5720	1497.7281
1499.8003	1500.5814	1503.2824
1506.7444	1507.7228	1508.6688
1520.0299	1523.9792	1537.9779
1541.4532	1548.2206	1550.1789
1550.6461	1564.4202	1594.3791
1629.2027	1639.3696	1671.0376
1671.3287	1672.0740	1676.8912
1681.3258	1686.3082	1688.8286
1691.2836	1695.3272	1698.3175
1703.2607	1725.1382	3070.9893
3077.7062	3079.7345	3093.8582
3125.1841	3139.5822	3151.2908
3154.1450	3158.8185	3160.0719
3165.2712	3174.4567	3178.0611
3188.4660	3190.0117	3192.0250
3200.6284	3205.7394	3205.8004
3206.4478	3206.8422	3210.5393
3212.6765	3215.4236	3216.1853
3221.6228	3222.4437	3224.9890
3225.4164	3225.7306	3227.3751
3228.9663	3230.0201	3231.3016
3231.9349	3235.0456	3236.4917
3242.6809	3247.5895	3250.0475

²TS5S

Zero-point correction=0.779100

Thermal correction to Energy=0.826101

Thermal correction to Enthalpy=0.827045
 Thermal correction to Gibbs Free Energy=0.697269
 Sum of electronic and zero-point Energies=-3207.945324
 Sum of electronic and thermal Energies=-3207.898324
 Sum of electronic and thermal Enthalpies=-3207.897380
 Sum of electronic and thermal Free Energies=-3208.027155

Cartesian coordinate

N	0.45301200	0.52223100	-2.20552900
N	1.27735900	1.45998300	-1.60371000
C	2.56696400	1.71383100	-2.25288400
C	0.93686800	-0.73537300	-2.53217400
C	0.11235300	-1.70353200	-2.97837500
C	-1.33108600	-1.51224500	-2.93097600
C	-1.73338300	-0.11422600	-2.84826400
C	-0.88286900	0.85536500	-2.42929500
C	-2.03159200	-2.41201200	-1.41552000
C	-1.23287500	-1.98980900	-0.32581400
C	-0.11889900	-2.73157700	0.11822600
O	0.29236200	-3.82040600	-0.32104800
S	1.33876100	1.31433900	0.09964300
O	0.01209500	0.84389100	0.47921000
C	1.55510000	2.99510800	0.58454300
O	2.51199700	0.54406700	0.51387400
C	2.78678000	3.41535800	1.07629400
C	2.93298800	4.74888800	1.44266400
C	1.87150400	5.65023900	1.31928400
C	0.64654800	5.19102700	0.81620600
C	0.47404400	3.86555600	0.44764500
C	2.02706000	7.08597700	1.74091500
H	2.37426600	1.88373600	-3.31296600
H	2.98384700	2.62564800	-1.81928600
H	3.28066700	0.89245700	-2.12594400
H	0.53180200	-2.65704800	-3.27415800
H	-2.75600600	0.16457100	-3.07490000
H	-1.83724300	-3.44101000	-1.72342100
H	3.60527300	2.70942400	1.17017900
H	3.88600100	5.09606100	1.82964500
H	-0.18264400	5.88455100	0.71002200
H	-0.47754000	3.50955200	0.06285100
H	3.07808900	7.37641600	1.78496000
H	1.50826600	7.75643100	1.05195700
H	1.59459600	7.23765800	2.73494900
C	-3.47657700	-2.02904900	-1.44083300

C	-4.31989800	-2.59985100	-2.40014700
C	-4.01344000	-1.08529500	-0.55624100
C	-5.65842100	-2.23046300	-2.48477900
H	-3.92317300	-3.34758800	-3.08317600
C	-5.35285800	-0.71531100	-0.63997200
H	-3.39608400	-0.64740500	0.22342700
C	-6.17910000	-1.28186300	-1.60706400
H	-6.29700900	-2.68734600	-3.23375700
H	-5.75214900	0.00951700	0.06294400
H	-7.22356900	-0.99547500	-1.66935800
H	-1.39535300	-1.01212900	0.11284400
C	4.34163700	-1.83342700	-0.75476100
C	3.27995800	-2.74055100	-0.64279500
C	2.77760100	-3.38656300	-1.76980500
C	3.29973400	-3.05523200	-3.02011800
C	4.30619300	-2.09539400	-3.14031100
C	4.84304400	-1.48696400	-2.00524600
C	4.88238900	-1.46639200	0.60007000
C	4.38498300	-2.65928000	1.44350400
C	3.01524500	-3.04970500	0.81611900
H	1.99979300	-4.13366200	-1.67059400
H	2.92832000	-3.55709500	-3.90793700
H	4.70198500	-1.85061200	-4.12087900
H	5.67160400	-0.79027500	-2.09223800
H	4.45319500	-0.51906300	0.93881000
H	5.04788100	-3.51057800	1.27116100
H	5.97087700	-1.38308100	0.62143600
H	2.74145700	-4.09067200	0.99252100
N	1.96301600	-2.23159300	1.50524900
O	4.36111400	-2.48134400	2.83835100
C	0.63802400	-2.13971000	1.27499400
C	2.19896300	-1.52892100	2.66013900
N	0.13696000	-1.43216300	2.28923100
N	1.10152800	-1.03118600	3.15258900
C	3.56279100	-1.40172700	3.25665000
H	3.99334300	-0.43171000	2.97720400
H	3.48390000	-1.44738900	4.34345100
C	-1.23965400	-1.16248900	2.59581800
C	-1.63696500	0.14944300	2.82017300
C	-2.13561600	-2.22560000	2.66498000
C	-2.97518300	0.40604900	3.09916400
C	-3.47353200	-1.96631000	2.93179700
C	-3.88024600	-0.65080700	3.14208900
H	-3.31636700	1.41954900	3.27449200

H	-4.19365900	-2.77436000	2.98082200
H	-1.79459300	-3.24357500	2.50754100
H	-0.91394500	0.95253600	2.74863800
Cl	-5.55615300	-0.32121300	3.46089000
H	-1.90608900	-2.10876000	-3.63859100
H	2.01116700	-0.85892300	-2.44769000
C	-1.32297300	2.25349400	-2.21340600
C	-0.64373300	3.34217100	-2.77186300
C	-2.46912400	2.47961700	-1.44594100
C	-1.10389900	4.63610800	-2.56166000
H	0.24068600	3.17242500	-3.37788000
C	-2.92680700	3.77839200	-1.23369100
H	-2.98751000	1.63202900	-1.00593900
C	-2.24378700	4.85757900	-1.78830900
H	-0.57522300	5.47383100	-3.00409800
H	-3.81614800	3.94568300	-0.63503800
H	-2.60151900	5.86914200	-1.62551900

Variable frequencies

-360.7437	17.0944	20.7354
24.2228	30.5066	34.5424
36.5961	39.5177	53.2945
56.7190	57.3145	67.6538
70.8310	72.6803	73.3672
81.0179	85.7898	90.6030
94.2696	99.6835	105.3033
111.5975	117.5227	133.3574
147.6946	155.0893	155.3976
170.7933	179.8274	191.7274
204.1394	207.1567	213.2088
220.5254	225.7710	230.7603
245.8054	255.8588	265.1226
267.9120	285.9159	287.5777
297.5022	308.6103	311.1846
315.8063	327.3916	348.7429
351.0266	356.8628	360.8496
382.6552	386.5365	390.4523
407.7425	415.4654	417.1002
420.3667	426.3741	434.5388
447.3645	452.4886	456.7620
462.0817	479.0733	488.7984
491.0128	503.1773	514.1033
526.1186	533.5382	544.3987
554.4770	558.9342	570.1191

574.2914	588.4745	593.8999
603.1392	607.3884	621.1276
627.9110	630.7161	634.9919
642.7446	643.1774	654.2600
661.9203	673.7401	682.0331
703.1910	711.9273	716.1732
720.2083	722.6951	724.6889
732.6648	753.6985	762.8484
764.6158	775.7157	780.8132
786.5102	787.6773	792.5103
809.8857	827.6872	840.0440
840.8648	846.9065	848.3998
851.4717	860.8766	869.6496
876.2420	876.8933	881.0040
883.6387	891.0387	899.6612
908.9155	914.6578	945.7512
952.7731	959.8575	964.2474
979.1622	988.7833	988.8883
994.0348	1000.7224	1004.6217
1006.3284	1009.0052	1015.0869
1016.3429	1019.6865	1025.5304
1025.8872	1027.3965	1030.8542
1033.8338	1038.8567	1040.9291
1055.5083	1060.6289	1068.0342
1069.4965	1070.5351	1073.9446
1078.3880	1090.2476	1098.0940
1114.5574	1118.8867	1120.0614
1122.2697	1128.3030	1132.8382
1135.5621	1144.3490	1146.7845
1154.2064	1158.9253	1163.8732
1167.8746	1173.7409	1175.2671
1180.8126	1182.0749	1182.9798
1199.5006	1205.7247	1206.2066
1207.7149	1212.1616	1213.0536
1218.9296	1227.0431	1238.3086
1251.5440	1255.9457	1263.8930
1280.4353	1286.8812	1289.7531
1300.1504	1312.7332	1316.9365
1319.5991	1321.0849	1325.9809
1330.6746	1338.3251	1338.6069
1341.3212	1342.9246	1353.4784
1358.0525	1359.5196	1362.5799
1363.7693	1364.5112	1370.2994
1378.2404	1382.9060	1423.0071

1427.8430	1446.3413	1448.3022
1457.3900	1459.7226	1460.7051
1480.8790	1488.8290	1496.6009
1500.2450	1500.3497	1502.0018
1504.7546	1506.3535	1514.6078
1519.9342	1525.0824	1534.5338
1537.7212	1546.8328	1548.8458
1549.3837	1580.2585	1590.8883
1635.7745	1643.9210	1668.0660
1670.2089	1671.7960	1672.6479
1674.0225	1681.6235	1684.9025
1689.8320	1693.5746	1695.8787
1701.4710	1715.1667	3067.5384
3080.4069	3089.6334	3111.5333
3143.5022	3151.3954	3152.5393
3156.3367	3160.1469	3162.8034
3165.4035	3177.5126	3179.7909
3190.0527	3196.4349	3198.1612
3201.4621	3201.9236	3206.5205
3207.0586	3210.5185	3212.6120
3214.8325	3221.3802	3222.3693
3223.1488	3223.8811	3225.6903
3230.8879	3236.1610	3237.9094
3238.2959	3242.2949	3244.2762
3246.9070	3247.4307	3261.0410
3261.4519	3262.4996	3266.0855

²TS5S^b

Zero-point correction=0.778753

Thermal correction to Energy=0.826326

Thermal correction to Enthalpy=0.827270

Thermal correction to Gibbs Free Energy=0.693221

Sum of electronic and zero-point Energies=-3207.922800

Sum of electronic and thermal Energies=-3207.875227

Sum of electronic and thermal Enthalpies=-3207.874283

Sum of electronic and thermal Free Energies=-3208.008332

Cartesian coordinate

C	6.97669000	-3.03323100	-0.14514800
C	5.79129200	-2.32978000	0.04421100
C	4.59090800	-2.75864300	-0.51264100
C	4.59258900	-3.92572000	-1.27092900
C	5.77741100	-4.64218800	-1.45965200

C	6.97466900	-4.20341700	-0.90020200
C	8.12995100	-2.36548600	0.55857400
C	7.58427200	-0.99993200	1.03896400
C	6.01877700	-1.10676500	0.90151300
H	3.67346600	-2.19202400	-0.36503700
H	3.67093700	-4.28319100	-1.71765500
H	5.76407500	-5.54988700	-2.05373600
H	7.89289800	-4.76121400	-1.05601800
H	9.00194400	-2.21271700	-0.08509700
H	7.84846300	-0.80099300	2.07721200
H	8.46354800	-2.96080000	1.41414700
H	5.52612200	-1.16785000	1.87265700
N	5.48646000	0.09208600	0.23656800
O	8.14050200	0.09422100	0.32662800
C	4.27384800	0.66227300	0.30639200
C	6.18426800	0.73278300	-0.74731200
N	4.29694000	1.64541900	-0.60413800
N	5.48237800	1.69552300	-1.27324600
C	7.60123900	0.30897900	-0.96097300
H	7.64414700	-0.59288400	-1.58741700
H	8.16776600	1.10711200	-1.44002200
C	0.79385300	0.55701800	1.79191500
C	1.86378000	0.52620600	0.85961600
C	3.18197700	0.26226700	1.27071500
O	3.55305100	-0.20311700	2.36395600
H	1.66833000	0.78512100	-0.17596300
C	3.26482300	2.59681100	-0.91456600
C	2.68253300	3.34289800	0.10597900
C	2.84305200	2.70110600	-2.23379900
C	1.61601500	4.17957800	-0.19574600
H	3.03976600	3.25614400	1.12663400
C	1.79070000	3.55706400	-2.53839100
H	3.32596000	2.11468900	-3.00766400
C	1.17767400	4.27427700	-1.51469900
H	1.12081000	4.74570800	0.58488700
H	1.43746300	3.65581900	-3.55791100
Cl	-0.15922900	5.31541900	-1.89197800
S	-3.74441800	-1.15089400	-1.56353900
O	-3.27282400	-1.85179400	-2.75210800
O	-3.16764700	0.12771600	-1.18123800
N	-3.50992900	-2.15893400	-0.18727100
N	-2.35251200	-1.86133700	0.51408100
C	-6.20135200	-1.67249800	-2.63060800
H	-5.66128800	-2.19086300	-3.41589400

C	-7.59124200	-1.59476100	-2.63040200
H	-8.15228800	-2.06455800	-3.43223600
C	-5.50507700	-1.06081200	-1.59526300
C	-6.15257800	-0.37597300	-0.56598900
H	-5.58298800	0.09864600	0.22870600
C	-8.27389700	-0.92223300	-1.61431000
C	-7.53678100	-0.31679800	-0.58602900
H	-8.05768700	0.20714500	0.21060900
C	-9.77642200	-0.83684300	-1.61373000
H	-10.18664600	-1.23313700	-0.68068700
H	-10.20819100	-1.39715200	-2.44450000
H	-10.10228400	0.20395600	-1.69745900
C	-1.11789600	-2.16867500	-0.02206300
H	-1.14784300	-2.66763300	-0.98448700
C	-2.44734900	-1.20456400	1.73123200
C	-1.31127200	-0.96210600	2.44374200
H	-1.42663600	-0.49770600	3.41732400
C	0.02582800	-1.87608300	0.62869900
H	0.96944200	-2.15296000	0.17221300
C	0.01777700	-1.18596200	1.91196200
C	-3.73835800	-3.58702300	-0.42977100
H	-4.74044200	-3.69914900	-0.84892300
H	-3.01142600	-4.02412500	-1.12172000
H	-3.69761700	-4.09987400	0.53194800
C	-3.78088700	-0.75527200	2.19793500
C	-4.84466800	-1.63786000	2.40877400
C	-3.95715100	0.61305000	2.42252300
C	-6.07369900	-1.15450700	2.84101600
H	-4.70802100	-2.70139500	2.24051000
C	-5.19464100	1.09420000	2.84659300
H	-3.13034900	1.29480300	2.24001900
C	-6.25193400	0.21285100	3.05568200
H	-6.89421600	-1.84419700	3.00867800
H	-5.32874700	2.15856800	3.00957300
H	-7.21387700	0.58776100	3.39039300
H	1.14490800	0.60592600	2.82377500
C	-0.27388400	1.55511600	1.49299800
C	-0.56000400	2.53752700	2.44575400
C	-0.94619800	1.57805300	0.26808000
C	-1.47100200	3.55371900	2.16304200
H	-0.04938900	2.51709700	3.40515200
C	-1.86597900	2.58471900	-0.00955500
H	-0.76722400	0.79999500	-0.47048600
C	-2.11838400	3.58418000	0.92982600

H	-1.67129100	4.31946100	2.90588800
H	-2.39112800	2.57646500	-0.95822000
H	-2.82433500	4.37672800	0.70378800
H	0.78382900	-1.51544600	2.61367100

Variable frequencies

-220.0149	13.3091	14.6606
19.9645	23.8723	25.9563
29.4110	37.4391	42.6935
50.3028	56.6169	58.2194
61.0445	63.8886	66.5380
76.5784	80.4550	82.0932
89.6350	93.9383	97.6741
98.9127	109.0679	116.0073
127.7124	131.9229	145.5512
155.5233	164.8173	177.2585
183.6729	199.5544	202.5552
213.1860	222.1558	230.2014
236.2437	249.3670	255.8521
258.2243	275.6720	286.3887
289.2732	305.4621	311.3531
314.8279	327.0509	344.0127
351.8009	353.0297	367.4287
377.4367	382.4127	387.7810
415.2000	417.9956	421.7878
423.6775	428.4821	432.9400
435.1119	441.8172	447.1191
476.0672	486.2882	490.8349
500.1184	511.6014	519.9335
522.7667	534.5656	542.8800
557.7237	558.3579	571.5540
574.1642	584.9371	595.2567
611.7582	617.1457	618.5573
629.7947	636.3054	640.0659
642.2802	648.8795	669.8432
674.0639	691.8753	706.4691
712.8658	718.5586	720.4543
722.5211	724.3155	728.7926
732.7582	755.9237	756.8472
769.1582	772.4299	784.9625
788.3288	794.8326	800.3328
818.8300	829.5585	837.6347
846.8756	847.4906	851.8215
855.9130	863.6571	876.2285

879.7044	879.9618	881.6801
883.7929	888.3468	895.8319
904.7885	918.3598	951.3349
955.2623	958.5547	962.8696
975.5534	981.6276	987.4589
997.6594	1003.9767	1006.7385
1011.2383	1011.8919	1014.2533
1015.4534	1016.5984	1023.9729
1027.0766	1027.6694	1029.1077
1032.4178	1034.3525	1046.4549
1054.4235	1059.3188	1065.4257
1067.4904	1068.4794	1070.9313
1075.9543	1085.7066	1109.0884
1115.8780	1120.2770	1121.1192
1123.9704	1130.6634	1133.9801
1141.1220	1145.0163	1150.3586
1154.3132	1156.5994	1166.2210
1171.0922	1179.9637	1183.1141
1183.5326	1184.9284	1185.9737
1200.9709	1203.5584	1205.0734
1208.0927	1212.7739	1219.3808
1226.2918	1232.6350	1242.5537
1249.9578	1253.8715	1262.0394
1273.8402	1281.5656	1291.3443
1311.7290	1312.5291	1314.2609
1315.8100	1321.6785	1322.4947
1331.4930	1332.8350	1339.7464
1343.6778	1350.4513	1356.3321
1356.9403	1359.4694	1366.1643
1370.4131	1375.7095	1377.0127
1380.6360	1382.3425	1424.3835
1425.9384	1456.1546	1456.3435
1460.2393	1461.8963	1474.2541
1484.0980	1489.4080	1494.4271
1498.1467	1498.6866	1499.5626
1502.4128	1507.0764	1512.3575
1522.0384	1529.5295	1534.9403
1542.8778	1544.2833	1545.9759
1549.1432	1562.9543	1570.8805
1626.8573	1658.2721	1665.7357
1671.1667	1674.7107	1676.4554
1685.7094	1687.3524	1690.7602
1691.1185	1692.3272	1695.5502
1700.9001	1721.5723	3069.5754

3076.4864	3079.0564	3092.6646
3137.8191	3138.9146	3148.5736
3153.5699	3165.5994	3171.5221
3172.1247	3180.7423	3189.5319
3189.9586	3190.5687	3190.8985
3206.6031	3208.2033	3208.4607
3211.1581	3214.1850	3221.4746
3221.8460	3222.3431	3223.4369
3224.2866	3225.2088	3225.6508
3226.7256	3230.2178	3233.1457
3233.3672	3233.5316	3236.0383
3240.8008	3241.1244	3242.8256
3244.7190	3251.3143	3252.4563

²TS5S^c

Zero-point correction=0.778770

Thermal correction to Energy=0.826288

Thermal correction to Enthalpy=0.827232

Thermal correction to Gibbs Free Energy=0.693787

Sum of electronic and zero-point Energies=-3207.929743

Sum of electronic and thermal Energies=-3207.882225

Sum of electronic and thermal Enthalpies=-3207.881281

Sum of electronic and thermal Free Energies=-3208.014725

Cartesian coordinate

N	2.90920200	0.56982500	1.96511400
N	4.12265000	0.60940400	1.28512400
C	5.28518800	0.99735600	2.08795300
C	2.40787500	1.72647900	2.53569500
C	1.10358000	1.83593700	2.85904800
C	0.16399000	0.79960700	2.45839300
C	0.78278000	-0.46411000	2.11252200
C	2.09826700	-0.54447300	1.77853200
C	-0.58025800	1.38399400	0.79650800
C	-1.75986400	0.63097000	0.54756400
C	-1.79515500	-0.48330200	-0.30214200
O	-0.85344300	-1.14097700	-0.78711100
S	3.96006100	1.46099800	-0.20803700
O	2.63199900	1.09664900	-0.68494600
C	5.22589900	0.67195900	-1.15063900
O	4.30120100	2.86613300	-0.02049500
C	6.23858400	1.45100200	-1.69908800
C	7.21699500	0.82201000	-2.46161700

C	7.19254100	-0.56025000	-2.66702700
C	6.15781400	-1.31292200	-2.09553600
C	5.16702900	-0.70901900	-1.33611600
C	8.27318900	-1.23704000	-3.46641200
H	5.33557500	0.32760000	2.94694800
H	6.17463200	0.85080600	1.47189200
H	5.25386400	2.03948200	2.42113200
H	0.75000600	2.74250800	3.33425900
H	0.16688400	-1.34892200	2.00077200
H	0.26455500	1.11219400	0.16124800
H	6.25019900	2.52250900	-1.53071700
H	8.01209800	1.41408400	-2.90450400
H	6.12809500	-2.38759100	-2.25053700
H	4.36476700	-1.29294500	-0.89393900
H	9.06302100	-1.60456900	-2.80330700
H	7.87818500	-2.09418900	-4.01600300
H	8.73013300	-0.54724600	-4.17842400
C	-0.75991100	2.85968900	0.92571100
C	0.16988200	3.70015500	0.30609600
C	-1.83574700	3.42615000	1.61853200
C	0.00185300	5.08284200	0.34173400
H	1.01796600	3.25969000	-0.21383400
C	-1.99940500	4.80581800	1.65668100
H	-2.55823600	2.78949000	2.12362700
C	-1.08652000	5.63813900	1.00900600
H	0.72233000	5.72465600	-0.15499400
H	-2.84681200	5.23551000	2.18171100
H	-1.22533700	6.71401400	1.02838600
H	-2.70620100	0.99788700	0.93124100
C	-3.53378500	-4.43996900	1.09948500
C	-2.51943800	-3.70325500	0.47868500
C	-1.31780100	-3.44666100	1.13005300
C	-1.16374500	-3.89248000	2.44139900
C	-2.19184200	-4.58804300	3.07969400
C	-3.37954100	-4.87779200	2.40934800
C	-4.66669900	-4.70595800	0.14143600
C	-3.96318400	-4.50344700	-1.21887600
C	-2.90151700	-3.40480500	-0.95193600
H	-0.51672700	-2.93004100	0.61409100
H	-0.22715200	-3.71400300	2.96108700
H	-2.05438300	-4.93299800	4.09931300
H	-4.16006500	-5.45521500	2.89486400
H	-5.47861200	-3.98393800	0.29203100
H	-3.41276100	-5.41322400	-1.46807300

H	-5.09489000	-5.70557800	0.23546400
H	-2.06808100	-3.40816400	-1.65488200
N	-3.59649600	-2.09291800	-1.12353100
O	-4.78353000	-4.24350100	-2.33347700
C	-3.16976800	-0.85559600	-0.80984900
C	-4.83758000	-1.95292500	-1.68876200
N	-4.14968000	-0.02947600	-1.19214700
N	-5.19870200	-0.70234300	-1.73204000
C	-5.62492600	-3.12682900	-2.18598500
H	-6.46217200	-3.32577400	-1.50528700
H	-6.03492900	-2.89172100	-3.16970500
C	-4.20652900	1.40714900	-1.11938100
C	-5.30747600	1.98401100	-0.49982500
C	-3.17075600	2.17445800	-1.64468100
C	-5.36963800	3.36879400	-0.38940300
C	-3.22348600	3.55582900	-1.51278600
C	-4.32380000	4.13889400	-0.88808600
H	-6.21831000	3.84633000	0.08567200
H	-2.41440100	4.17648600	-1.88094000
H	-2.32539900	1.70149400	-2.13288800
H	-6.10351800	1.35842200	-0.11151200
Cl	-4.39756700	5.86706800	-0.73398800
H	-0.75747200	0.75257300	3.03306100
H	3.13491000	2.50979900	2.71339900
C	2.70947700	-1.76502800	1.20781300
C	3.86405400	-2.33220200	1.75714800
C	2.11835500	-2.34068500	0.07989400
C	4.41808600	-3.47102700	1.18712500
H	4.32177400	-1.88119800	2.63280500
C	2.67837100	-3.48531600	-0.48721000
H	1.25007400	-1.86107300	-0.36585800
C	3.82601400	-4.04926100	0.06279600
H	5.31136400	-3.91051000	1.61812300
H	2.22302900	-3.92575900	-1.36814600
H	4.26232500	-4.93798100	-0.38152500

Variable frequencies

-183.2942	11.4605	15.7219
23.7240	26.4248	29.7085
32.9754	36.7658	38.9878
43.0261	51.2732	53.4822
58.9505	68.5468	73.5067
75.1904	81.4357	86.6475
90.2305	96.3348	99.0128

108.1432	111.4278	121.5101
140.3500	143.2627	152.7561
170.4918	178.1489	179.1187
187.0768	192.7225	206.7870
212.5821	218.2547	222.1753
244.8149	251.0549	253.6549
257.0071	268.8601	279.1542
288.6005	307.8084	308.9062
312.4850	329.7601	342.5091
345.3312	357.2703	361.1011
374.2885	384.1608	387.7594
403.1696	415.1074	418.5594
420.6074	421.3643	426.2148
441.7805	442.7855	459.6299
464.5331	484.4925	497.2480
498.7329	499.8811	523.5397
530.9798	534.7102	543.6276
553.2085	560.9902	574.0821
577.6023	589.4928	594.6095
601.7196	607.7673	621.9123
629.1692	630.3126	638.9740
642.2012	643.6597	654.7375
669.3185	683.8833	684.1073
707.9656	716.2074	717.5931
721.9700	725.8758	728.1087
730.7631	760.3762	763.7337
770.1561	780.0514	781.2653
784.2791	788.2073	793.5763
812.9639	826.5773	838.3789
840.2547	843.4062	843.8683
847.0055	855.5988	860.0215
862.0311	871.4904	872.8192
885.4870	892.0650	900.9572
913.4331	918.4691	948.0801
966.3556	968.6243	976.5205
985.0709	989.1084	989.7303
990.7332	995.4057	1007.4987
1009.0034	1012.8590	1014.5736
1016.7752	1017.6646	1024.5920
1026.4086	1031.1900	1033.1477
1034.1784	1038.3159	1045.1958
1054.1997	1066.7045	1067.1891
1073.8283	1074.5501	1076.2790
1087.8698	1097.2307	1113.6913

1116.7862	1118.8790	1125.6431
1128.6467	1131.3994	1134.2779
1141.3347	1143.5168	1150.7541
1155.8963	1159.8451	1167.8001
1172.6387	1175.8577	1181.0938
1183.3460	1186.7980	1194.4093
1203.1935	1204.4617	1206.5886
1208.3798	1210.0396	1215.0185
1217.7562	1234.7630	1237.5875
1249.7161	1253.8690	1265.8017
1271.7775	1278.3314	1292.5688
1298.8580	1302.2035	1313.5721
1322.4284	1324.1606	1324.8204
1330.1613	1337.0369	1344.0630
1346.6809	1354.6999	1354.7492
1355.9351	1362.8111	1367.6555
1370.1914	1371.8640	1375.9439
1376.9629	1384.9037	1423.5402
1424.4575	1451.0109	1453.2883
1454.4333	1455.4003	1463.3066
1485.2604	1498.5801	1499.2768
1500.4195	1502.5196	1503.5376
1507.3732	1508.1004	1512.8424
1517.0539	1525.0437	1536.1081
1542.1447	1544.7656	1548.8147
1555.2258	1571.8359	1573.6775
1627.2076	1652.0622	1669.4079
1671.2550	1676.0569	1677.0957
1679.4692	1683.9909	1686.1226
1689.9945	1692.7754	1701.7821
1709.7449	1724.7282	3073.6503
3079.3972	3080.0490	3091.0027
3145.4002	3146.0376	3159.8369
3161.5252	3164.9876	3165.4147
3171.1487	3176.0461	3184.4141
3188.3626	3192.7203	3194.6764
3199.9399	3203.8877	3205.5948
3207.5632	3209.1983	3210.1870
3212.7643	3215.4613	3215.9339
3219.1271	3226.7164	3227.2059
3227.7110	3229.2408	3231.4179
3233.5921	3234.6550	3239.4184
3241.1077	3242.1954	3244.8923
3251.8641	3264.9397	3267.9254

²TS5S^d

Zero-point correction=0.778494

Thermal correction to Energy=0.825801

Thermal correction to Enthalpy=0.826745

Thermal correction to Gibbs Free Energy=0.694048

Sum of electronic and zero-point Energies=-3207.930186

Sum of electronic and thermal Energies=-3207.882880

Sum of electronic and thermal Enthalpies=-3207.881936

Sum of electronic and thermal Free Energies=-3208.014633

Cartesian coordinate

C	-0.99005400	0.57209100	-1.76586300
C	-2.10396300	0.44427500	-0.85387400
C	-3.38295900	0.06667200	-1.29937400
O	-3.70043300	-0.34616500	-2.42660100
H	-1.97642300	0.67565000	0.19917600
S	4.99271000	-1.24765600	-1.48500400
O	4.25922400	-2.47146800	-1.20636900
O	5.51455100	-0.97714000	-2.82030900
N	3.90920900	0.01253800	-1.03025300
N	2.58536900	-0.29953000	-1.29335200
C	6.02332200	-1.31926600	1.03116900
H	5.05378300	-1.70848100	1.32886000
C	7.03236100	-1.12136700	1.96168800
H	6.84412600	-1.35129500	3.00677200
C	6.28185400	-1.01022800	-0.30345000
C	7.51420300	-0.52204400	-0.72308400
H	7.67976500	-0.29940900	-1.77200100
C	8.28781700	-0.63328100	1.57535300
C	8.51294200	-0.33806700	0.22801900
H	9.48263400	0.03931300	-0.08201500
C	9.38204200	-0.45904800	2.59421000
H	8.98230900	-0.09750300	3.54436100
H	9.87639800	-1.41640400	2.78739500
H	10.14083900	0.24394000	2.24548800
C	2.15592000	-0.41558200	-2.60766300
H	2.92526400	-0.25830400	-3.35596400
C	1.80079200	-0.81643700	-0.26310200
C	0.52252800	-1.17153000	-0.52480500
H	-0.07445000	-1.57425500	0.28722400
C	0.89037400	-0.75441400	-2.90250300
H	0.59594000	-0.86461400	-3.93946200

C	-0.11538900	-0.89175900	-1.82624500
C	2.40172100	-0.95375000	1.08627100
C	2.92704900	0.15598100	1.75654100
C	2.40993000	-2.20373200	1.70720600
C	3.45187200	0.01352000	3.03605500
H	2.92135200	1.12614800	1.26735200
C	2.93836000	-2.34389300	2.98960900
H	2.02870800	-3.06571500	1.16888300
C	3.45974500	-1.23704000	3.65434100
H	3.86052200	0.87735900	3.55017600
H	2.95211900	-3.32038400	3.46236100
H	3.87493600	-1.34760700	4.65091600
C	-0.08387800	1.73432600	-1.44414700
C	0.30888300	2.03758300	-0.13501800
C	0.35195500	2.56073000	-2.48258900
C	1.09531600	3.15615400	0.12707500
H	0.00631900	1.40104300	0.69259500
C	1.14318200	3.67782800	-2.22324600
H	0.05960900	2.33060900	-3.50382300
C	1.50836500	3.98531100	-0.91531300
H	1.37239900	3.38991000	1.15082000
H	1.46298300	4.31261800	-3.04322600
H	2.10607000	4.86642700	-0.70551000
H	-1.36227200	0.63891400	-2.79283500
H	-0.90625300	-1.60291500	-2.07829400
C	-4.93052100	-3.62137600	0.73313400
C	-4.61061400	-2.88283900	-0.41081800
C	-3.41827100	-3.10055000	-1.09684400
C	-2.52229000	-4.04012100	-0.58927200
C	-2.82542500	-4.75587400	0.57019000
C	-4.03644400	-4.56153500	1.23213100
C	-6.30465900	-3.26896700	1.24286800
C	-6.93737100	-2.58666100	0.01037800
C	-5.74724500	-1.94538200	-0.74956600
H	-3.20383300	-2.56489200	-2.01515200
H	-1.58872000	-4.22839300	-1.10982000
H	-2.12004600	-5.48907400	0.94725700
H	-4.28300900	-5.14519300	2.11349200
H	-6.23421000	-2.58610600	2.09808900
H	-7.35280200	-3.35291000	-0.64722400
H	-6.88441600	-4.13535900	1.56700200
H	-5.92628200	-1.79830100	-1.81488400
N	-5.54906300	-0.58908600	-0.15407900
O	-7.99632900	-1.68676800	0.25106000

C	-4.51206400	0.24476700	-0.31716600
C	-6.39911300	0.00813000	0.73847200
N	-4.75882600	1.29586600	0.46564300
N	-5.93117600	1.15977800	1.13655900
C	-7.69279300	-0.63630900	1.13601600
H	-7.63651900	-0.97117300	2.17900800
H	-8.49655700	0.09781000	1.05730300
C	-3.93499500	2.45725600	0.65906600
C	-3.44294800	3.14529500	-0.44638300
C	-3.60932500	2.82310800	1.95911300
C	-2.56075200	4.19919700	-0.24483400
H	-3.73469100	2.85959200	-1.45174300
C	-2.74602800	3.89401200	2.15880100
H	-4.02113100	2.27578200	2.79981200
C	-2.21691000	4.55935300	1.05603400
H	-2.13662300	4.73243200	-1.08792400
H	-2.47426900	4.20168800	3.16154500
Cl	-1.10491600	5.86769500	1.30917400
C	4.30267400	1.35890000	-1.45253100
H	5.30439100	1.55651700	-1.06483400
H	4.30771400	1.47873800	-2.54154400
H	3.59467500	2.06021500	-1.00569300

Variable frequencies

-39.3476	12.0562	16.7741
20.0782	24.7164	27.8726
32.0485	37.1998	42.6605
47.8927	51.2473	60.5653
64.7253	67.8805	69.7347
74.0919	80.8126	88.8364
98.2490	101.3637	102.1054
112.1006	123.2429	128.1911
143.5395	146.7583	155.2495
170.9114	175.2697	184.2621
189.3948	191.9405	208.4890
216.2241	220.2245	243.1744
247.4256	258.0153	258.4772
262.0752	270.0580	281.2570
288.3852	302.2675	311.5090
324.6905	326.9114	342.5891
344.0875	357.3427	365.7007
374.5613	383.5851	387.4476
400.7447	414.6427	419.3287
420.4181	423.4946	425.8166

439.2968	448.5342	459.2959
468.3938	489.0261	496.1277
504.0661	511.1115	513.8007
535.4253	539.4063	546.4213
557.5549	559.5161	569.9292
581.5759	591.4129	595.0572
607.1485	620.7756	624.3043
629.3925	633.9025	641.4249
642.7641	644.0139	654.4242
662.9543	676.0086	697.8460
702.5328	708.6674	718.4241
720.1580	722.8875	726.3575
730.5985	750.8646	760.7407
767.0732	774.9179	781.1343
784.8744	787.1795	793.8174
814.0947	824.7290	834.5473
839.2491	841.6647	842.2389
847.0697	853.8006	854.2052
861.3435	872.2685	875.1435
878.4475	889.1073	900.4396
913.6610	922.0022	940.2158
948.6783	956.7570	973.1684
977.4203	988.8068	990.0650
992.8240	997.4899	1002.3388
1008.6516	1011.9033	1015.1956
1015.5582	1018.0817	1025.1469
1025.3684	1027.5318	1033.7610
1033.8548	1035.5465	1043.1375
1053.1408	1064.2475	1065.1763
1071.6181	1073.9312	1075.9360
1081.4584	1097.9296	1104.7994
1115.0252	1118.1383	1120.4121
1126.6462	1135.3700	1137.0899
1139.4666	1141.8035	1148.9736
1160.1789	1164.7649	1166.8615
1179.1167	1181.9250	1182.2143
1184.8266	1192.1678	1200.9193
1205.8647	1206.9380	1207.6169
1209.8157	1211.5678	1219.9587
1222.0848	1243.3934	1248.3588
1253.2682	1254.2853	1266.3667
1269.5285	1281.7423	1284.4037
1305.3420	1308.3527	1311.4536
1318.1217	1320.8193	1328.4406

1328.5870	1337.2147	1339.8312
1345.9041	1355.1136	1355.8477
1357.9558	1360.2608	1361.3970
1364.7157	1368.9217	1375.8514
1376.4450	1385.3143	1422.8042
1423.8708	1447.2520	1453.0312
1453.9863	1455.2631	1459.5408
1464.8677	1495.3585	1496.8230
1497.8319	1499.4270	1500.7211
1505.0894	1506.4259	1507.8510
1523.9461	1528.6132	1537.1819
1543.0713	1547.8243	1548.6738
1550.3091	1562.6897	1587.4758
1623.3194	1661.0157	1664.2652
1666.8045	1673.6114	1675.5031
1681.6807	1682.5610	1685.4266
1689.9510	1693.3085	1697.6231
1704.4585	1731.5389	3066.5633
3077.4146	3079.5925	3092.1119
3108.2316	3112.9169	3147.2584
3150.1237	3154.3546	3158.9992
3169.5561	3172.4198	3175.2796
3184.2532	3196.1836	3196.9843
3202.9803	3205.2452	3211.7626
3212.3370	3212.6311	3213.6867
3214.1395	3215.0246	3216.5466
3220.5144	3223.1279	3228.1532
3228.3321	3229.0004	3230.7185
3233.0197	3234.5265	3235.3191
3237.9869	3238.6839	3242.3929
3244.1177	3247.3946	3256.0167

²TS5S^e

Zero-point correction=0.779137

Thermal correction to Energy=0.826094

Thermal correction to Enthalpy=0.827038

Thermal correction to Gibbs Free Energy=0.696172

Sum of electronic and zero-point Energies=-3207.918655

Sum of electronic and thermal Energies=-3207.871697

Sum of electronic and thermal Enthalpies=-3207.870753

Sum of electronic and thermal Free Energies=-3208.001620

Cartesian coordinate

N	-0.09496200	-1.61459200	-1.08082700
N	-0.94024100	-2.11620800	-0.09663900
C	-0.35757200	-2.06629100	1.24230700
C	-0.57416100	-0.60716300	-1.92073300
C	0.24998600	-0.13700600	-2.89057900
C	1.62459700	-0.60995600	-3.00330900
C	1.82580200	-1.93779100	-2.43797400
C	1.01413700	-2.36152200	-1.45127700
C	2.81668900	0.50933700	-2.07112000
C	2.27637000	0.72821200	-0.77189500
C	1.71605700	1.98337800	-0.46861900
O	1.67998000	2.97389200	-1.22531500
S	-1.64457900	-3.63016000	-0.54322700
O	-1.91342100	-3.48592800	-1.96285600
C	-3.13062600	-3.58372400	0.40321700
O	-0.80165000	-4.71190100	-0.04624200
C	-3.30324900	-4.49812400	1.43691300
C	-4.48656600	-4.45477900	2.16639400
C	-5.47951200	-3.51590300	1.87249300
C	-5.26836800	-2.60945000	0.82446300
C	-4.09985700	-2.63720600	0.07760600
C	-1.97550900	-0.15934600	-1.72625100
C	-2.90496100	-0.37407400	-2.74360000
C	-4.23326300	0.01589400	-2.56857500
C	-4.63301900	0.61323500	-1.37747000
C	-3.70253300	0.83398900	-0.36002700
C	-2.37984000	0.45153200	-0.53474900
C	-6.76938900	-3.49486800	2.64743700
H	-0.17373200	-1.01391600	1.47382700
H	-1.08778900	-2.46330900	1.95019100
H	0.57651500	-2.63480400	1.32449400
H	-0.12003300	0.63877500	-3.55123100
H	2.66827200	-2.54700000	-2.73851500
H	1.13556900	-3.30269100	-0.92554400
H	2.76081700	1.41023900	-2.68447700
H	-2.52787400	-5.22585500	1.65207300
H	-4.64225500	-5.16346200	2.97398400
H	-6.03352300	-1.87473000	0.58946100
H	-3.93837800	-1.94344000	-0.74219100
H	-2.59084300	-0.87504100	-3.65374800
H	-4.95462100	-0.16084900	-3.35942200
H	-5.66677700	0.91527700	-1.24067000
H	-4.01181100	1.31132600	0.56446900
H	-1.64761500	0.62235900	0.25176500

H	-7.54174700	-4.05653300	2.11249000
H	-6.64863400	-3.94961900	3.63239200
H	-7.13609100	-2.47409100	2.77660000
C	4.12334700	-0.20516600	-2.22352700
C	4.85165500	-0.01986200	-3.40202700
C	4.63405200	-1.06511000	-1.24501600
C	6.06441600	-0.67258100	-3.60035400
H	4.46749500	0.65204600	-4.16586500
C	5.84687500	-1.71849900	-1.44211900
H	4.08808100	-1.22681400	-0.32002900
C	6.56587500	-1.52469200	-2.61983700
H	6.61850600	-0.51130300	-4.51913400
H	6.23206800	-2.37891100	-0.67138100
H	7.51292500	-2.03178800	-2.77038100
H	2.27161800	-0.06576200	-0.03297200
C	-2.64014700	4.25307900	-0.30236400
C	-1.36221100	3.83990700	-0.69587900
C	-1.16386700	3.26719800	-1.95201800
C	-2.26282600	3.09586000	-2.79067900
C	-3.53353100	3.51338400	-2.39816900
C	-3.72911000	4.10096000	-1.15085400
C	-2.62364600	4.88557100	1.06067600
C	-1.14079100	5.26267200	1.22274100
C	-0.32961100	4.26695100	0.32868700
H	-0.17177200	2.98126400	-2.27790400
H	-2.12502400	2.64829200	-3.77015700
H	-4.37458500	3.38174300	-3.07149900
H	-4.71400700	4.44320200	-0.84746100
H	-2.95622500	4.16799200	1.82016500
H	-0.98450600	6.24870000	0.78033000
H	-3.26785500	5.76344800	1.14222100
H	0.54049500	4.73400600	-0.12953500
N	0.24265600	3.18661400	1.20406300
O	-0.67827800	5.38027500	2.54961700
C	1.14604500	2.22624400	0.90575800
C	0.07699000	3.15469500	2.56500700
N	1.47213200	1.66205400	2.07505200
N	0.80697900	2.22759500	3.11533600
C	-0.74460200	4.17990600	3.27875300
H	-1.77349600	3.82917000	3.42047400
H	-0.30377700	4.35863100	4.26000200
C	2.50230600	0.70257500	2.36429300
C	2.17697900	-0.42149400	3.11303700
C	3.80023200	0.94228600	1.92353800

C	3.16732200	-1.35731900	3.39029100
C	4.78737300	0.00447000	2.19565300
C	4.45899700	-1.14245500	2.91644400
H	2.94079800	-2.24476200	3.96936200
H	5.80292700	0.15913400	1.85012800
H	4.03796200	1.84168100	1.36548900
H	1.16701100	-0.55496500	3.48566800
Cl	5.68916000	-2.32286200	3.23434100
H	2.08644400	-0.44710100	-3.97626000

Variable frequencies

-283.4818	13.1942	18.6086
22.8503	24.0944	28.1823
35.1548	41.1436	46.5998
54.0851	58.1749	61.4258
65.0116	70.0848	72.1388
78.1801	85.2538	86.4331
91.9821	95.2334	104.7239
114.7647	133.5370	145.5027
148.9103	149.1625	156.6803
173.4779	179.7976	186.5570
193.9111	208.1219	212.9280
217.9143	242.6567	246.8586
251.4501	254.5882	267.6425
274.1340	282.5198	288.6451
293.7071	304.1851	319.0202
328.3545	336.8644	343.9654
355.1212	362.9538	374.9496
381.5526	385.9139	396.8214
410.0094	416.0080	417.9797
420.9354	422.4518	426.8848
442.9855	452.6698	454.5010
471.1127	478.8929	493.1265
498.7163	511.8182	521.4914
525.1838	529.2818	536.6125
557.2055	560.7222	579.9896
586.7763	592.3426	597.2771
607.0231	611.4657	623.5389
626.4539	632.7970	641.0451
643.1346	644.2722	653.3174
664.6454	668.2545	698.5062
707.3711	710.3493	711.2570
718.5349	719.1108	720.1725
728.8706	751.5545	762.1445

765.4466	772.8000	779.6259
783.9329	785.9958	804.1067
813.3083	818.9351	829.0120
840.0418	844.0058	846.9628
849.6268	852.6496	862.0496
865.3327	866.2136	871.2734
871.6504	888.4702	900.7363
911.7296	916.3800	939.8456
946.2445	955.4142	980.5009
981.2070	989.8498	990.0647
991.1888	996.9595	1000.9688
1005.9232	1008.5412	1014.2690
1017.5135	1018.9147	1021.8745
1023.9789	1024.6776	1027.3587
1035.8725	1039.2004	1039.4634
1056.5174	1063.8445	1065.9675
1070.3445	1073.4350	1075.6602
1084.4479	1099.9478	1105.4803
1113.2017	1118.2908	1121.6550
1123.8296	1134.2006	1136.5611
1139.1274	1147.9355	1151.8897
1159.1454	1161.0460	1170.8464
1175.8040	1181.5724	1182.2391
1185.0689	1185.5094	1186.6802
1201.2010	1202.9474	1204.2049
1205.8827	1215.8912	1215.9966
1227.8953	1233.6020	1241.9611
1248.0312	1254.7694	1259.7459
1280.1596	1281.4209	1287.9605
1299.8818	1303.6990	1315.3621
1319.9848	1321.7955	1330.4502
1333.2274	1335.1058	1337.4918
1349.5326	1354.1040	1358.2008
1358.9867	1359.5265	1360.6810
1366.0145	1369.7871	1377.6492
1379.8479	1384.7090	1423.8432
1425.0530	1446.2465	1453.2454
1456.6740	1462.3103	1462.8344
1483.1226	1490.2733	1494.5552
1497.5017	1502.0052	1502.4039
1503.7252	1504.1405	1512.9063
1514.2798	1520.6855	1533.1884
1536.9949	1545.2905	1546.7128
1550.1379	1567.9751	1574.2165

1629.9502	1642.6434	1669.7236
1671.8407	1672.5520	1677.8790
1679.0630	1681.7813	1687.4486
1688.8094	1695.4509	1696.7463
1700.5409	1720.6415	3065.6485
3074.6572	3077.4127	3096.0220
3144.9627	3147.9308	3155.9059
3158.4098	3161.1658	3174.5688
3177.7852	3181.8272	3183.8281
3185.4117	3188.3434	3195.7338
3197.6980	3201.7358	3202.4602
3203.3705	3212.6835	3213.7337
3216.0412	3216.1502	3217.5618
3218.4077	3222.3640	3230.1756
3231.5819	3232.6412	3233.2607
3234.4871	3234.7030	3234.8008
3235.6791	3238.5608	3247.5835
3252.7905	3254.4815	3270.8479

²TS5S^f

Zero-point correction=0.778927

Thermal correction to Energy=0.826542

Thermal correction to Enthalpy=0.827486

Thermal correction to Gibbs Free Energy=0.691516

Sum of electronic and zero-point Energies=-3207.924980

Sum of electronic and thermal Energies=-3207.877365

Sum of electronic and thermal Enthalpies=-3207.876421

Sum of electronic and thermal Free Energies=-3208.012391

Cartesian coordinate

N	2.42025400	-0.15267100	0.20828500
N	3.55370900	-0.71494900	-0.37016700
C	3.28976000	-1.50088700	-1.57771300
C	2.45388700	1.19272200	0.55296800
C	1.40349400	1.72059500	1.23961100
C	0.20307200	0.95356500	1.51153700
C	0.38697500	-0.48179100	1.40193100
C	1.44540700	-0.98182800	0.73209400
C	-1.02215700	1.44380800	0.13703900
C	-2.20235600	0.65943500	0.24554200
C	-2.38395400	-0.49557900	-0.53113000
O	-1.54286000	-1.09373800	-1.23176500
S	4.55424800	-1.49870500	0.80283100

O	4.42608600	-0.66933200	1.98878700
C	6.13709300	-1.29728400	0.05289400
O	4.21605900	-2.91652800	0.84577000
C	6.80599100	-2.41245000	-0.43894100
C	8.04995500	-2.22786800	-1.03456700
C	8.61601600	-0.95466500	-1.13993200
C	7.91059200	0.14602600	-0.63423700
C	6.67220800	-0.01220200	-0.03158900
C	3.64417300	1.99553300	0.18428000
C	4.33093000	2.68704800	1.18446100
C	5.43966100	3.46652500	0.85908300
C	5.86368900	3.55912800	-0.46386400
C	5.17617000	2.87248700	-1.46527000
C	4.07176400	2.09270600	-1.14392500
C	9.97196800	-0.76283100	-1.76413700
H	2.77207400	-0.85580400	-2.28881600
H	4.25243000	-1.79559900	-2.00017300
H	2.69460500	-2.39912500	-1.38267200
H	1.44340300	2.77149200	1.50024300
H	-0.36087700	-1.15960500	1.79552200
H	1.61869700	-2.04251100	0.58361000
H	-0.40130900	1.14660800	-0.70940500
H	6.35818600	-3.39660000	-0.34895400
H	8.58897100	-3.08679900	-1.42241000
H	8.33957900	1.14089500	-0.71519100
H	6.12918000	0.84090700	0.36568000
H	4.01045800	2.58738000	2.21664300
H	5.97395800	3.99322800	1.64253600
H	6.72779700	4.16477600	-0.71682900
H	5.50284100	2.94391300	-2.49735900
H	3.53748000	1.55684100	-1.92287900
H	10.73188400	-0.62967200	-0.98784100
H	10.25768400	-1.62553600	-2.36840900
H	9.99034500	0.12750400	-2.39711500
C	-1.16279500	2.92161600	0.28902200
C	-0.38822000	3.76395200	-0.51531900
C	-2.04876700	3.49566000	1.20879100
C	-0.51499000	5.14760400	-0.42403300
H	0.31529400	3.32711700	-1.21996500
C	-2.17288900	4.87731300	1.30293500
H	-2.65542100	2.86521300	1.85409600
C	-1.41156900	5.70809000	0.48178100
H	0.08703500	5.78635500	-1.06202100
H	-2.87045100	5.30723100	2.01443500

H	-1.51566700	6.78567100	0.55188900
H	-3.02010500	0.99521700	0.87255600
C	-3.31509000	-4.74461700	1.05029300
C	-2.58144300	-3.83055200	0.28736500
C	-1.31141600	-3.42405700	0.68446000
C	-0.80425800	-3.91076000	1.88892800
C	-1.55040100	-4.79452200	2.67005500
C	-2.80695400	-5.22676400	2.25057600
C	-4.60078100	-5.11638400	0.36011500
C	-4.29370100	-4.71591200	-1.09870100
C	-3.32307500	-3.50800300	-0.99027100
H	-0.73829700	-2.74987800	0.05780300
H	0.18766500	-3.61471000	2.21850100
H	-1.13710800	-5.16752300	3.60131400
H	-3.37067300	-5.94194200	2.84135300
H	-5.43954400	-4.54491400	0.77577600
H	-3.73085300	-5.52252200	-1.57319700
H	-4.85303100	-6.17514200	0.44549400
H	-2.68168700	-3.37175100	-1.86100000
N	-4.16909700	-2.27786200	-0.89713200
O	-5.39965300	-4.48637300	-1.94019800
C	-3.80212400	-1.00563100	-0.64743100
C	-5.52393100	-2.26593100	-1.10460100
N	-4.93127500	-0.29019600	-0.70484900
N	-6.01163100	-1.06442200	-0.98027500
C	-6.28691500	-3.50243200	-1.47039900
H	-6.87652900	-3.84704100	-0.61195600
H	-6.97551100	-3.26579600	-2.28313000
C	-5.11124200	1.12868600	-0.55094900
C	-5.97765600	1.57599300	0.43740000
C	-4.40844400	2.00740700	-1.36897000
C	-6.13032500	2.94502100	0.62985800
C	-4.54514700	3.37335600	-1.16184700
C	-5.40359900	3.82802500	-0.16283200
H	-6.80100200	3.32398200	1.39182500
H	-3.98835300	4.08126800	-1.76490400
H	-3.74783300	1.63145100	-2.14268000
H	-6.52145000	0.86379500	1.04813700
Cl	-5.56841600	5.53655000	0.09890400
H	-0.40117000	1.30194000	2.34688400

Variable frequencies

-173.1659	6.3187	11.5749
17.6047	19.7437	22.0284

25.2684	31.4377	35.2299
41.4046	50.1497	53.1193
58.5520	67.9637	70.2535
72.6158	78.8893	83.9956
85.7871	89.3986	103.3543
104.8591	115.6523	123.6421
138.7853	146.3389	147.1687
162.5715	176.0848	180.6351
189.8989	200.8591	206.1986
207.6292	216.1655	243.3574
246.6793	255.4835	256.4040
259.0274	265.5810	282.5777
291.0583	300.0083	307.5052
313.2667	328.5284	342.6519
345.8316	359.0394	365.1734
375.5720	380.2280	383.1385
406.7838	410.7200	415.0340
416.9446	423.4427	427.4002
442.4201	447.9195	457.7085
464.8515	487.7980	495.2662
498.2239	506.3060	518.3822
528.9424	541.1899	542.2020
558.3549	562.6875	575.2045
582.3135	587.5552	593.1397
607.7045	607.9971	622.6745
627.8996	629.3780	640.4903
642.3472	644.2984	653.6912
665.3014	681.4629	699.9443
707.9012	712.5984	717.8214
718.5603	720.0365	726.8208
730.6586	758.9077	763.5127
768.1902	775.7663	785.9155
791.0999	792.5922	803.3038
814.3314	826.5653	829.6845
838.3559	844.1013	845.9788
850.3860	854.4116	863.1337
868.0920	879.9365	880.7879
885.1477	889.8942	900.3101
913.3159	915.1509	946.6888
959.1538	976.4441	981.4301
988.5133	990.0077	995.8089
996.4011	1004.3002	1005.4236
1008.8962	1009.2538	1015.0096
1015.7772	1019.2752	1025.8406

1033.3947	1033.8024	1034.2145
1035.3759	1038.9875	1046.3249
1051.6190	1067.7266	1069.1202
1071.4486	1072.9022	1074.1931
1094.8789	1099.5643	1105.6758
1115.9106	1118.3591	1121.7531
1126.3657	1131.6837	1134.4323
1138.0347	1144.6595	1147.6622
1153.2536	1159.3089	1160.8157
1174.5025	1179.8343	1185.4750
1186.6382	1187.8121	1193.6989
1198.9389	1205.0309	1205.3893
1208.1132	1212.2803	1212.5999
1219.8642	1232.9297	1239.3890
1248.1540	1252.4359	1265.2354
1271.4123	1280.5795	1293.6210
1300.4769	1303.5399	1314.8871
1319.3397	1321.4939	1324.6228
1330.5304	1336.5213	1338.6138
1347.2375	1353.3095	1356.3145
1357.7383	1358.8933	1364.8125
1367.0245	1371.7459	1377.3177
1381.9357	1384.5381	1423.6128
1429.4115	1449.6388	1454.6923
1455.7798	1457.1262	1461.9299
1489.8824	1493.9430	1498.4496
1499.4405	1500.1970	1501.7876
1503.3026	1506.2144	1509.4379
1510.1209	1526.4903	1533.4975
1541.1408	1545.9986	1547.5690
1549.0534	1569.9094	1571.9418
1627.9516	1638.4370	1667.8378
1669.2466	1670.3939	1671.3714
1680.1808	1682.7413	1685.2254
1686.7278	1693.0133	1695.1488
1705.9013	1723.2727	3071.3732
3075.5481	3083.9001	3090.7796
3146.1909	3154.6288	3156.0806
3158.0273	3162.0935	3167.1773
3173.3858	3179.3093	3181.7086
3187.6900	3201.9548	3208.9251
3209.5583	3210.4657	3210.4751
3211.7873	3212.9592	3215.1482
3223.5947	3226.3382	3229.1118

3229.2117	3230.7502	3231.7698
3234.5944	3235.4302	3238.0670
3239.0738	3240.7635	3243.7494
3244.3156	3244.9782	3247.4806
3250.2280	3251.4658	3257.1227

²M5R

Zero-point correction=0.780169

Thermal correction to Energy=0.827864

Thermal correction to Enthalpy=0.828808

Thermal correction to Gibbs Free Energy=0.694887

Sum of electronic and zero-point Energies=-3207.948658

Sum of electronic and thermal Energies=-3207.900964

Sum of electronic and thermal Enthalpies=-3207.900019

Sum of electronic and thermal Free Energies=-3208.033940

Cartesian coordinate

N	-0.24365000	-3.16172900	-0.84817000
N	0.72096300	-3.21282400	0.15549600
C	0.81842300	-4.48818300	0.86841900
C	-1.59984900	-3.24588100	-0.48888700
C	-2.58251400	-2.72670700	-1.22884600
C	-2.31834100	-1.86927700	-2.43798200
C	-0.86219700	-1.94249500	-2.81326700
C	0.09240200	-2.47702000	-2.03809600
C	-2.73636400	-0.36671800	-2.20088400
C	-2.00539500	0.17258200	-1.02947800
C	-1.16118700	1.31329000	-1.08988500
O	-0.86723900	1.95288500	-2.10532300
S	0.75610900	-1.82751200	1.14190800
O	0.53801500	-0.72356700	0.20401800
C	2.42824300	-1.80547900	1.69472100
O	-0.13935000	-1.93317600	2.29434300
C	2.68241000	-1.55873000	3.03765500
C	4.00555600	-1.40757800	3.44294100
C	5.05499200	-1.50335100	2.52666600
C	4.75917000	-1.76104800	1.18014100
C	3.45017200	-1.90775200	0.75040900
H	0.96669700	-5.26792700	0.12127500
H	1.69278100	-4.44804300	1.52115400
H	-0.06666800	-4.71160800	1.47247900
H	-3.60924200	-2.91772600	-0.93544900
H	-2.94441100	-2.20138100	-3.27692200

H	-0.55857100	-1.51771600	-3.76537300
H	-2.43920800	0.20088700	-3.08947300
H	1.86089400	-1.49003100	3.74326400
H	4.22530800	-1.21805500	4.48917200
H	5.56865500	-1.84809900	0.46018300
H	3.21855300	-2.10253000	-0.29338000
C	-4.23995500	-0.21568300	-2.01231000
C	-4.85785500	-0.39446700	-0.77052500
C	-5.03146600	0.08525100	-3.12330300
C	-6.24006800	-0.27526500	-0.64550500
H	-4.26566600	-0.62821500	0.11154700
C	-6.41243300	0.19932400	-3.00035800
H	-4.55880100	0.23344300	-4.09074100
C	-7.02046000	0.02130800	-1.75956400
H	-6.70502400	-0.41440800	0.32599200
H	-7.01284900	0.43423600	-3.87309700
H	-8.09685100	0.11535300	-1.66135400
H	-2.06092900	-0.36654300	-0.08909100
C	3.60481300	3.67397300	-0.97574800
C	2.22997600	3.47674000	-1.06475600
C	1.36544700	4.49469000	-1.45255100
C	1.90812400	5.74419500	-1.73766700
C	3.28634800	5.95519400	-1.64168700
C	4.14421100	4.92392200	-1.26715700
C	4.31659800	2.40397100	-0.58374700
C	3.20098400	1.42222300	-0.15714100
C	1.86850800	2.05422300	-0.71239900
H	0.29878800	4.30965300	-1.54223200
H	1.25937200	6.55903200	-2.04035600
H	3.69363800	6.93586600	-1.86517000
H	5.21436600	5.09398400	-1.20091900
H	5.02850400	2.53638200	0.23656300
H	3.33406100	0.42796900	-0.58824100
H	4.87475300	1.99487000	-1.43296400
H	1.50168500	1.49232100	-1.57320200
N	0.81470800	1.99957400	0.30538800
O	3.19500900	1.19422000	1.24293600
C	-0.48090600	1.69355500	0.19684100
C	1.09631900	2.07430900	1.63839300
N	-0.94964300	1.64715300	1.44175800
N	0.02985300	1.86394200	2.35981200
C	2.53621800	2.17577900	2.01901600
H	2.92490600	3.18596500	1.83337600
H	2.66891300	1.91799400	3.06963200

C	-2.29455500	1.37428400	1.85953400
C	-3.33340800	2.16013000	1.37236700
C	-2.50871300	0.30917200	2.72838000
C	-4.63418900	1.87302200	1.76980500
C	-3.81006300	0.03186000	3.12960000
C	-4.85680100	0.81672500	2.64916500
H	-5.46616000	2.46438000	1.40587000
H	-4.01437200	-0.78996200	3.80587400
H	-1.67245400	-0.29982600	3.05721000
H	-3.13273800	2.99088000	0.70315400
Cl	-6.48111800	0.46173300	3.15312400
H	-1.79267500	-3.82935200	0.40515900
C	1.53157700	-2.41219500	-2.38600500
C	2.35855000	-3.53854300	-2.32357700
C	2.07828400	-1.18595100	-2.76979400
C	3.71114900	-3.43282100	-2.62954100
H	1.93505300	-4.49634800	-2.03542700
C	3.43387200	-1.07739500	-3.07270600
H	1.42305500	-0.32058200	-2.82157600
C	4.25478200	-2.20040000	-2.99447600
H	4.34414800	-4.31288000	-2.58426300
H	3.84656700	-0.11729200	-3.36927200
H	5.31148900	-2.12071000	-3.22787600
C	6.48503100	-1.33676300	2.96433800
H	7.08024000	-2.21072900	2.68595600
H	6.93659600	-0.46635500	2.47918600
H	6.55911200	-1.20201900	4.04463700

Variable frequencies

10.4578	17.3502	20.7626
26.7066	29.5944	32.8102
36.9309	40.8547	44.1966
47.6230	49.7776	55.2347
63.4531	70.9597	76.4350
79.6637	83.2898	87.5420
89.3134	101.3206	107.2045
114.3201	118.8988	123.8538
136.3389	143.5770	158.1306
166.7679	176.5640	191.6488
198.9131	209.6907	217.9479
220.0198	227.4183	231.0060
249.0655	254.3444	261.7065
268.8256	272.4697	288.9922
310.5652	314.0616	323.9481

331.3702	338.7676	351.2701
356.9803	365.9524	372.8217
390.5560	405.3770	407.6339
416.6002	417.6770	421.0682
423.6679	426.8902	439.9953
450.0423	453.7991	471.1553
481.3943	487.8365	494.6580
498.8120	513.1324	520.0616
523.6465	535.9824	549.6702
563.9701	566.9562	572.4450
586.2356	602.2046	616.5920
619.8848	626.9146	628.3181
630.7367	640.3478	641.1626
645.7490	658.3417	663.8888
678.8547	709.3996	715.6322
717.9863	720.2778	723.7514
725.9705	730.3722	733.1499
740.5859	760.7664	763.7775
768.5700	779.3831	788.1465
791.9489	798.0913	813.1987
816.6654	830.8097	838.4780
839.9546	840.7096	844.6983
856.6433	865.9326	868.0897
873.0026	880.4176	886.5075
887.8535	890.6915	892.9152
903.2755	919.4382	947.1599
955.2132	957.4082	973.6461
974.9680	989.3795	990.6817
992.2433	1001.0905	1006.5966
1008.7460	1010.5701	1014.4141
1015.1242	1017.0797	1023.7815
1027.8898	1028.8312	1032.2042
1033.3874	1033.5286	1039.4233
1047.9816	1054.9533	1067.0329
1067.2236	1067.5689	1073.1293
1077.2321	1081.6636	1106.0766
1112.8289	1115.9930	1119.3027
1123.2318	1133.5845	1135.8182
1141.8057	1143.3934	1144.9649
1150.2993	1164.2588	1166.9672
1173.5949	1180.8214	1181.5176
1185.2422	1195.4088	1202.7417
1205.1423	1206.1476	1209.7441
1210.3153	1221.6725	1222.9489

1226.8318	1233.9340	1248.3002
1254.9116	1256.1272	1270.6740
1278.7802	1283.0546	1289.9968
1297.3284	1301.0225	1306.2858
1313.6201	1324.3432	1327.2013
1331.2840	1332.8402	1333.7011
1337.7306	1347.0223	1349.5479
1359.2206	1363.0641	1363.3891
1368.1691	1373.2828	1374.6844
1379.9829	1386.6432	1425.6228
1427.1865	1431.3324	1444.2603
1455.1075	1456.7966	1465.0585
1476.9032	1482.4558	1495.0618
1497.2744	1498.3662	1500.7575
1501.6963	1505.2385	1516.4743
1518.7966	1519.8583	1541.8398
1545.5471	1548.8045	1552.4419
1554.8436	1563.9457	1610.2186
1632.3551	1668.1175	1669.1632
1675.9300	1677.2231	1684.0796
1685.2036	1691.5548	1692.3103
1695.6126	1697.8993	1703.4185
1732.5480	1779.1097	3057.0992
3077.2677	3079.6067	3080.3658
3081.5648	3109.0567	3127.7593
3148.6472	3156.6241	3164.1944
3166.8050	3175.1623	3186.0332
3198.3916	3198.8934	3200.6343
3204.0192	3205.3833	3206.9048
3208.1130	3211.6807	3212.8557
3213.3570	3218.8972	3219.6296
3220.3696	3221.2215	3221.2318
3223.0077	3230.1028	3231.7646
3232.6052	3233.5895	3235.3630
3235.6440	3236.2128	3240.2321
3241.3981	3243.5882	3244.9308

²M5S

Zero-point correction=0.781294

Thermal correction to Energy=0.828308

Thermal correction to Enthalpy=0.829252

Thermal correction to Gibbs Free Energy=0.699180

Sum of electronic and zero-point Energies=-3207.950817

Sum of electronic and thermal Energies=-3207.903804
Sum of electronic and thermal Enthalpies=-3207.902860
Sum of electronic and thermal Free Energies=-3208.032931

Cartesian coordinate

N	0.57737100	0.37432500	-2.44195200
N	1.53957900	1.18560400	-1.86519900
C	2.81827900	1.26559400	-2.57537500
C	0.82966700	-0.99330900	-2.61303100
C	-0.14282200	-1.87531200	-2.85906700
C	-1.60167600	-1.52192900	-2.75792000
C	-1.76444900	-0.02603100	-2.70488900
C	-0.75480200	0.83625500	-2.49663800
C	-2.20422900	-2.22935500	-1.47741500
C	-1.37957000	-1.80141600	-0.32414900
C	-0.62038800	-2.68849700	0.48354500
O	-0.55938500	-3.91789700	0.38401400
S	1.67945300	1.04240300	-0.17381300
O	0.32066300	0.76308100	0.28785000
C	2.14875000	2.67781900	0.29024900
O	2.74749900	0.11485800	0.21075000
C	3.42982600	2.91428400	0.77747300
C	3.77818500	4.21586200	1.12327200
C	2.86712300	5.26689900	0.98355800
C	1.58609800	4.99135900	0.48652000
C	1.21349600	3.70205600	0.13780700
C	3.24161800	6.66959900	1.37869800
H	2.59904300	1.50599600	-3.61582800
H	3.40234700	2.07768500	-2.13663400
H	3.39568000	0.33616600	-2.51699500
H	0.13066300	-2.90497700	-3.06053600
H	-2.75821400	0.38823500	-2.83605600
H	-2.09622300	-3.31170100	-1.61081500
H	4.13408900	2.09494500	0.87935500
H	4.77400300	4.41881500	1.50512300
H	0.87108500	5.80014000	0.36534700
H	0.21916700	3.49305400	-0.24688700
H	4.32483000	6.79544100	1.42227300
H	2.83414400	7.39748700	0.67352900
H	2.83593400	6.90630100	2.36742700
C	-3.67469600	-1.89546800	-1.29114800
C	-4.62882300	-2.67245900	-1.95212400
C	-4.10400800	-0.81177600	-0.51926200
C	-5.98348500	-2.37365300	-1.84762900

H	-4.30557900	-3.52100600	-2.54987600
C	-5.46083000	-0.51518900	-0.40892400
H	-3.38461800	-0.19468400	0.01496300
C	-6.40358100	-1.29421300	-1.07343400
H	-6.71209400	-2.98854000	-2.36574900
H	-5.77794500	0.32608200	0.20009400
H	-7.46020400	-1.06419300	-0.98639200
H	-1.25235500	-0.73575800	-0.15205500
C	3.96933000	-2.68944800	-0.47694800
C	2.72983400	-3.28796400	-0.22258000
C	2.03289900	-3.93876300	-1.23781500
C	2.56971900	-3.93704800	-2.52477900
C	3.77628600	-3.28908500	-2.79186000
C	4.48855500	-2.66776000	-1.76636700
C	4.62610000	-2.22394900	0.79265200
C	3.86373700	-3.03690100	1.85799000
C	2.44331700	-3.28889200	1.26319100
H	1.10439100	-4.45943300	-1.03030800
H	2.05159800	-4.45739300	-3.32402200
H	4.18092000	-3.30084100	-3.79884400
H	5.45423800	-2.21155600	-1.96233600
H	4.48670600	-1.14724200	0.91786700
H	4.32753600	-4.02185600	1.94711600
H	5.69652700	-2.43750300	0.82377400
H	2.00181400	-4.22313900	1.61428500
N	1.53353300	-2.21121800	1.76709400
O	3.86534000	-2.51031600	3.16436100
C	0.22729100	-2.01205400	1.52685800
C	1.88327900	-1.30206700	2.73138100
N	-0.16191700	-1.04082200	2.34691000
N	0.86356900	-0.57713600	3.09844200
C	3.27369000	-1.23790000	3.27076400
H	3.83348300	-0.46517000	2.72929800
H	3.24044700	-0.97388800	4.32817600
C	-1.47948000	-0.49976000	2.50605800
C	-1.64069900	0.88153600	2.48349100
C	-2.55117800	-1.36716600	2.69589400
C	-2.91608100	1.40617500	2.65081600
C	-3.82694300	-0.83851800	2.85555700
C	-3.99482400	0.54321300	2.83528200
H	-3.07556000	2.47804800	2.63968500
H	-4.68029900	-1.49056400	3.00025500
H	-2.39397800	-2.44047800	2.73507300
H	-0.78183200	1.52121000	2.31947900

Cl	-5.58380600	1.21022200	3.04760000
H	-2.16698500	-1.93129100	-3.60520000
H	1.87890200	-1.27422300	-2.59165500
C	-0.98051800	2.29449100	-2.34788500
C	-0.21176900	3.23536000	-3.04139700
C	-1.98736000	2.73824300	-1.48614800
C	-0.44740100	4.59482100	-2.87442500
H	0.56723300	2.89641600	-3.71749900
C	-2.22556300	4.10121800	-1.32115900
H	-2.56769700	2.00522200	-0.93253400
C	-1.45243300	5.03176800	-2.01086600
H	0.15185400	5.31627900	-3.41997300
H	-3.01004700	4.43476100	-0.64950600
H	-1.63423500	6.09381900	-1.88139800

Variable frequencies

12.9237	17.5814	23.0341
27.0225	34.4937	36.9783
40.1194	47.9562	57.1543
58.2015	68.1160	71.6069
74.9437	78.5745	82.7616
90.8068	98.6460	100.5009
104.2165	108.8328	114.4829
116.8182	135.5336	145.6677
151.0664	158.8292	171.8627
187.6775	190.0963	203.3365
204.7139	211.7052	218.7173
229.2416	232.8815	238.2944
256.5329	265.3349	267.2675
285.4880	287.4181	297.8140
302.3868	311.2202	322.2943
327.5236	341.0339	350.1908
356.0080	360.5686	367.7622
385.1346	396.8401	407.4526
415.8087	418.9787	424.1607
425.3614	428.8513	442.5753
453.1674	460.3865	463.9986
478.4542	486.2406	495.6658
500.6674	513.7361	526.9479
532.2078	537.4038	549.0506
554.4743	565.6566	573.7802
590.6068	607.7003	613.8421
620.4452	625.5594	628.3148
629.2687	638.1360	641.6685

642.3468	651.3283	656.9518
672.2917	683.7406	704.9270
705.5879	717.1421	719.6767
722.6208	726.0593	730.9389
745.5280	757.7633	763.2635
769.9743	783.5839	786.7910
792.2686	804.0901	810.7174
820.6148	837.7418	839.6869
841.2523	843.6697	848.0250
861.1995	866.8369	867.5970
877.5664	881.2702	886.9351
888.4607	895.7065	906.3216
914.0290	921.9883	952.7247
958.3150	975.4010	976.4296
984.0424	986.4309	989.1337
994.7014	1000.7733	1002.8481
1006.0777	1006.4577	1014.6746
1017.6413	1020.1682	1024.5745
1026.0115	1026.8157	1032.2385
1035.3574	1037.1456	1040.8502
1055.2851	1064.6891	1065.5078
1071.3394	1073.8063	1075.4077
1078.2549	1095.5812	1107.4822
1112.2790	1117.0496	1119.6410
1129.5623	1132.6490	1136.1180
1138.4556	1141.5956	1149.0383
1164.2426	1165.7303	1170.1735
1177.3657	1180.6098	1183.5276
1187.3236	1197.1490	1199.5528
1203.9452	1205.0575	1209.8024
1212.5760	1222.6693	1224.0828
1225.4314	1238.0436	1246.8518
1253.7960	1259.7076	1261.3536
1280.8394	1289.2381	1294.8139
1303.9235	1310.3937	1316.9710
1318.7623	1326.0150	1327.8266
1331.6680	1336.3763	1338.6015
1343.8333	1352.1609	1359.0738
1360.0069	1360.1779	1360.6552
1367.1191	1368.2061	1372.1216
1377.4810	1383.0200	1421.9607
1424.2195	1431.3872	1443.5607
1450.1736	1452.6410	1454.4432
1461.6303	1487.4818	1498.8515

1499.5926	1500.0134	1501.7342
1504.5740	1505.3821	1515.1769
1520.4146	1521.9672	1536.8601
1539.5950	1547.7143	1552.2424
1552.2798	1556.9269	1606.9377
1629.2091	1665.1191	1668.0783
1671.8752	1677.6172	1677.9528
1681.1956	1684.7889	1687.9422
1696.3066	1698.4241	1701.9439
1725.5617	1773.7775	3064.9309
3066.7129	3077.8981	3083.6458
3105.4668	3114.5236	3146.8334
3152.7258	3154.7230	3157.3566
3166.8677	3178.4333	3182.9639
3183.1333	3199.0375	3199.4423
3201.2172	3205.2065	3207.4970
3209.5376	3210.7426	3212.6548
3213.0019	3219.3817	3219.4190
3221.2550	3222.0726	3228.0756
3228.6499	3229.1502	3229.3578
3233.6882	3235.2155	3235.9175
3238.1876	3239.9971	3241.2496
3241.9405	3245.8031	3252.9634

²TS6R

Zero-point correction=0.776643

Thermal correction to Energy=0.823573

Thermal correction to Enthalpy=0.824517

Thermal correction to Gibbs Free Energy=0.691592

Sum of electronic and zero-point Energies=-3207.923097

Sum of electronic and thermal Energies=-3207.876167

Sum of electronic and thermal Enthalpies=-3207.875223

Sum of electronic and thermal Free Energies=-3208.008148

Cartesian coordinate

N	2.38153800	-1.73526700	-1.00395200
N	3.75288200	-1.76672400	-1.24004500
C	4.17417500	-2.68109400	-2.30524400
C	1.76996000	-0.49644500	-0.89178300
C	0.46807000	-0.44714200	-0.49578300
C	-0.32759200	-1.62096500	-0.16424200
C	0.43575200	-2.86306100	-0.22062600
C	1.72446000	-2.89123600	-0.62569200

C	-1.20021800	-1.43019900	1.16618500
C	-2.29263700	-0.44944800	0.90312500
C	-2.92363800	-0.45315500	-0.29904100
O	-2.73136600	-1.27870800	-1.27994000
S	4.63948000	-1.91941200	0.24467300
O	3.87657100	-1.12543600	1.19108300
C	6.13709800	-1.10669400	-0.20829100
O	4.90648200	-3.33046000	0.48905500
C	7.30083400	-1.85372500	-0.36046700
C	8.46761100	-1.19083200	-0.72363700
C	8.47563000	0.19195100	-0.93420900
C	7.28347100	0.90955200	-0.77503100
C	6.10732800	0.27216500	-0.40761800
C	2.55902000	0.72939900	-1.15810500
C	2.62444100	1.70798700	-0.16209000
C	3.33932200	2.88392300	-0.38870000
C	3.98270100	3.08564300	-1.60766800
C	3.91635600	2.10919600	-2.60232700
C	3.21091400	0.93311900	-2.37840800
C	9.75288600	0.90045800	-1.29652400
H	3.61988100	-2.42186600	-3.20798000
H	5.23754200	-2.50749200	-2.48153400
H	4.02349900	-3.73627400	-2.05619500
H	0.00898400	0.53269600	-0.40347500
H	-0.03265000	-3.79615600	0.07589900
H	2.32299900	-3.79340400	-0.65597000
H	-1.62085200	-2.42935100	1.35164700
H	7.28358100	-2.92537400	-0.19205300
H	9.38746500	-1.75488300	-0.84491700
H	7.27726300	1.98306400	-0.93999700
H	5.18457000	0.82976600	-0.27397800
H	2.14186600	1.52730800	0.79601200
H	3.39709600	3.63567500	0.39162800
H	4.53707700	4.00178000	-1.78371200
H	4.41463700	2.26525400	-3.55319200
H	3.15863100	0.17206600	-3.15121700
H	9.55266600	1.82591500	-1.83997900
H	10.31121400	1.16000200	-0.39144700
H	10.39603200	0.26709700	-1.91095100
C	-0.28842200	-1.03411200	2.30740900
C	0.33343800	-2.00999400	3.08575500
C	0.01809300	0.31045700	2.53998800
C	1.24148400	-1.65320700	4.07924500
H	0.10648500	-3.05918600	2.91196900

C	0.92467600	0.67045500	3.53246100
H	-0.45255700	1.08576200	1.93704900
C	1.54094200	-0.31250800	4.30376300
H	1.71733500	-2.42435100	4.67601100
H	1.14870800	1.71985800	3.70164100
H	2.25067600	-0.03472400	5.07580900
H	-2.53395600	0.29695000	1.64968900
C	-7.30399600	-1.69055400	-0.06784000
C	-5.97981400	-1.79034800	-0.50461900
C	-5.10754700	-2.72554200	0.04592400
C	-5.57849100	-3.54518000	1.06933600
C	-6.89448600	-3.43653300	1.52089000
C	-7.76959300	-2.51402200	0.95061800
C	-8.05954100	-0.64786200	-0.85063300
C	-7.17206200	-0.47705100	-2.10209400
C	-5.73088100	-0.82005100	-1.63727700
H	-4.09336800	-2.81207200	-0.32934400
H	-4.91839000	-4.28398400	1.51171300
H	-7.24521100	-4.08872900	2.31416100
H	-8.79928300	-2.44792300	1.28810300
H	-8.13694300	0.28053600	-0.27252300
H	-7.45147300	-1.23326800	-2.83883100
H	-9.07515500	-0.94970700	-1.11473800
H	-5.08865800	-1.20853800	-2.42819200
N	-5.10421500	0.45254600	-1.17913200
O	-7.26666200	0.75590200	-2.78330500
C	-3.91969700	0.61746100	-0.56818500
C	-5.66714200	1.69612400	-1.30224100
N	-3.81544900	1.92768500	-0.33657200
N	-4.90116500	2.61565800	-0.78608100
C	-6.98314800	1.88584800	-1.99412700
H	-7.76988600	2.08986400	-1.25791900
H	-6.91484300	2.74392500	-2.66474300
C	-2.68663100	2.62269400	0.21747700
C	-2.77025900	3.13649900	1.50481800
C	-1.53581300	2.74770200	-0.55214000
C	-1.65761500	3.76587500	2.05311900
C	-0.42318100	3.37853600	-0.00722600
C	-0.49407000	3.86842700	1.29523200
H	-1.68825100	4.16390400	3.06050200
H	0.49128500	3.48414900	-0.58080600
H	-1.50730900	2.35078700	-1.56238100
H	-3.68731200	3.03087000	2.07440300
Cl	0.90983700	4.61818900	1.99393700

H -1.26076200 -1.66129700 -0.90736600

Variable frequencies

-168.1004	11.2981	18.0133
19.9211	22.9352	24.1265
27.9744	30.6688	38.5517
41.9300	51.0200	56.9896
60.5368	64.6032	69.1763
72.5758	75.3015	77.8517
81.4022	93.8061	106.2163
111.9648	129.3354	139.2852
147.5736	149.2315	154.4771
168.6682	178.2654	182.5301
190.4679	208.0452	212.8093
221.6918	232.2381	243.2320
250.9147	258.5366	259.6209
279.6210	285.6934	299.2340
305.5171	310.4730	316.4383
328.7862	336.3260	343.9588
347.8567	355.5812	371.2743
377.5006	386.0893	405.9051
416.8759	418.0051	420.0780
425.9452	437.3158	441.8049
446.0926	461.1103	466.3392
472.1506	490.4931	495.2375
508.7100	517.6739	524.8581
535.2215	545.5501	558.8375
563.7759	576.1522	583.8702
591.3931	605.9439	608.4792
617.3848	626.3324	629.9209
639.1213	642.5388	642.9262
649.0580	656.3302	660.7130
678.5130	695.4608	705.3404
707.6103	717.9919	721.4859
726.8295	728.4125	734.8781
747.8180	758.2923	765.6376
781.9975	785.1162	790.9382
791.1034	802.2604	813.3162
814.3664	825.0265	834.3846
840.1813	846.6775	849.3760
852.9017	853.3616	863.0384
865.2427	876.3449	887.5398
889.2601	902.5904	915.2937
924.2874	936.3959	952.6621

969.3712	975.0746	979.5977
984.3242	989.9431	994.9193
1000.7436	1002.0858	1006.1075
1010.1967	1013.4781	1016.4867
1017.5522	1022.8439	1026.1479
1027.2741	1032.6563	1032.8462
1035.5429	1039.1575	1040.3998
1052.7572	1060.5767	1063.8500
1071.9479	1074.1809	1076.8321
1085.8190	1098.0683	1101.4041
1116.6526	1118.0869	1119.8968
1129.7186	1131.1531	1132.3187
1133.7280	1144.1833	1147.0041
1155.3293	1158.2534	1166.1741
1176.7262	1177.5459	1180.8589
1184.2817	1185.8074	1187.4324
1196.5788	1197.2616	1201.3398
1208.4166	1211.1945	1213.2434
1216.8989	1220.5479	1229.9323
1241.1944	1253.4461	1255.1170
1263.2013	1279.9154	1290.7468
1296.7532	1304.1172	1305.4620
1315.7916	1317.2565	1329.5035
1329.5950	1335.8989	1339.9955
1341.8318	1354.7290	1356.3571
1358.1707	1359.2469	1361.3215
1364.7230	1368.9677	1376.3009
1380.8126	1384.6910	1421.2638
1427.9560	1429.5757	1455.0287
1455.3679	1457.2695	1458.6898
1467.6777	1475.0368	1494.7320
1495.4082	1502.0905	1504.3061
1506.7836	1507.2709	1508.9003
1513.6734	1520.2813	1524.5557
1542.6618	1543.4708	1545.6607
1549.6151	1554.0315	1594.4987
1608.7757	1648.7398	1666.9724
1670.5618	1670.7505	1678.1718
1679.1635	1681.4692	1688.5068
1690.2043	1693.8276	1699.7225
1705.2299	1736.2924	1875.4782
3051.4922	3076.8721	3077.6530
3078.9524	3095.5676	3144.9764
3150.9036	3156.7695	3164.4981

3169.2764	3170.3282	3175.9129
3178.0933	3192.8822	3193.3620
3203.4166	3205.1149	3205.5083
3206.1144	3207.1342	3209.5820
3214.6887	3215.4701	3216.5811
3217.0331	3219.7078	3224.8850
3224.9658	3226.2576	3226.5807
3228.3259	3230.3637	3233.1720
3233.7723	3235.6928	3238.0160
3240.3851	3243.0689	3273.6853

²TS6R¹

Zero-point correction=0.774834

Thermal correction to Energy=0.822357

Thermal correction to Enthalpy=0.823301

Thermal correction to Gibbs Free Energy=0.689003

Sum of electronic and zero-point Energies=-3207.898966

Sum of electronic and thermal Energies=-3207.851443

Sum of electronic and thermal Enthalpies=-3207.850499

Sum of electronic and thermal Free Energies=-3207.984797

Cartesian coordinate

C	7.21771800	1.14663800	0.33448900
C	6.21872800	0.99653800	-0.63353900
C	5.39715600	2.06177500	-0.99326000
C	5.57128400	3.28127500	-0.33952200
C	6.54939000	3.42660700	0.64532800
C	7.38600500	2.36371800	0.98361000
C	8.01735700	-0.12163400	0.49036700
C	7.70167900	-0.85719400	-0.82983500
C	6.26855700	-0.40026900	-1.20851400
H	4.65054800	1.94762600	-1.77246300
H	4.94150400	4.12476900	-0.60308900
H	6.67395100	4.38519800	1.13864200
H	8.16424800	2.49000400	1.72966800
H	7.67203700	-0.68833100	1.36384500
H	8.36794400	-0.48470100	-1.61066400
H	9.08859600	0.04796100	0.61480200
H	6.04675200	-0.46521000	-2.27461400
N	5.33148900	-1.33539600	-0.52205800
O	7.86490400	-2.25817900	-0.83703500
C	3.99934000	-1.22453100	-0.39175900
C	5.69826500	-2.49125800	0.11575300

N	3.61323200	-2.29517700	0.30353200
N	4.66526400	-3.09283200	0.63569200
C	7.12644900	-2.94583900	0.14319800
H	7.54189000	-2.81088000	1.14948400
H	7.16806900	-4.00829900	-0.10250800
C	1.33401900	1.58848000	-0.78064500
C	2.23689400	0.52165700	-0.18596100
C	3.16689400	-0.14772900	-1.01681500
O	3.34596500	0.02916400	-2.23890700
H	2.33227000	0.46823500	0.89773000
C	2.27381800	-2.69589200	0.61461400
C	1.31062900	-2.67789000	-0.39028600
C	1.97772500	-3.09864300	1.91060700
C	0.00490900	-3.03470800	-0.07803800
H	1.57474300	-2.38886800	-1.40401800
C	0.67517700	-3.47400000	2.21698700
H	2.75562000	-3.11926000	2.66589200
C	-0.29759400	-3.42819400	1.22246400
H	-0.76647100	-3.02138000	-0.84058900
H	0.41441700	-3.79181300	3.21948800
Cl	-1.92795900	-3.89208500	1.60906200
S	-4.67855200	0.32617500	-1.92913300
O	-4.73462400	-0.14930400	-3.30624800
O	-4.05691700	1.59922600	-1.60335500
N	-3.80924900	-0.82083000	-0.97232200
N	-2.46962200	-0.47512300	-0.82201900
C	-7.31032600	-0.40635500	-1.91155300
H	-7.12727300	-0.79844600	-2.90660900
C	-8.56417500	-0.49313200	-1.31478700
H	-9.37960300	-0.96794100	-1.85173600
C	-6.28239900	0.20791200	-1.20441500
C	-6.47248500	0.73586800	0.07198700
H	-5.65336700	1.21941500	0.59626600
C	-8.79071800	0.02302900	-0.03604000
C	-7.73010200	0.63407400	0.64659200
H	-7.89349900	1.03730200	1.64207200
C	-10.15622400	-0.04629600	0.59274000
H	-10.08636400	-0.25595800	1.66260700
H	-10.77143000	-0.81762100	0.12595200
H	-10.67449500	0.91104000	0.47818900
C	-1.65737600	-0.46054500	-1.94857500
H	-2.10394400	-0.88904300	-2.83943300
C	-2.11276500	0.27898900	0.29842400
C	-0.88233200	0.84976300	0.34967700

H	-0.62355900	1.43248300	1.22651100
C	-0.43162100	0.09971600	-1.93965800
H	0.16364600	0.10918600	-2.84605400
C	0.10086300	0.67694000	-0.70963500
C	-4.03875100	-2.22124600	-1.32778400
H	-5.11609000	-2.39840100	-1.31624100
H	-3.64806200	-2.48184900	-2.31773100
H	-3.57016800	-2.84005100	-0.56028000
C	-3.11186300	0.49174400	1.37220000
C	-3.82609000	-0.56699300	1.94286300
C	-3.32659600	1.79479500	1.83095900
C	-4.74010500	-0.32278100	2.96058600
H	-3.65996300	-1.58017500	1.59200100
C	-4.24661300	2.03613000	2.84894000
H	-2.79171000	2.61758900	1.36576100
C	-4.95519300	0.97882400	3.41336800
H	-5.28755400	-1.14947600	3.40102200
H	-4.41410200	3.05143500	3.19246900
H	-5.67400700	1.16619200	4.20448500
C	1.25489400	2.91556800	-0.07012200
C	0.16209700	3.75753500	-0.30486300
C	2.26782700	3.34025800	0.78804100
C	0.08884600	5.00234600	0.31029000
H	-0.63333900	3.43171500	-0.97140200
C	2.19945400	4.59255800	1.39715500
H	3.12680300	2.69928800	0.96884600
C	1.10922600	5.42395800	1.16257800
H	-0.76313300	5.64707600	0.12006800
H	3.00031600	4.91392200	2.05586700
H	1.05209200	6.39703100	1.63911900
H	1.61576300	1.73913400	-1.82864700
H	0.95538800	-0.23339700	-0.25729800

Variable frequencies

-1074.8191	11.6637	15.0540
18.6237	23.8945	26.8761
31.9149	34.1930	36.9868
43.6985	46.5154	55.6504
58.5209	62.6666	65.3768
67.0377	73.0848	79.4191
88.7190	92.2932	96.7778
108.1570	120.5817	132.6523
139.1455	145.8251	151.8537
155.3012	172.1171	180.2823

184.4028	204.1843	212.9994
220.1468	226.6096	238.0719
245.1908	251.3494	263.0709
265.4106	278.6461	287.5528
288.5341	307.6268	311.0315
319.0229	329.6662	336.4313
344.9035	356.0697	363.9658
369.7383	385.2139	389.0020
405.6195	414.0048	415.6424
421.8957	423.2011	439.4309
439.9045	449.1381	461.0979
461.3517	468.7132	486.9993
491.0268	497.1990	511.0390
525.4936	531.0785	540.9751
553.6295	558.9601	575.9177
586.5698	589.9964	605.8233
611.9808	618.7499	626.3174
629.2217	640.2368	642.9870
647.6196	653.0548	654.3960
661.5157	680.2126	693.2704
706.0905	709.1199	716.3391
718.8501	724.9015	727.4170
729.4438	735.5440	758.5107
772.0466	780.0756	784.9894
787.5837	800.5730	810.2504
813.4273	823.9630	837.3245
840.3114	841.1030	843.6868
851.6669	853.3999	856.8635
869.3182	876.2270	885.4221
887.7098	891.6885	904.3907
913.8846	935.3852	951.5134
961.3518	963.9913	974.8317
976.9501	986.6437	990.3495
992.4327	1003.0390	1005.1211
1009.1889	1014.1473	1015.9809
1016.8280	1018.6398	1024.7994
1027.8038	1031.8157	1033.2473
1033.7160	1042.7937	1043.2880
1058.1194	1059.7623	1066.5005
1069.3497	1071.2708	1073.7422
1090.5324	1099.7574	1103.5985
1118.0637	1119.9870	1122.1243
1131.7511	1133.4313	1135.2117
1137.0784	1140.0550	1142.3053

1156.8559	1160.7326	1165.9327
1178.3749	1179.8132	1183.1337
1184.4063	1190.9567	1193.1272
1199.2507	1201.7134	1203.2570
1208.5747	1211.2225	1212.7548
1221.2252	1226.2341	1241.0142
1246.5080	1250.2964	1254.8455
1266.2039	1277.2006	1282.7357
1297.9002	1301.8209	1304.3435
1319.6755	1329.5564	1330.7674
1332.7746	1339.0306	1341.7134
1344.4429	1346.8030	1356.3855
1357.1492	1360.1880	1362.0327
1363.4715	1367.5911	1374.3778
1377.0934	1382.0779	1420.5536
1422.5358	1444.4369	1450.7329
1453.3115	1455.5703	1459.9676
1465.0253	1471.8836	1490.3148
1498.2589	1498.3273	1499.9954
1503.8396	1505.2554	1508.0700
1509.9984	1520.4048	1525.1558
1540.0966	1542.2946	1547.6287
1550.6604	1552.2933	1581.3658
1635.0037	1643.7901	1666.4918
1666.8342	1671.8151	1676.7154
1679.3282	1683.9365	1686.1237
1690.5799	1695.4211	1697.9249
1703.5680	1710.1483	1744.4023
3065.3738	3072.6899	3074.6532
3086.5729	3102.1538	3145.2505
3147.6317	3153.7880	3156.3880
3165.0249	3168.4709	3170.8873
3182.1057	3188.4685	3193.5476
3196.4517	3208.1834	3208.6102
3213.9936	3214.4131	3215.7776
3219.0667	3219.6036	3222.6584
3224.1075	3227.3272	3228.5803
3230.1915	3230.5525	3231.9520
3234.0139	3234.4874	3238.1014
3239.0111	3244.4888	3245.0264
3248.2080	3250.8961	3251.9037

²TS6S

Zero-point correction=0.775827
 Thermal correction to Energy=0.823129
 Thermal correction to Enthalpy=0.824073
 Thermal correction to Gibbs Free Energy=0.688339
 Sum of electronic and zero-point Energies=-3207.916941
 Sum of electronic and thermal Energies=-3207.869639
 Sum of electronic and thermal Enthalpies=-3207.868695
 Sum of electronic and thermal Free Energies=-3208.004428

Cartesian coordinate

N	2.57579400	0.93858900	0.11827000
N	3.87545800	1.24069500	-0.27777800
C	2.40000000	0.20845300	1.28372900
C	1.15076500	-0.24849200	1.58451700
C	-0.01645400	-0.03151300	0.74389700
C	0.29273300	0.65737600	-0.50327900
C	1.53429400	1.11479100	-0.77501800
C	-0.94202900	-1.32372600	0.56590000
C	-2.30964200	-0.90693300	0.13791400
C	-2.89034900	0.11764400	0.81789700
O	-2.31743000	0.80976100	1.75867700
S	4.46346500	0.08920700	-1.43397800
O	4.21459400	0.60161800	-2.77528900
C	6.19011600	0.16470000	-1.08661500
O	3.89008600	-1.17116200	-0.99770300
C	6.64057500	-0.31533600	0.14336500
C	7.99701700	-0.24717900	0.41805100
C	8.89915400	0.28500500	-0.51485900
C	8.41203800	0.74938500	-1.73916900
C	7.05353100	0.69700800	-2.03694800
C	3.57823800	-0.08360500	2.13334200
C	4.39801900	0.93307500	2.63273900
C	5.48828200	0.61619400	3.43358400
C	5.76975200	-0.71634200	3.73790600
C	4.95507500	-1.73110200	3.24311300
C	3.85950700	-1.41688500	2.44116300
C	10.36559900	0.36149500	-0.18557100
H	1.03638500	-0.80233900	2.51189100
H	-0.87278800	0.57183400	1.35630800
H	-0.48761400	0.79435000	-1.24566200
H	1.80376300	1.59862000	-1.70644500
H	-1.00858400	-1.72142400	1.58893300
H	5.94106900	-0.73469300	0.86072900
H	8.36630400	-0.61551000	1.37104300

H	9.10379400	1.15588500	-2.47030500
H	6.66503100	1.05321300	-2.98522800
H	4.17828600	1.96997400	2.39727600
H	6.12002600	1.40812400	3.82146700
H	6.62378200	-0.96164800	4.36073100
H	5.17514200	-2.76852000	3.47134400
H	3.23826600	-2.20076600	2.01800400
H	10.95827400	0.62223400	-1.06374100
H	10.72743800	-0.59278000	0.20539200
H	10.54585000	1.11963500	0.58284300
C	-0.25294200	-2.33550600	-0.31764100
C	0.58077400	-3.29739600	0.25661400
C	-0.36879300	-2.28726200	-1.70813100
C	1.28458600	-4.19476200	-0.54042300
H	0.67225400	-3.34794400	1.33962400
C	0.33300400	-3.18444300	-2.50811100
H	-1.00998400	-1.54164900	-2.17207200
C	1.16291200	-4.13880800	-1.92643900
H	1.92618600	-4.93902400	-0.07994200
H	0.23396900	-3.13549700	-3.58761200
H	1.71327500	-4.83502500	-2.55028900
H	-2.81848100	-1.42274100	-0.66660100
C	-3.84471200	4.38379500	-0.95419200
C	-3.21876500	3.47364000	-0.09680300
C	-1.87498800	3.15350300	-0.25428100
C	-1.17354600	3.72822400	-1.31239600
C	-1.80325000	4.61424700	-2.18688000
C	-3.14207900	4.95589900	-2.00795700
C	-5.26780400	4.63499400	-0.53453300
C	-5.26361100	4.13572800	0.92595300
C	-4.17404100	3.02734100	0.98791000
H	-1.39135600	2.48864600	0.45170100
H	-0.12144400	3.49634300	-1.44647500
H	-1.24054400	5.05793100	-3.00186400
H	-3.62295400	5.66857800	-2.67079600
H	-5.95733600	4.06247600	-1.16532300
H	-4.91707500	4.94423500	1.57317900
H	-5.56307100	5.68410700	-0.60018400
H	-3.71197900	2.91146900	1.96792400
N	-4.84234800	1.72832000	0.68597000
O	-6.50879900	3.74038900	1.45419600
C	-4.29809100	0.50291600	0.53358900
C	-6.19525300	1.58674200	0.51035700
N	-5.32468100	-0.30824400	0.25417400

N	-6.51089700	0.35627200	0.23124800
C	-7.14573400	2.72648900	0.71628500
H	-7.52839600	3.08592900	-0.24608400
H	-7.99235300	2.37430000	1.30760100
C	-5.33118900	-1.73307600	0.06664700
C	-5.73852700	-2.23730900	-1.16079900
C	-4.96845400	-2.56277400	1.12147200
C	-5.77090800	-3.61504700	-1.34615800
C	-4.99487400	-3.93802200	0.93416400
C	-5.39329300	-4.44986700	-0.29898400
H	-6.08596500	-4.03805600	-2.29275500
H	-4.71650900	-4.61020800	1.73706600
H	-4.66539500	-2.13916800	2.07288700
H	-6.03073100	-1.56246800	-1.95788800
Cl	-5.42634000	-6.17083100	-0.53184300
C	4.09713200	2.64361900	-0.63685200
H	5.16679000	2.77145300	-0.81378400
H	3.55030900	2.95259000	-1.53361700
H	3.80514200	3.25880300	0.21507400

Variable frequencies

-351.1889	8.3280	9.3947
16.6463	21.8603	25.1066
26.2003	31.5243	34.7293
39.4108	46.7576	48.9465
50.9470	56.7355	60.0428
67.3947	71.2245	75.0195
82.2366	85.6637	95.3681
103.0375	126.5432	143.3392
151.7502	154.6254	157.5151
164.1253	172.6691	183.7032
195.1475	209.1202	210.9671
214.3535	224.9765	230.4703
242.7313	252.4734	253.4838
275.8024	280.8527	286.6734
299.3630	301.5413	314.1050
330.9692	333.1611	343.5773
351.7091	354.1054	365.8832
373.1790	390.2037	408.8237
411.9726	416.9047	418.1159
421.3723	435.9366	438.9783
443.1663	456.1698	463.5810
467.4410	494.3148	495.7314
513.7144	518.3993	521.6391

539.2350	549.6837	557.3624
561.6401	578.2121	585.6017
592.3739	605.3809	610.8637
620.0483	623.3472	630.3822
639.5534	642.4417	643.6680
648.2966	654.7122	655.9262
674.3737	693.3317	700.5944
710.7226	718.5503	719.5701
721.0340	725.6296	731.4463
748.3833	756.2770	759.2992
774.8566	781.9401	787.3342
789.1381	792.2249	814.3174
823.9737	824.4928	837.9191
843.1985	844.9565	846.1872
847.8193	851.6635	860.2457
870.2725	877.7079	880.5006
884.7295	889.5852	899.7534
920.7724	924.3758	938.8443
952.5342	960.7639	977.5596
983.5118	990.3287	990.8247
996.2107	997.6022	1005.3168
1007.1594	1012.4297	1015.3750
1017.8338	1017.9856	1022.1487
1025.8448	1027.0521	1030.4359
1033.4093	1034.7465	1037.0592
1054.5843	1055.7207	1062.6168
1069.1870	1070.6108	1075.3354
1079.7555	1095.7142	1099.5888
1112.9972	1118.4576	1120.9241
1126.5784	1131.0319	1133.8929
1136.0210	1144.9351	1147.3743
1157.4746	1159.9410	1162.2442
1176.8797	1181.2082	1183.2761
1184.3474	1187.7586	1190.9148
1198.2778	1203.2001	1205.3436
1209.1067	1212.5460	1213.9216
1217.7281	1227.4005	1233.4212
1235.7389	1251.4131	1254.9789
1263.4293	1279.4528	1288.2807
1296.1201	1297.1582	1307.1837
1319.0150	1321.8113	1322.5445
1333.5446	1336.8062	1337.2250
1341.9350	1351.3724	1355.9474
1359.2332	1360.4943	1361.3076

1363.0292	1368.9606	1376.5515
1384.9129	1385.2594	1423.1823
1426.9747	1427.4533	1447.6870
1457.1520	1459.3493	1460.0223
1465.1382	1480.1568	1491.3523
1498.2149	1500.3591	1502.7166
1504.5303	1506.8324	1509.1497
1512.8245	1513.4922	1520.9065
1533.0755	1542.6427	1544.5983
1550.0133	1552.5048	1583.5349
1605.7427	1618.6281	1668.3712
1671.5523	1671.9334	1679.1827
1680.6735	1682.2207	1689.7404
1691.4716	1694.8008	1700.0403
1705.3432	1734.9279	1763.1943
3042.8230	3078.6382	3084.0603
3084.0691	3095.9426	3143.9782
3154.6802	3154.8982	3165.7793
3171.6078	3181.6370	3189.7188
3190.3543	3190.4551	3193.7026
3205.5875	3208.1033	3209.2833
3209.8295	3211.9953	3212.6553
3220.2545	3224.4705	3226.3116
3227.5851	3227.7284	3227.7853
3230.7990	3231.2012	3232.6003
3233.7507	3240.1264	3244.9283
3247.2468	3250.5035	3250.8332
3251.7232	3252.6913	3269.6290

²M6R

Zero-point correction=0.780037

Thermal correction to Energy=0.827865

Thermal correction to Enthalpy=0.828810

Thermal correction to Gibbs Free Energy=0.693388

Sum of electronic and zero-point Energies=-3207.948632

Sum of electronic and thermal Energies=-3207.900803

Sum of electronic and thermal Enthalpies=-3207.899859

Sum of electronic and thermal Free Energies=-3208.035281

Cartesian coordinate

N	2.31381900	-1.88380900	-0.42596000
N	3.66824100	-2.03227300	-0.71659900
C	3.98603400	-3.17247900	-1.57560300

C	1.80337700	-0.57018700	-0.42756500
C	0.63436300	-0.31877300	0.22875900
C	-0.07494000	-1.31071400	0.95942200
C	0.53429600	-2.58768300	1.04051600
C	1.69391600	-2.85436000	0.38018600
C	-1.25584400	-0.90297500	1.82165800
C	-2.35214500	-0.22320400	1.03888700
C	-2.64377400	-0.40895400	-0.25201300
O	-2.08730200	-1.25430600	-1.15520900
S	4.67941300	-1.88356500	0.67507500
O	4.03253700	-0.86609600	1.48690800
C	6.14953200	-1.24250500	-0.06904300
O	4.96578000	-3.20565600	1.22141400
C	7.28851300	-2.03762000	-0.12225200
C	8.43470400	-1.51710100	-0.71541000
C	8.44530700	-0.22639300	-1.24972900
C	7.27738000	0.54566700	-1.18142000
C	6.12516100	0.05092700	-0.58951800
C	2.55035200	0.48990300	-1.13015800
C	2.72331100	1.72500000	-0.49254600
C	3.41022300	2.75774500	-1.12861700
C	3.94137200	2.56210000	-2.40171100
C	3.77912300	1.33123000	-3.03860000
C	3.09055100	0.30158900	-2.40862400
C	9.69415900	0.34309800	-1.86774400
H	3.38215200	-3.08699200	-2.47994800
H	5.04158000	-3.10492200	-1.84714200
H	3.80710300	-4.13984000	-1.09415000
H	0.24548400	0.69465300	0.18401900
H	0.09213900	-3.37542800	1.64344800
H	2.20427800	-3.80734700	0.42761400
H	-1.68161400	-1.81110800	2.27335900
H	7.26890100	-3.03778500	0.29807600
H	9.33479400	-2.12255500	-0.76182400
H	7.27350600	1.54943800	-1.59729300
H	5.22316500	0.65326600	-0.52803900
H	2.35117100	1.85402600	0.52060700
H	3.54588300	3.70678400	-0.61937400
H	4.48409600	3.36211200	-2.89451000
H	4.19306500	1.17446500	-4.02931100
H	2.96714900	-0.65520500	-2.90625600
H	9.45932200	0.92734700	-2.76064500
H	10.19809900	1.01037500	-1.16131600
H	10.39724200	-0.44524300	-2.14304700

C	-0.77689400	0.00314500	2.95418300
C	-0.32646800	-0.55669300	4.14980000
C	-0.70767100	1.38880700	2.78745300
C	0.17806300	0.25256900	5.16284100
H	-0.36600300	-1.63462300	4.28565000
C	-0.20087900	2.20044200	3.79865300
H	-1.05222100	1.84345100	1.85995800
C	0.24221200	1.63363400	4.99042200
H	0.52341900	-0.19575300	6.08872100
H	-0.15361500	3.27560200	3.65204400
H	0.63684100	2.26365300	5.78047400
H	-2.96482700	0.49739200	1.57386200
C	-6.71601600	-2.21802600	-0.06892100
C	-5.38401100	-2.25296000	-0.49337800
C	-4.42708000	-2.99379800	0.19365800
C	-4.81761100	-3.67729500	1.34258100
C	-6.14145600	-3.62649000	1.78233700
C	-7.10213100	-2.90479800	1.07599400
C	-7.56716500	-1.41063100	-1.01656100
C	-6.69058100	-1.39072500	-2.28776100
C	-5.23145700	-1.45740700	-1.76679700
H	-3.40507000	-3.04902200	-0.16651200
H	-4.09073500	-4.26603200	1.89209800
H	-6.42968600	-4.17222100	2.67471300
H	-8.13582400	-2.89206800	1.40667200
H	-7.73403900	-0.40298100	-0.61687900
H	-6.86475400	-2.30999200	-2.85117600
H	-8.54748000	-1.85163500	-1.20644400
H	-4.52715900	-1.87150100	-2.48990200
N	-4.80419000	-0.04854200	-1.51455400
O	-6.90761700	-0.34372800	-3.20629300
C	-3.71295300	0.39015700	-0.86767000
C	-5.50198000	1.06546500	-1.90451200
N	-3.77829600	1.72059200	-0.89598400
N	-4.89613700	2.15833800	-1.52876600
C	-6.78535100	0.95141700	-2.67108500
H	-7.62936100	1.21593200	-2.02248500
H	-6.76709300	1.65043600	-3.50877700
C	-2.77284400	2.63948600	-0.43842900
C	-3.10678800	3.60169700	0.50448500
C	-1.48627600	2.52375900	-0.95590000
C	-2.11494300	4.46501500	0.95965100
C	-0.49653800	3.38443100	-0.49957700
C	-0.82041500	4.34160900	0.46040900

H	-2.34068500	5.22238800	1.70116800
H	0.51576300	3.31207100	-0.88295300
H	-1.25764700	1.76575500	-1.69986200
H	-4.12138000	3.67104800	0.88101300
Cl	0.42307200	5.40054200	1.04712200
H	-1.29645500	-1.65467500	-0.74395500

Variable frequencies

9.5872	16.9445	18.2419
22.1120	24.0525	27.0424
30.3762	34.3113	39.9438
50.1839	55.1509	57.4993
61.7151	65.4855	67.4648
70.0281	73.7878	85.3296
96.1552	106.1262	106.4770
110.9312	135.6824	139.9104
146.2052	149.1094	161.5006
177.1426	182.6523	186.4400
199.0155	205.8365	212.2387
223.8563	239.1639	252.2332
256.8259	262.1387	263.5284
276.7732	282.3066	294.9867
299.5912	305.8894	315.3966
328.7232	331.8839	337.8037
346.2568	360.1425	364.5145
384.6384	387.2839	402.8446
416.1429	417.8458	420.6325
420.7696	426.7992	438.8506
450.0232	462.2785	464.0210
471.2104	494.2366	496.2557
502.8774	516.4065	523.7445
534.8213	546.2553	549.0212
560.0223	570.5155	581.1216
589.9157	594.7322	604.0510
610.2387	614.5330	628.7504
630.7281	634.5365	641.0317
644.2867	650.7784	652.6834
663.6426	672.4692	677.3512
706.2165	707.3292	718.9595
721.8705	723.0792	729.0826
730.1032	732.9348	738.4285
761.1262	780.2559	781.0015
786.9507	789.8800	798.4957
813.2842	817.1577	834.9762

842.2350	843.6205	851.0295
858.8813	861.8692	872.2889
875.8256	877.5387	882.5958
883.1937	892.1094	902.5642
906.2027	918.3380	925.8344
936.2965	952.0209	958.3900
989.3091	992.2377	992.9885
1001.0163	1004.8259	1007.7419
1009.2534	1013.3181	1015.2199
1016.6675	1017.1959	1018.2657
1026.3582	1029.0507	1034.1308
1034.7743	1035.4742	1036.4413
1041.4055	1052.4301	1066.8604
1069.5116	1072.7494	1075.0986
1086.1782	1094.8623	1103.2319
1119.8643	1120.9413	1124.7286
1130.8908	1132.5009	1136.4320
1139.0957	1142.0933	1143.6545
1154.9101	1167.1414	1179.1590
1181.4643	1182.9020	1185.1779
1185.3689	1191.4576	1201.6997
1203.8128	1206.3500	1208.0811
1210.4637	1212.3778	1214.6648
1218.3052	1234.4926	1248.8306
1254.3755	1254.6105	1267.7267
1274.8792	1278.1879	1278.7035
1286.9717	1308.4182	1320.2387
1325.8903	1332.0216	1333.1633
1336.3519	1343.9327	1346.7544
1351.5887	1356.1167	1357.4015
1357.4691	1360.3492	1362.5525
1364.2874	1368.6300	1377.6782
1378.7352	1384.3611	1400.8848
1420.3127	1422.9570	1427.1407
1453.5440	1454.4471	1457.1523
1463.1441	1465.8163	1495.8186
1496.9909	1498.0309	1503.1626
1504.2210	1506.4223	1507.1826
1513.1235	1521.0467	1532.5816
1541.7844	1542.4700	1548.6176
1549.4350	1551.6123	1567.9199
1622.9895	1664.3545	1666.4063
1667.5532	1677.9810	1679.7057
1682.4032	1683.7852	1688.5691

1692.2881	1698.3278	1705.1029
1711.6761	1777.6903	3046.1525
3071.1284	3074.1346	3077.7736
3088.0370	3147.1413	3149.0447
3155.8402	3161.0249	3164.8243
3170.6827	3171.9813	3185.7240
3186.1350	3195.7685	3198.3152
3202.4864	3203.2431	3204.7021
3207.9876	3211.0871	3213.4620
3216.3644	3216.8288	3217.5379
3218.1178	3220.5878	3222.9352
3227.6845	3229.7551	3230.9123
3231.1097	3234.2862	3235.3415
3235.4045	3238.1288	3242.9583
3247.9635	3256.3774	3621.0763

²M6S

Zero-point correction=0.779822

Thermal correction to Energy=0.827876

Thermal correction to Enthalpy=0.828820

Thermal correction to Gibbs Free Energy=0.691545

Sum of electronic and zero-point Energies=-3207.947397

Sum of electronic and thermal Energies=-3207.899343

Sum of electronic and thermal Enthalpies=-3207.898399

Sum of electronic and thermal Free Energies=-3208.035674

Cartesian coordinate

N	-2.46155300	-1.20565100	0.39914500
N	-3.84600400	-1.39448500	0.31790600
C	-2.01201800	-0.07167000	1.10863400
C	-0.74911900	-0.08921600	1.64497400
C	0.13266700	-1.18411400	1.51339100
C	-0.37341200	-2.32679800	0.83048700
C	-1.63118000	-2.33691600	0.31361800
C	1.58721300	-1.08349600	1.92009300
C	2.50143300	-0.60607800	0.81345500
C	2.21663400	-0.28919100	-0.45624500
O	1.05867900	-0.32079300	-1.16055500
S	-4.32427800	-1.79793000	-1.27913400
O	-4.14664100	-3.22978700	-1.50587100
C	-6.05579500	-1.45691100	-1.19304700
O	-3.63751700	-0.84578100	-2.13906700
C	-6.48650700	-0.17249900	-0.86233200

C	-7.84956900	0.07938800	-0.83106000
C	-8.77887200	-0.92506100	-1.13501700
C	-8.31205400	-2.19989000	-1.46283100
C	-6.94920300	-2.47872500	-1.49341600
C	-2.85139100	1.13872200	1.15623700
C	-3.43554200	1.65451400	-0.00920300
C	-4.13147600	2.85742400	0.03454200
C	-4.25882400	3.55707800	1.23475700
C	-3.68456600	3.04650100	2.39567900
C	-2.98610300	1.84235500	2.35913000
C	-10.25252900	-0.62041000	-1.12122000
H	-0.40967500	0.81417100	2.14224000
H	0.24717800	-3.20785400	0.69338100
H	-2.05920200	-3.17914300	-0.21654500
H	1.93510100	-2.09469000	2.18093000
H	-5.76631200	0.60256300	-0.61782100
H	-8.20446100	1.07103600	-0.56571900
H	-9.02330400	-2.98683100	-1.69441000
H	-6.57607200	-3.46684400	-1.74045600
H	-3.32432200	1.11430300	-0.94586900
H	-4.56943700	3.25539100	-0.87578900
H	-4.80439600	4.49443700	1.26347100
H	-3.78749300	3.57932300	3.33542500
H	-2.54978300	1.43459300	3.26669400
H	-10.53004200	-0.04280900	-2.00844100
H	-10.52165900	-0.02524100	-0.24523700
H	-10.84783200	-1.53493100	-1.11577400
C	1.77505100	-0.21081000	3.15627200
C	1.59302100	-0.76427900	4.42524900
C	2.06283500	1.15080900	3.04492400
C	1.70434600	0.02736300	5.56339000
H	1.35977400	-1.82198500	4.51830300
C	2.16525300	1.94721600	4.18374600
H	2.19508100	1.59711400	2.06178700
C	1.98998400	1.38686500	5.44533500
H	1.56843400	-0.41675600	6.54415800
H	2.38234000	3.00582300	4.07917200
H	2.07432200	2.00390200	6.33387100
H	3.54369400	-0.48531900	1.10242400
H	0.34085200	-0.65466300	-0.59808300
C	2.40967300	4.06956300	-0.58263900
C	1.66745400	2.92772700	-0.91036700
C	0.54866400	2.56208200	-0.16789800
C	0.21203900	3.32728500	0.94845800

C	0.98828700	4.42827200	1.31323000
C	2.08632900	4.81463700	0.54464800
C	3.43757900	4.36523300	-1.64635300
C	2.83838100	3.60276800	-2.84985500
C	2.17367300	2.35551300	-2.21445700
H	-0.06731700	1.71872900	-0.46167200
H	-0.67511300	3.07561600	1.52299700
H	0.71181900	5.01254600	2.18496900
H	2.65474700	5.70269500	0.80234600
H	4.42265500	3.97358500	-1.36309000
H	2.03211800	4.20071400	-3.27999500
H	3.55484900	5.43051400	-1.85346900
H	1.41076200	1.89225300	-2.84118800
N	3.26977600	1.34797500	-2.04978400
O	3.69647500	3.30078400	-3.92350500
C	3.29635100	0.21875700	-1.31710000
C	4.49239200	1.43841600	-2.66671000
N	4.49578400	-0.32504800	-1.52188200
N	5.25823900	0.43375000	-2.34960800
C	4.85026200	2.58156800	-3.56754800
H	5.59643700	3.21510500	-3.07171200
H	5.29060900	2.19077300	-4.48639100
C	5.00318600	-1.57951100	-1.04172500
C	6.27043900	-1.60681800	-0.47478100
C	4.23189400	-2.72768800	-1.18777200
C	6.77821100	-2.82019600	-0.02594900
C	4.73841200	-3.93676900	-0.73121300
C	6.00573200	-3.97110900	-0.15293900
H	7.76406300	-2.87493900	0.42024800
H	4.16440700	-4.85008400	-0.83444800
H	3.25567300	-2.67940700	-1.65956000
H	6.85146500	-0.69494800	-0.39403800
Cl	6.63828800	-5.48452600	0.41069500
C	-4.37986500	-2.28101600	1.36335400
H	-5.46513700	-2.32261500	1.26276700
H	-3.96351500	-3.29190700	1.30435000
H	-4.13161800	-1.82685700	2.32448000

Variable frequencies

5.4534	8.6205	14.4847
22.2845	25.7001	26.8326
31.0100	33.5154	37.1360
48.2500	53.4315	58.2180
62.7351	65.8434	73.6699

74.1384	81.0315	87.0594
91.6461	94.2651	99.3901
108.0540	127.9568	132.1585
140.1559	151.8648	168.6103
173.7416	185.4410	189.7853
206.3023	212.2001	215.9695
224.8995	232.0470	246.5522
251.2094	256.0465	264.2736
273.6383	276.3331	290.5734
297.3529	301.7768	317.7006
321.1071	331.3086	338.3747
345.0501	363.3498	367.6490
384.9350	392.8090	398.6393
399.3072	412.1112	420.1513
421.0134	423.4950	425.0472
437.5714	443.4080	462.4684
465.4821	467.8960	495.7152
500.0566	512.6989	518.8964
526.4042	542.5588	544.2516
548.8879	556.6705	571.4283
580.1249	591.0211	599.8528
607.8252	612.3379	629.4625
630.6494	636.3026	639.5864
643.5848	652.2252	655.3786
663.8754	672.3021	684.9175
704.5748	707.5482	719.0352
723.3010	724.4581	727.0771
728.3916	730.8541	761.4518
774.6375	777.9493	788.1259
791.3702	797.7306	805.2303
813.8365	823.0003	834.8244
837.0071	841.1486	848.4123
856.7310	861.2086	864.6010
866.0423	883.0723	888.5157
890.8168	897.6546	905.4722
912.0578	920.0037	929.0079
954.0761	958.0869	964.7348
982.5298	985.2359	991.0883
995.0754	998.8387	1002.1796
1007.6864	1012.7143	1013.3255
1014.4287	1017.4745	1019.0242
1029.9124	1031.7479	1032.8363
1035.0278	1037.5879	1039.5523
1044.6704	1054.0354	1067.2700

1071.1010	1072.2286	1073.6600
1074.5063	1081.9007	1100.1751
1121.0575	1121.6876	1122.7848
1129.3192	1131.9991	1134.8129
1137.7481	1139.6305	1145.9260
1154.0825	1160.1864	1174.3373
1179.9567	1181.6822	1183.2697
1191.3548	1192.2891	1201.3527
1204.0399	1207.4512	1208.3775
1211.4100	1213.1984	1214.4965
1217.4167	1238.2105	1245.1855
1246.7565	1255.1697	1259.6221
1266.4136	1277.5641	1280.0456
1289.0441	1300.5310	1302.6628
1323.0413	1327.8185	1331.3963
1335.1913	1337.6633	1342.5521
1353.8594	1355.3342	1357.2640
1360.7774	1364.0170	1364.4402
1366.9150	1367.1398	1372.2647
1376.5183	1384.5309	1396.4039
1421.2440	1425.9694	1428.1533
1451.7755	1454.6545	1456.1259
1462.7168	1469.1566	1493.6881
1494.1684	1499.0436	1501.2454
1504.9689	1505.2452	1506.0751
1506.2616	1522.6661	1527.9998
1539.5970	1540.4545	1551.4508
1552.1240	1553.4853	1563.8636
1622.1069	1665.3699	1666.4998
1670.0243	1678.8258	1679.3874
1685.8761	1688.8836	1692.3438
1692.7952	1698.9176	1701.9731
1702.6580	1775.7583	3032.8829
3069.6592	3074.6111	3082.8629
3087.2195	3149.5354	3154.0960
3159.5650	3164.4377	3169.8509
3172.0960	3177.7385	3182.8684
3190.6611	3194.4568	3201.5517
3202.0386	3202.1362	3203.7902
3205.2517	3210.0459	3212.8172
3214.1616	3219.0494	3220.0137
3220.9381	3222.3276	3222.6282
3224.3147	3229.1700	3230.2909
3235.0916	3236.0684	3239.0062

3240.6110	3244.6760	3249.2333
3250.0108	3255.4928	3762.0094

²TS7R

Zero-point correction=0.777918

Thermal correction to Energy=0.825963

Thermal correction to Enthalpy=0.826908

Thermal correction to Gibbs Free Energy=0.690477

Sum of electronic and zero-point Energies=-3207.925346

Sum of electronic and thermal Energies=-3207.877300

Sum of electronic and thermal Enthalpies=-3207.876356

Sum of electronic and thermal Free Energies=-3208.012787

Cartesian coordinate

N	2.59840700	1.15692700	-0.32358500
N	4.31333200	0.93891800	-0.61794300
C	4.79924900	2.18478300	-1.19755900
C	2.21068700	0.37722300	0.73697000
C	1.09169000	-0.44044600	0.64501400
C	0.35033100	-0.50924300	-0.53115400
C	0.75769100	0.29760700	-1.60423900
C	1.85698000	1.11019500	-1.47134300
C	-0.94090800	-1.30750600	-0.65137200
C	-2.06523500	-0.34413600	-0.37589800
C	-3.02568600	-0.00422000	-1.23626400
O	-3.24850300	-0.45941600	-2.50026700
S	4.51643300	-0.40500400	-1.61418700
O	3.69224200	-1.45976200	-1.03457700
C	6.22774800	-0.76042800	-1.32629400
O	4.34726700	-0.05701400	-3.02655600
C	7.14470500	-0.58794100	-2.35507500
C	8.48734800	-0.86180900	-2.10538700
C	8.90998400	-1.29715300	-0.84836600
C	7.95845900	-1.45506900	0.16995300
C	6.61721300	-1.18927800	-0.05687700
C	3.02888000	0.45161600	1.96083800
C	3.19707800	-0.68104100	2.76402300
C	3.96121900	-0.61145000	3.92494900
C	4.56630500	0.58759400	4.29234500
C	4.41194500	1.71693100	3.48927000
C	3.65362200	1.64908500	2.32755300
C	10.35958000	-1.60245000	-0.57910200
H	4.55777700	2.98703900	-0.49889500

H	5.88823700	2.12445800	-1.29760800
H	4.37556300	2.40325500	-2.18504000
H	0.79535000	-1.01384700	1.51746800
H	0.20494900	0.30373800	-2.54007500
H	2.20671400	1.73912800	-2.28389500
H	-0.99705700	-1.64806200	-1.69392500
H	6.80264200	-0.25193900	-3.32824800
H	9.21668500	-0.73548200	-2.89984700
H	8.28117700	-1.79001300	1.15165600
H	5.87655600	-1.30211200	0.72936500
H	2.75753200	-1.62607200	2.45860600
H	4.09298000	-1.49829800	4.53637600
H	5.16268700	0.64061400	5.19733400
H	4.88534700	2.65205500	3.77061800
H	3.52536500	2.52451000	1.69813000
H	10.71567000	-1.05897700	0.30042600
H	10.49851900	-2.66969600	-0.38199300
H	10.98765700	-1.33021800	-1.42910900
C	-1.03311000	-2.55037800	0.22138200
C	-0.70526200	-3.79196500	-0.32726100
C	-1.45009100	-2.48993300	1.55364500
C	-0.79420400	-4.95212900	0.43753800
H	-0.36991600	-3.85046300	-1.35953200
C	-1.53673300	-3.64858400	2.32124400
H	-1.72036600	-1.53898400	2.00353600
C	-1.21237500	-4.88281800	1.76469300
H	-0.53482900	-5.90882000	-0.00385600
H	-1.86347000	-3.58538600	3.35410300
H	-1.28122600	-5.78608900	2.36177400
H	-2.06638800	0.15224200	0.59047000
C	-6.62813400	-1.77089300	0.54958600
C	-5.72538400	-1.66449100	-0.51298600
C	-4.68231100	-2.57477400	-0.65807500
C	-4.51560500	-3.56411100	0.30773800
C	-5.39859800	-3.65203600	1.38495900
C	-6.46964200	-2.76818300	1.50506100
C	-7.70871900	-0.72405700	0.45522600
C	-7.59896100	-0.28107000	-1.02023300
C	-6.10966800	-0.49730700	-1.39442500
H	-4.01891600	-2.52792700	-1.51401500
H	-3.69373200	-4.26864200	0.21970700
H	-5.25758200	-4.42959100	2.12869800
H	-7.17308300	-2.86161300	2.32648700
H	-7.50435700	0.10216700	1.14684700

H	-8.18281300	-0.96283300	-1.64180100
H	-8.70497600	-1.10378900	0.69004600
H	-5.93749000	-0.63643000	-2.46222700
N	-5.39417000	0.75564500	-0.99592700
O	-8.06713500	1.01004700	-1.33913100
C	-4.07132500	0.95273400	-0.86287300
C	-6.00505600	1.89725600	-0.54910700
N	-3.92731100	2.17325400	-0.34625000
N	-5.12822100	2.77053200	-0.13666000
C	-7.49664800	2.05030200	-0.58371800
H	-7.88934900	2.08957800	0.43957800
H	-7.74896700	2.98873600	-1.08128600
C	-2.71045200	2.85198600	0.00402300
C	-2.62899100	3.44238400	1.25958500
C	-1.65404100	2.88853200	-0.89930000
C	-1.44749100	4.07303000	1.62991200
C	-0.47173300	3.51085100	-0.52247500
C	-0.37688500	4.09026500	0.74011300
H	-1.35264600	4.53899600	2.60356700
H	0.37027000	3.54937800	-1.20283700
H	-1.74785100	2.43854800	-1.88201500
H	-3.47689100	3.40707100	1.93432900
Cl	1.10932100	4.85345900	1.21065700
H	-2.59118000	-1.12757900	-2.73769200

Variable frequencies

-649.1236	11.4171	14.9336
19.5370	21.1232	29.3569
31.7676	32.2041	37.3065
38.6138	39.8999	41.5858
49.3332	53.8011	58.8331
63.8904	65.9278	67.9284
76.1780	85.5967	94.3774
103.5411	114.2672	128.9059
142.4402	147.0230	155.6125
164.9937	178.3686	183.2569
185.3694	194.7384	208.0876
216.8003	229.6825	230.2443
241.8608	252.9270	262.5582
266.1553	271.6017	279.0969
289.8386	304.0761	305.0071
315.2417	323.8485	332.6189
345.4976	351.3592	359.8191
370.3840	380.4470	381.9501

391.4261	408.1224	412.0098
416.6480	418.3170	423.2665
430.9992	443.5496	453.4681
461.5051	465.0639	475.3207
488.6231	495.2896	496.7551
514.9991	519.7960	536.8191
541.7756	549.0253	554.0426
569.6649	582.4046	594.5656
606.7190	611.2748	626.0188
628.0736	631.9826	637.1244
642.9193	648.5166	648.9032
655.7863	665.4678	670.5149
697.1265	707.4864	716.5532
717.3499	720.9189	723.1490
730.4105	736.3313	743.7288
760.3693	774.4032	776.1227
791.0092	794.0076	794.8199
809.2524	824.0170	833.2419
841.4495	846.4116	853.1858
856.1279	861.5167	869.8987
871.7658	872.7354	876.2898
887.2618	894.4734	901.6436
920.2202	926.8275	932.3741
946.4289	953.7970	957.2603
960.6067	986.1677	986.9905
992.7013	997.7557	999.6603
1006.1529	1007.9902	1008.2007
1015.9763	1016.5434	1017.7255
1021.4197	1023.4704	1025.0604
1035.4278	1037.1957	1038.4188
1043.2969	1055.6673	1064.1022
1066.2535	1071.4313	1073.1708
1077.1040	1091.5638	1100.5572
1105.8856	1119.0352	1119.5269
1120.5164	1133.5002	1136.5055
1143.8289	1146.1367	1149.8105
1155.2555	1161.4707	1163.1335
1174.2892	1177.9798	1180.6046
1181.8965	1185.2163	1191.3054
1197.9289	1204.1777	1204.3061
1205.9273	1206.7583	1214.3903
1216.7799	1233.2194	1238.6515
1243.3145	1254.0079	1261.6287
1266.2769	1277.5428	1282.3992

1295.7514	1299.4035	1313.7213
1317.5274	1323.9007	1327.8104
1335.8422	1339.7184	1341.5026
1347.5532	1349.3551	1351.6131
1352.9590	1360.4549	1362.7376
1364.3565	1366.5882	1373.8357
1380.1494	1386.3293	1418.7728
1422.9969	1426.4983	1441.2692
1456.0182	1457.1717	1458.7277
1471.6196	1484.3635	1496.8931
1497.4649	1500.3182	1504.6036
1505.9779	1506.7417	1507.9120
1511.5158	1525.1632	1529.6037
1540.9758	1552.0827	1554.1913
1554.2839	1555.2842	1572.7453
1624.4774	1659.7088	1664.3639
1672.1488	1675.9297	1680.1177
1683.8044	1686.7402	1689.9943
1692.1860	1694.6803	1697.5021
1704.6209	1781.8071	3056.2261
3057.1010	3074.1430	3078.0452
3088.5265	3132.2958	3143.0674
3147.5352	3158.7525	3163.3184
3167.8828	3170.2606	3174.0006
3195.2736	3198.0456	3198.7286
3201.9960	3202.2045	3205.9328
3206.8921	3210.0468	3213.4852
3213.7377	3214.2186	3215.7254
3218.8455	3219.8784	3221.8055
3231.4405	3232.9046	3233.5097
3237.0890	3238.9218	3239.0689
3240.7547	3240.8175	3242.3769
3251.9730	3256.8165	3858.7314

M7R

Zero-point correction=0.604896

Thermal correction to Energy=0.640172

Thermal correction to Enthalpy=0.641116

Thermal correction to Gibbs Free Energy=0.535133

Sum of electronic and zero-point Energies=-2294.228443

Sum of electronic and thermal Energies=-2294.193167

Sum of electronic and thermal Enthalpies=-2294.192223

Sum of electronic and thermal Free Energies=-2294.298207

Cartesian coordinate

N	-4.32846000	0.90875700	0.73241300
C	-3.92216500	0.76180100	-0.53549000
C	-2.63691400	1.13848900	-0.94670900
C	-1.76259200	1.70830100	-0.02858400
C	-2.19652000	1.86993000	1.28641100
C	-3.48213600	1.44757300	1.60906300
C	-0.32215700	2.01579800	-0.42631500
C	0.45609000	0.79935200	-0.00768400
C	1.00830600	-0.10556000	-0.81775700
O	1.11517800	-0.10144200	-2.17450700
C	-4.87935900	0.11794300	-1.47247800
C	-4.80261000	0.32122600	-2.85445700
C	-5.69798400	-0.31086400	-3.71042900
C	-6.67901700	-1.15581300	-3.19660800
C	-6.76766900	-1.35678500	-1.82081800
C	-5.87848000	-0.71980400	-0.96264500
H	-2.31217000	0.95651400	-1.96727800
H	-1.55371900	2.31571800	2.03900900
H	-3.85037800	1.54437600	2.62789600
H	-0.30514800	2.11816100	-1.52037700
H	-4.06461400	1.00352800	-3.26558800
H	-5.63686600	-0.13501200	-4.77940400
H	-7.37695400	-1.64832500	-3.86570900
H	-7.53376000	-2.00920400	-1.41484500
H	-5.94771200	-0.85394600	0.11256700
C	0.22474500	3.30729900	0.16721100
C	-0.55468000	4.46751000	0.12277100
C	1.50754300	3.37135200	0.70882000
C	-0.05611100	5.66903300	0.61220500
H	-1.55813400	4.42573300	-0.29259000
C	2.00834600	4.57698400	1.19909000
H	2.13040600	2.48160400	0.73938900
C	1.22796700	5.72704200	1.15292300
H	-0.67098000	6.56208600	0.57419300
H	3.00975700	4.61120900	1.61726700
H	1.61488500	6.66519900	1.53649200
H	0.48740900	0.59725900	1.06030200
C	5.50294800	-0.15697100	-0.19916900
C	4.35776500	0.01045300	-0.98506800
C	3.87262700	1.28130500	-1.27924600
C	4.53168900	2.38830400	-0.74750700
C	5.66006900	2.22112400	0.05588800

C	6.15912500	0.94861800	0.32819800
C	5.87210400	-1.61218400	-0.07523500
C	5.09986000	-2.24130700	-1.25405000
C	3.85484900	-1.33536300	-1.45647000
H	3.01098400	1.41419400	-1.92431200
H	4.16484300	3.38633300	-0.96432800
H	6.16587900	3.09324300	0.45721200
H	7.05383400	0.82460900	0.93034700
H	5.54036100	-2.01066300	0.89070900
H	5.70111500	-2.15257700	-2.16117700
H	6.94517600	-1.79800600	-0.15095900
H	3.46464600	-1.35155400	-2.47495200
N	2.77714000	-1.88221700	-0.57718300
O	4.78155700	-3.61009100	-1.14962100
C	1.58708300	-1.33794100	-0.27031600
C	2.86817900	-3.04703900	0.13897200
N	1.01454600	-2.16623400	0.60343400
N	1.80831600	-3.23160000	0.87653800
C	4.05002900	-3.95902400	-0.00025500
H	4.65813500	-3.92803600	0.91150700
H	3.69485000	-4.98179500	-0.13744300
C	-0.29206000	-2.06607800	1.19712000
C	-0.38834200	-2.05318100	2.58237600
C	-1.41114500	-1.99388000	0.37467700
C	-1.64643100	-1.95209600	3.16440900
C	-2.66719900	-1.89553000	0.95874400
C	-2.77178000	-1.86919100	2.34784200
H	-1.75571500	-1.93702200	4.24221700
H	-3.55922200	-1.84668100	0.34357900
H	-1.30662100	-2.01922700	-0.70540700
H	0.50548300	-2.12094200	3.19298000
Cl	-4.33961800	-1.73691300	3.07537500
H	0.77921600	0.72712300	-2.54265800

Variable frequencies

14.3655	18.4841	25.3118
26.6718	38.4546	39.9711
48.9153	52.3724	57.6608
65.6971	76.0722	79.5374
90.3813	101.6311	105.0875
120.9842	140.1425	144.4695
166.9915	174.6951	205.8099
212.3282	214.5816	225.2561
239.8460	249.1004	255.1595

266.6614	271.8289	286.4558
306.7914	340.0518	342.7595
351.5913	358.1324	371.4193
380.6261	404.7661	412.1168
417.8338	419.2546	425.1774
443.8365	452.8310	460.9703
467.5492	472.0730	492.6156
496.8186	519.1009	532.5300
540.0004	556.0739	586.0527
598.4160	605.3820	614.7346
628.5013	631.0376	637.9148
647.9051	652.2155	658.8732
668.7724	675.9503	707.7977
717.8423	721.3939	723.3663
726.2772	750.5599	758.9213
766.0319	773.0642	778.5697
781.9753	784.1872	803.7235
813.3154	844.5892	847.1573
851.1041	861.5452	874.7285
878.8105	881.1025	882.8723
888.2634	893.6313	900.5260
912.6847	921.2414	942.5234
961.2313	962.8868	974.3558
978.9286	997.0398	1002.0427
1004.7098	1006.8621	1007.1452
1016.2938	1019.3225	1020.5433
1022.3227	1023.9532	1028.7436
1033.9167	1035.9910	1042.3722
1052.4247	1065.9823	1070.6092
1072.5172	1091.7871	1098.3809
1107.4246	1121.7458	1125.7060
1132.1566	1134.3127	1138.8200
1147.7756	1154.1675	1163.6424
1176.5986	1182.9551	1183.4039
1185.7134	1196.8466	1202.3561
1203.1901	1207.0698	1215.3513
1220.2930	1225.3781	1234.3600
1244.1276	1260.5031	1263.0303
1274.3359	1284.9897	1298.4361
1312.5320	1313.7162	1320.1359
1323.3729	1325.6757	1335.0696
1340.4212	1345.3993	1350.1266
1352.3262	1356.4042	1365.4502
1367.8452	1370.0642	1373.2920

1382.2303	1417.3032	1423.6355
1455.6008	1457.1099	1466.0850
1494.3087	1502.0367	1504.7050
1505.7448	1522.2327	1529.4002
1535.5908	1536.1977	1550.5134
1553.4552	1563.5191	1624.0786
1655.2114	1664.1103	1676.6631
1679.9257	1680.9687	1682.7579
1686.1469	1686.6615	1697.9226
1701.0397	1704.1912	1788.6992
3047.0693	3082.0235	3093.1681
3148.8142	3157.7417	3164.5028
3165.5441	3193.9466	3199.8665
3200.2660	3202.4228	3204.3994
3204.6280	3206.3412	3213.3252
3213.9885	3219.6380	3221.1737
3222.8480	3224.2362	3225.3287
3226.6250	3231.7720	3232.1781
3234.8810	3236.5358	3247.6259
3247.7636	3250.0548	3871.8080

TS8R

Zero-point correction=0.600346

Thermal correction to Energy=0.634819

Thermal correction to Enthalpy=0.635763

Thermal correction to Gibbs Free Energy=0.532719

Sum of electronic and zero-point Energies=-2294.124813

Sum of electronic and thermal Energies=-2294.090340

Sum of electronic and thermal Enthalpies=-2294.089396

Sum of electronic and thermal Free Energies=-2294.192440

Cartesian coordinate

N	-2.41654900	-2.65848600	-1.19622700
C	-1.24107200	-2.09492600	-1.51653900
C	-1.10482000	-0.70961000	-1.62794100
C	-2.19091400	0.12584900	-1.37068500
C	-3.40470400	-0.46973400	-1.03945000
C	-3.46004100	-1.86109400	-0.98244500
C	-1.96894700	1.63523500	-1.31358500
C	-1.36319000	1.91052800	0.09161600
C	0.04259400	1.73579100	0.14872400
O	0.62544700	2.74824600	-0.39026500
C	-0.07268300	-3.00983700	-1.64667100

C	1.13278100	-2.60152300	-2.22970700
C	2.21689100	-3.47203900	-2.29764000
C	2.11828400	-4.75804500	-1.77026100
C	0.92350600	-5.17227800	-1.18576600
C	-0.16424500	-4.30837800	-1.12984700
H	-0.14202600	-0.27168300	-1.88262500
H	-4.28555000	0.12757400	-0.83038100
H	-4.39595000	-2.35666000	-0.73426600
H	-1.21899000	1.88804700	-2.07471400
H	1.23234200	-1.61182800	-2.66601800
H	3.13943000	-3.13667100	-2.76020300
H	2.96411900	-5.43571400	-1.82441100
H	0.83527200	-6.17369500	-0.77760300
H	-1.10388400	-4.62870400	-0.69256700
C	-3.22074900	2.44577200	-1.59444500
C	-3.90939700	2.20831900	-2.78998000
C	-3.70027400	3.41930700	-0.72147000
C	-5.05307700	2.93124900	-3.10310800
H	-3.54510800	1.44756500	-3.47625000
C	-4.85080000	4.14422800	-1.03370000
H	-3.17311600	3.62221300	0.20562000
C	-5.52886900	3.90264700	-2.22230800
H	-5.57387100	2.73821000	-4.03513100
H	-5.21383800	4.89823500	-0.34303200
H	-6.42289400	4.46697300	-2.46528100
H	-2.00147700	1.52916300	0.88330100
C	5.29517000	1.69203800	0.18319000
C	3.94251200	1.96895700	0.35876600
C	3.49899200	2.84338600	1.34748500
C	4.44336400	3.43565100	2.17884300
C	5.80341600	3.15858100	2.01244100
C	6.23855000	2.29231800	1.01420300
C	5.53038800	0.74692000	-0.96496600
C	4.12273200	0.33726300	-1.46052100
C	3.09794600	1.21461000	-0.63965700
H	2.44278200	3.07144100	1.46087000
H	4.12440400	4.12130500	2.95629500
H	6.52865300	3.62853500	2.66834100
H	7.29659900	2.08723500	0.88502000
H	6.10440300	-0.14071300	-0.67956000
H	3.99567700	0.55727700	-2.52044200
H	6.08715400	1.23428600	-1.77019600
H	2.52025200	1.86695700	-1.29168100
N	2.12324800	0.34489000	0.06704300

O	3.88117000	-1.05448900	-1.36649300
C	0.88605300	0.59968700	0.55035300
C	2.43513600	-0.92469500	0.44637600
N	0.52540600	-0.50574500	1.21595100
N	1.47691100	-1.45964700	1.15656300
C	3.71035600	-1.52318800	-0.04702000
H	4.54783500	-1.24394600	0.60687200
H	3.61570100	-2.60923100	-0.07916300
C	-0.68585400	-0.76072500	1.93203700
C	-1.18232700	0.19701100	2.81040600
C	-1.31365900	-1.98619600	1.73624400
C	-2.37791300	-0.05594300	3.46987600
C	-2.50851400	-2.23458200	2.39639100
C	-3.03524400	-1.26467900	3.24762400
H	-2.79159800	0.66993900	4.15946900
H	-3.03141600	-3.17178500	2.24507000
H	-0.88019700	-2.72272700	1.06815700
H	-0.64308000	1.12258900	2.98848900
Cl	-4.53353900	-1.57196900	4.06047700
H	-0.56579100	3.12490200	-0.32249000

Variable frequencies

-2284.1302	23.2113	26.1642
27.8639	33.2171	36.8953
38.1804	48.7925	52.2056
65.2857	75.3632	80.2504
91.1249	99.9884	116.3746
127.6673	128.1350	140.6954
145.5380	158.1431	171.9626
211.9281	219.7009	223.9135
235.5769	240.7219	243.7638
269.3009	276.5617	285.3574
300.2043	311.3362	346.7717
360.4083	363.2690	377.4674
402.4606	415.6329	416.5547
420.5683	425.8450	435.1138
438.5165	453.7287	459.0875
474.4265	480.2530	485.9117
501.5235	511.5007	525.0236
530.3911	569.4029	590.7307
598.6313	607.4581	623.8363
629.7560	632.0764	641.2140
646.7286	651.5140	662.4234
674.8374	700.2415	712.6609

715.4749	719.6411	726.0070
727.7864	749.1139	757.5525
765.3151	768.5454	780.4952
788.6239	806.3073	812.0260
829.0615	841.8810	852.1677
858.3439	871.9436	872.6785
874.1813	875.3145	879.4584
881.0176	896.9565	910.8867
925.4996	928.6461	936.9038
952.4848	958.3421	965.8673
988.9670	990.4044	1000.0882
1007.2196	1011.3464	1015.2310
1016.4235	1019.4820	1022.0139
1024.0868	1026.6748	1028.1595
1029.7097	1033.6868	1036.0928
1057.7047	1065.4965	1071.5521
1072.5752	1077.6373	1083.7609
1093.8369	1123.8012	1128.0094
1128.2121	1139.4171	1145.8403
1146.0959	1153.7554	1163.8499
1174.3222	1185.0905	1187.4942
1190.7911	1193.1327	1205.5237
1207.2136	1209.0063	1216.3066
1224.6912	1225.9231	1235.2290
1242.6309	1252.5993	1263.6678
1276.6044	1284.7805	1301.0645
1315.3765	1317.7994	1323.2768
1326.2510	1327.8848	1336.7397
1339.6928	1349.8978	1352.7269
1354.6806	1356.2287	1366.8734
1370.4633	1371.2587	1377.8314
1381.6420	1417.0348	1425.6796
1455.5464	1468.5827	1474.7535
1485.1536	1495.0350	1502.2428
1505.9782	1509.0511	1520.4177
1532.7498	1541.8632	1546.5288
1554.4636	1560.4125	1562.5453
1592.4313	1654.9300	1662.1070
1673.0471	1680.5004	1683.7488
1685.4304	1685.8823	1687.2542
1698.2328	1702.5991	1703.9998
1972.8728	3072.1720	3075.1756
3098.9427	3140.8390	3167.3888
3185.2660	3188.6744	3193.1909

3198.5030	3203.4109	3204.0108
3204.4413	3205.3247	3210.2465
3213.2392	3218.5410	3218.5988
3219.0817	3222.4402	3225.8043
3225.9137	3232.2756	3233.3893
3238.6289	3239.0115	3239.4084
3241.4317	3253.2182	3266.2445

TS8R^H

Zero-point correction=0.626372

Thermal correction to Energy=0.662956

Thermal correction to Enthalpy=0.663900

Thermal correction to Gibbs Free Energy=0.555526

Sum of electronic and zero-point Energies=-2370.560782

Sum of electronic and thermal Energies=-2370.524199

Sum of electronic and thermal Enthalpies=-2370.523255

Sum of electronic and thermal Free Energies=-2370.631629

Cartesian coordinate

N	4.54139900	0.57868200	-0.44748500
C	3.99724800	0.29847300	0.74469800
C	2.73446500	0.78042900	1.11224300
C	2.02609700	1.59331700	0.23257100
C	2.60146400	1.88290200	-1.00371300
C	3.85236600	1.34692200	-1.28976400
C	0.63440100	2.09330900	0.59627400
C	-0.39142200	1.11986100	0.01765200
C	-0.89375100	0.07030700	0.79351600
O	-1.11544600	0.07850500	2.03503800
C	4.77377900	-0.60900700	1.63197400
C	4.55034700	-0.65982700	3.01235100
C	5.27252500	-1.53882000	3.81244100
C	6.22619800	-2.38042900	3.24476200
C	6.46186300	-2.33015700	1.87274200
C	5.74575500	-1.44729700	1.07220000
H	2.29348600	0.50652600	2.06643400
H	2.09583800	2.52185700	-1.72110300
H	4.32685400	1.54648000	-2.24810300
H	0.54957000	2.04670600	1.68930400
H	3.83147300	0.00961200	3.47438000
H	5.09653500	-1.55968400	4.88297800
H	6.78923100	-3.06536100	3.87028800
H	7.20840500	-2.97828000	1.42535200

H	5.93360000	-1.38654000	0.00471000
C	0.43753300	3.54172800	0.16943000
C	1.19497600	4.52888700	0.80836000
C	-0.44030300	3.92149100	-0.84516300
C	1.07071100	5.86410000	0.44763300
H	1.88974100	4.24042000	1.59361900
C	-0.56477500	5.26212100	-1.21222800
H	-1.03391300	3.17237700	-1.36375100
C	0.18837800	6.23538500	-0.56696900
H	1.66216900	6.61799400	0.95670100
H	-1.24890700	5.54140400	-2.00713500
H	0.09285400	7.27777500	-0.85188700
H	-0.33280100	0.94973900	-1.05528700
C	-6.02878300	-0.61171200	0.69421500
C	-4.70570300	-0.23721700	0.48207100
C	-4.37801900	0.86712900	-0.30205500
C	-5.41080400	1.63209700	-0.83955600
C	-6.74223700	1.28304600	-0.59806200
C	-7.05930100	0.15670600	0.15756200
C	-6.11675500	-1.87799900	1.50760200
C	-4.66410700	-2.40076600	1.61405200
C	-3.76318900	-1.18332800	1.19106900
H	-3.34086200	1.09942600	-0.54196600
H	-5.18173200	2.49198100	-1.45983500
H	-7.53768400	1.88548200	-1.02340900
H	-8.09593100	-0.12387400	0.31558700
H	-6.75215800	-2.63917300	1.04474200
H	-4.41906100	-2.70707000	2.63076700
H	-6.52409300	-1.68257800	2.50444100
H	-3.27329900	-0.73454000	2.05718500
N	-2.69641500	-1.62604000	0.29001900
O	-4.43149700	-3.56444800	0.83789400
C	-1.48277500	-1.10570900	0.05265800
C	-2.90933400	-2.60390600	-0.63798200
N	-0.99331400	-1.80443000	-0.97124600
N	-1.87161300	-2.74577400	-1.41428500
C	-4.19967400	-3.35536200	-0.54020400
H	-5.01003400	-2.78799800	-1.01864100
H	-4.11050700	-4.32968900	-1.01971900
C	0.32237300	-1.72985500	-1.54092800
C	0.44099900	-1.56802700	-2.91606100
C	1.42865500	-1.86500400	-0.70979700
C	1.71111800	-1.51898100	-3.47527200
C	2.69688700	-1.83255300	-1.27515400

C	2.82552000	-1.64757300	-2.64867500
H	1.83956000	-1.38623100	-4.54294000
H	3.57882700	-1.95028800	-0.65575400
H	1.30791500	-2.01751200	0.35870100
H	-0.44572000	-1.48703800	-3.53516300
Cl	4.41250600	-1.58169000	-3.34550700
H	-1.86153100	1.62185900	2.16592800
O	-2.10531300	2.38076600	1.55336300
H	-1.57003700	1.95109900	0.63736200
H	-3.06911500	2.42011000	1.43149100

Variable frequencies

-945.0186	10.6272	23.7763
30.0788	31.1039	37.1756
42.1187	47.0589	54.7694
56.1949	60.0429	72.6320
78.5463	88.4212	97.4630
108.2169	114.6077	133.2998
141.1672	156.4670	161.7978
178.6939	183.2580	208.2720
221.7260	226.5745	233.0757
239.7709	251.3398	261.1810
267.4747	274.7046	304.7724
309.0452	333.1676	351.7098
358.6697	385.9762	398.1518
413.0863	416.2507	418.8890
425.4425	426.9161	433.9291
440.7293	453.1993	473.3872
475.7832	482.5933	486.1350
490.5568	516.7570	525.1311
532.8287	553.4570	561.8144
593.2754	609.3892	615.1468
618.9793	625.1160	627.4084
632.5031	644.5387	650.0499
656.1124	673.5555	701.1849
710.6834	718.2848	722.9673
725.0412	725.7897	736.9373
752.0858	766.0475	768.1816
773.9922	783.4256	793.4807
804.2480	817.0976	825.3186
839.5692	841.2165	852.9477
861.8826	866.8880	874.5838
878.8778	881.4800	882.6806
893.2062	909.5052	915.0352

922.5757	927.0547	954.9934
961.4690	962.5131	971.3439
989.0479	996.0220	999.7498
1010.0189	1011.5556	1015.9913
1019.4485	1021.1823	1024.1438
1026.6284	1029.6286	1030.7438
1031.7963	1050.0142	1052.7474
1059.3714	1060.8760	1069.0887
1071.9742	1076.5454	1092.0538
1097.3747	1117.9397	1122.9890
1127.5597	1136.3230	1137.2190
1138.6413	1154.7865	1161.2144
1181.9907	1182.2032	1186.8259
1199.2961	1200.3494	1203.7185
1204.7412	1215.0881	1217.6154
1228.2965	1233.8410	1251.0807
1252.7375	1278.9681	1280.8266
1287.5504	1299.9621	1307.3843
1308.9589	1318.1798	1318.8271
1320.6130	1327.7545	1336.8980
1341.9389	1350.5167	1354.3312
1356.3002	1357.4620	1364.8925
1367.2579	1375.6996	1378.0351
1381.7250	1419.0552	1455.9266
1465.5329	1472.7657	1480.3080
1487.8864	1501.9195	1502.8750
1505.3695	1515.9112	1535.5820
1538.3856	1543.9032	1546.6869
1553.6192	1559.1728	1596.6107
1614.3971	1644.8837	1653.1468
1675.2614	1675.3596	1681.8745
1682.3646	1685.2437	1686.5283
1687.9711	1697.8060	1698.7398
1702.4882	1812.3290	3071.2139
3083.0236	3093.1428	3139.7892
3161.3826	3172.1317	3182.4078
3186.3293	3188.5882	3189.3315
3193.0027	3197.1494	3199.8056
3201.1389	3205.1769	3206.0777
3211.1031	3211.4511	3216.0977
3217.4448	3218.7130	3219.2394
3223.9336	3224.1287	3227.8493
3230.8242	3235.1064	3238.8101
3239.9559	3250.2757	3797.9164

TS8R^M

Zero-point correction=0.655336
Thermal correction to Energy=0.693834
Thermal correction to Enthalpy=0.694779
Thermal correction to Gibbs Free Energy=0.580366
Sum of electronic and zero-point Energies=-2409.815490
Sum of electronic and thermal Energies=-2409.776992
Sum of electronic and thermal Enthalpies=-2409.776048
Sum of electronic and thermal Free Energies=-2409.890461

Cartesian coordinate

N	4.53824800	0.53539800	-0.84153200
C	4.15427200	0.49634200	0.44095100
C	2.90106100	0.97015600	0.85256700
C	2.03428600	1.52369000	-0.08357300
C	2.44503600	1.56523500	-1.41606100
C	3.69632600	1.05259000	-1.73636700
C	0.66089400	2.02650900	0.33314000
C	-0.39251900	0.99548900	-0.06118100
C	-0.85528400	0.04530500	0.85706900
O	-1.00904600	0.16705200	2.09682900
C	5.10160700	-0.13551000	1.39785900
C	5.04901100	0.12865500	2.77078600
C	5.93363300	-0.49545700	3.64366700
C	6.88099000	-1.39362900	3.15747500
C	6.94536400	-1.65691800	1.79101600
C	6.06618200	-1.02920200	0.91589100
H	2.59260700	0.88836600	1.89057000
H	1.81144800	1.99975900	-2.18370000
H	4.04457500	1.06079400	-2.76700900
H	0.65672100	2.09174500	1.42814400
H	4.33575100	0.84728200	3.16237900
H	5.88945000	-0.27308500	4.70484300
H	7.57039200	-1.87971700	3.84006300
H	7.68398400	-2.35178400	1.40481300
H	6.11537700	-1.21494800	-0.15253600
C	0.40139000	3.42488400	-0.21776400
C	1.16611000	4.48850100	0.27104400
C	-0.56164700	3.68553800	-1.19342600
C	0.96257500	5.78241200	-0.19197000
H	1.92848200	4.29463500	1.02187300
C	-0.76766000	4.98450100	-1.66182300

H	-1.15687900	2.87219700	-1.60249400
C	-0.00909500	6.03557900	-1.16043300
H	1.56180000	6.59648200	0.20264300
H	-1.51750800	5.16852900	-2.42482700
H	-0.16718800	7.04546400	-1.52376900
H	-0.39896900	0.69670200	-1.10771000
C	-6.01547100	-0.69709600	0.54268700
C	-4.68695600	-0.33236600	0.34270100
C	-4.32183700	0.57842700	-0.64533300
C	-5.32491600	1.15267400	-1.42186800
C	-6.66265300	0.80817800	-1.21097800
C	-7.01662000	-0.11965000	-0.23449200
C	-6.13956000	-1.73250100	1.63154900
C	-4.69249200	-2.19103100	1.92456300
C	-3.77689700	-1.07678900	1.29502600
H	-3.27579400	0.82790300	-0.82285100
H	-5.06766700	1.86292600	-2.20047200
H	-7.43364500	1.26004900	-1.82605700
H	-8.05620200	-0.39652400	-0.08983900
H	-6.75070100	-2.59251500	1.34322100
H	-4.49971100	-2.27413900	2.99397500
H	-6.59009500	-1.30442400	2.53264800
H	-3.32787400	-0.44354500	2.06353200
N	-2.67109300	-1.69287200	0.55974900
O	-4.41031800	-3.48682200	1.42115500
C	-1.45285800	-1.21600800	0.26986800
C	-2.85236200	-2.82929300	-0.17521200
N	-0.93211000	-2.08255000	-0.59813500
N	-1.79347700	-3.10048800	-0.88383300
C	-4.13643100	-3.56705800	0.03648900
H	-4.93876400	-3.13126300	-0.57479400
H	-4.01829900	-4.61876500	-0.22340100
C	0.39144800	-2.09840300	-1.15248100
C	0.52642800	-2.25972700	-2.52613900
C	1.48856100	-2.01271100	-0.30294100
C	1.80250200	-2.32716800	-3.06896200
C	2.76385800	-2.09676800	-0.84777300
C	2.90781400	-2.24752000	-2.22429100
H	1.94285400	-2.44907900	-4.13642900
H	3.63983900	-2.05761700	-0.21011900
H	1.35248800	-1.91268100	0.76981000
H	-0.35336000	-2.33781100	-3.15519500
Cl	4.50037500	-2.35074700	-2.90265000
H	-1.84378500	1.87114400	2.15829700

C	-3.19481000	3.20297200	1.28941400
H	-3.11058800	3.80741000	0.38748100
H	-4.01404900	2.48835000	1.20836800
H	-3.30520800	3.84358700	2.16209300
O	-1.92953800	2.51296000	1.41698700
H	-1.52129600	1.91834900	0.55380900

Variable frequencies

-624.8782	2.0593	24.1701
28.5923	30.8644	37.9504
41.7215	44.2012	50.3160
54.8442	65.8377	69.8496
70.2984	84.0286	88.9609
97.0132	103.2361	110.3543
119.5259	130.9978	149.2927
155.4297	160.8577	172.1165
188.0607	195.8877	208.8764
220.0309	221.6161	232.0863
238.7243	247.4554	256.2841
264.0492	269.4442	287.0287
308.4429	325.6709	351.4592
358.1485	381.8991	390.3471
410.3793	418.1932	418.9511
422.9360	427.0791	434.3444
441.5380	450.7817	471.8506
482.5215	487.4569	490.2297
518.6737	526.5474	536.1114
558.4895	571.0103	593.2035
609.3945	612.8423	624.7409
628.2273	630.9599	643.2154
650.9884	657.8824	673.0166
691.3788	708.3138	718.1065
725.0245	726.1191	728.3863
734.4573	751.8091	761.0201
765.2831	771.6683	775.8641
791.3742	803.3930	804.2181
822.8151	841.2929	845.6284
847.8918	852.7673	864.5091
865.0596	878.4029	882.4343
883.1367	884.2699	895.8143
910.5302	915.9170	920.4428
932.7800	957.4735	959.8084
962.8375	978.5272	987.7619
999.6585	1004.7329	1008.4295

1014.0029	1015.9634	1017.5085
1020.8965	1023.7639	1025.5058
1029.3237	1030.8674	1032.0167
1048.7134	1052.2009	1055.8023
1061.0180	1070.6127	1071.4541
1074.2531	1092.2238	1098.8219
1115.5682	1121.7295	1122.2882
1127.9862	1136.1457	1136.6120
1147.1419	1151.3717	1158.0027
1172.1153	1183.4818	1183.7278
1185.3031	1196.2229	1199.3236
1200.8457	1207.7142	1209.5936
1216.5271	1225.2570	1226.5414
1232.9878	1245.0799	1250.6507
1273.9772	1278.4551	1282.2238
1296.8398	1303.1839	1316.1196
1318.8739	1321.5489	1326.3940
1332.3979	1337.9153	1347.2014
1349.8707	1352.8581	1357.1196
1364.2557	1370.2704	1373.4476
1376.6786	1377.3315	1418.3961
1420.5055	1458.7238	1465.3487
1471.1749	1484.0244	1486.9625
1496.9277	1497.2378	1502.3584
1502.6661	1505.1197	1517.9745
1529.2105	1535.4544	1538.4600
1543.5673	1547.8197	1551.0213
1563.9499	1596.0440	1645.9337
1653.3019	1674.5266	1674.7421
1677.8964	1683.3779	1684.6649
1686.5598	1687.9677	1700.2997
1700.8737	1701.3195	1833.9853
3076.5823	3080.3897	3091.8981
3111.8627	3145.0017	3153.3068
3169.2631	3176.1107	3188.2302
3188.4595	3192.2719	3194.3891
3199.2994	3203.3620	3207.6547
3208.7116	3211.9259	3212.0897
3215.2528	3216.1280	3220.0562
3221.2491	3222.1461	3222.7091
3228.1223	3228.2028	3233.0977
3235.0044	3237.1255	3239.1621
3250.1036	3252.4095	3556.3077

TS8R^P

Zero-point correction=0.749514

Thermal correction to Energy=0.793357

Thermal correction to Enthalpy=0.794301

Thermal correction to Gibbs Free Energy=0.668773

Sum of electronic and zero-point Energies=-2640.962628

Sum of electronic and thermal Energies=-2640.918786

Sum of electronic and thermal Enthalpies=-2640.917841

Sum of electronic and thermal Free Energies=-2641.043370

Cartesian coordinate

N	-4.96002500	0.89310600	-0.46928400
C	-4.09228600	0.33111700	-1.32632500
C	-2.73750500	0.67351300	-1.32881100
C	-2.25968100	1.63551100	-0.44074400
C	-3.16763400	2.22641900	0.43195700
C	-4.49845600	1.81275200	0.37565500
C	-0.76232500	1.92560200	-0.42667100
C	-0.07037800	0.79904500	0.35437300
C	0.40298600	-0.31499200	-0.35992600
O	0.83638600	-0.29775300	-1.54220300
C	-4.62564800	-0.71468400	-2.23941900
C	-3.97132200	-1.03875500	-3.43335300
C	-4.46866400	-2.03711700	-4.26354700
C	-5.62704200	-2.72565200	-3.91224200
C	-6.29210200	-2.40087400	-2.73174500
C	-5.79910800	-1.39902900	-1.90302700
H	-2.04343500	0.17491200	-2.00060500
H	-2.86080600	2.99180700	1.13652700
H	-5.23009500	2.24692200	1.05321600
H	-0.42793400	1.85381200	-1.46709100
H	-3.08686200	-0.48797300	-3.73814900
H	-3.95729200	-2.26923300	-5.19202500
H	-6.01541400	-3.50407200	-4.56074000
H	-7.20003400	-2.92800400	-2.45735500
H	-6.31992200	-1.12723300	-0.99091200
C	-0.41577500	3.31997700	0.06177400
C	-0.27269200	4.34961400	-0.87094200
C	-0.25475100	3.61272200	1.41849900
C	0.01149300	5.64989100	-0.45801600
H	-0.39203800	4.13191500	-1.92979900
C	0.02612200	4.91156800	1.83459500
H	-0.34919600	2.82338200	2.15987400

C	0.15715300	5.93456400	0.89748400
H	0.11827000	6.43832100	-1.19626100
H	0.14481100	5.12440600	2.89196700
H	0.37681300	6.94622900	1.22194700
H	-0.44907000	0.61627700	1.35648800
C	5.11803200	-2.74291100	-0.30274400
C	4.03208200	-1.90377300	-0.06643800
C	4.14770300	-0.76628200	0.72493400
C	5.38939900	-0.47213600	1.28316700
C	6.48615300	-1.30379400	1.04343000
C	6.35910500	-2.44262000	0.25157600
C	4.73222500	-3.90059300	-1.18727500
C	3.18976300	-3.86182200	-1.25700000
C	2.80162100	-2.40992000	-0.78496400
H	3.29705500	-0.11690200	0.91492100
H	5.50341100	0.40657500	1.90989700
H	7.44703800	-1.06326500	1.48614600
H	7.21290900	-3.08944700	0.07515900
H	5.06273500	-4.87114800	-0.80620700
H	2.82018100	-4.03486800	-2.26763000
H	5.15800600	-3.78413600	-2.18896700
H	2.51123800	-1.78532000	-1.62897000
N	1.64419100	-2.46870800	0.12537300
O	2.58320900	-4.88573300	-0.48480800
C	0.63293000	-1.61541900	0.36263500
C	1.52893800	-3.48621400	1.02864600
N	-0.06270900	-2.15761100	1.36607800
N	0.48345100	-3.32410800	1.79163600
C	2.48615100	-4.62717900	0.90080200
H	3.45555400	-4.37736900	1.35244700
H	2.07922500	-5.51493500	1.38433500
C	-1.30247700	-1.70820400	1.93792300
C	-1.33462400	-1.41492400	3.29584100
C	-2.42439900	-1.59961000	1.12470600
C	-2.52546500	-0.96767500	3.85376000
C	-3.61616900	-1.16029400	1.68798700
C	-3.65005600	-0.83591500	3.04149600
H	-2.58341200	-0.72090500	4.90707600
H	-4.51018400	-1.06734100	1.08176900
H	-2.38088300	-1.86228900	0.07216500
H	-0.44191000	-1.53034700	3.90099900
Cl	-5.13184100	-0.25800200	3.73271700
H	1.23941200	1.31221800	0.40970000
C	2.58718500	2.34662900	-0.86517600

O	2.29068900	1.92475900	0.28381800
O	2.09615400	1.84733100	-1.94791300
H	1.53253000	0.98997300	-1.82103000
C	3.61872100	3.43791700	-1.02057600
C	3.31186700	4.29046500	-2.25615200
H	4.08780500	5.05334300	-2.35819900
H	3.29563200	3.68687500	-3.16522800
H	2.34712700	4.79431800	-2.15007200
C	3.64370200	4.29956500	0.24351800
H	3.90585400	3.70666800	1.12203400
H	4.38812100	5.09013600	0.11958900
H	2.66759000	4.76308700	0.41731400
C	4.96373800	2.70349400	-1.20603800
H	5.75733700	3.44874100	-1.30475400
H	5.19065700	2.06614500	-0.34612300
H	4.95353500	2.08731000	-2.10919900

Variable frequencies

-1259.5327	7.2653	18.8135
19.4661	24.6452	26.7519
30.1250	41.4629	43.7292
46.7359	48.5993	59.4412
60.1735	72.6740	77.8416
81.8101	87.0479	93.8391
103.6762	110.1703	112.9868
120.3291	134.4851	141.4748
155.6875	163.5046	175.6690
198.3498	209.4377	224.1247
228.7391	232.7375	235.6855
241.4336	243.7319	258.1937
263.3237	269.0310	278.5089
286.3087	298.2534	301.4902
311.4930	323.5779	347.6842
358.1765	363.5898	369.2032
383.9613	386.5843	412.7338
413.6459	415.9522	418.5941
424.1952	427.4807	440.3410
443.0072	444.8276	477.3846
483.3710	487.3656	497.1905
508.2958	517.7258	526.5070
536.6443	560.4497	584.7503
595.7193	605.5507	614.3185
623.1983	627.3679	629.3052
641.7089	649.9642	651.9979

653.9069	675.6368	707.6945
711.2370	716.9916	721.9820
725.0952	730.6300	736.5033
754.9696	759.5978	766.1892
771.4117	777.4434	790.1753
792.2781	802.4445	805.7019
817.2976	822.8104	839.4315
841.9450	855.2070	859.7158
871.8098	876.3225	878.3926
880.1094	882.3636	896.0886
909.3837	913.3359	927.0576
937.6331	944.3669	952.3285
962.2417	963.6272	965.9330
971.9316	974.7892	980.3406
981.3632	990.1331	1003.7160
1006.2431	1017.8444	1018.6695
1020.7222	1021.9909	1022.3262
1023.5073	1028.4347	1029.5102
1031.0428	1048.6458	1050.2978
1052.5659	1055.7314	1065.4153
1066.9024	1073.9017	1075.0395
1084.6344	1103.0706	1109.0716
1118.1550	1122.1848	1127.1762
1134.6135	1139.1608	1148.5779
1153.5217	1161.9796	1175.4412
1181.3054	1184.0139	1192.1167
1199.8369	1201.4565	1206.6478
1215.9556	1219.3211	1226.7780
1228.4157	1239.2375	1244.8117
1248.5510	1250.9742	1267.1590
1269.5885	1278.9589	1280.3626
1294.7604	1308.1689	1310.4726
1313.6578	1320.1133	1323.6480
1325.3447	1334.3827	1343.8634
1346.5737	1348.4273	1359.0511
1364.0692	1369.8813	1371.3292
1373.8096	1376.7239	1377.9930
1403.9190	1415.2978	1421.8545
1423.0933	1430.8790	1452.3740
1459.0096	1461.4731	1467.5760
1483.8028	1484.2211	1490.0295
1491.4995	1497.5409	1499.3389
1504.5266	1505.5008	1512.7620
1514.6045	1516.1643	1531.4283

1535.8801	1537.5181	1540.3817
1544.8787	1556.4777	1565.9838
1588.6160	1595.4593	1656.2828
1673.2755	1675.5085	1676.4310
1680.4834	1680.7881	1683.9680
1686.9630	1691.1751	1700.2021
1700.7202	1702.9068	1706.8909
2568.9406	3073.5182	3082.9792
3083.9056	3085.6343	3095.7711
3110.3824	3141.5610	3159.6619
3163.0878	3164.3365	3167.1336
3168.8487	3179.5701	3181.8732
3186.0619	3193.4542	3199.1499
3201.4183	3201.7689	3202.0562
3205.4630	3205.7921	3206.0301
3209.5393	3214.7399	3215.1705
3216.1689	3222.7440	3224.3954
3226.3284	3226.9492	3227.7196
3228.8848	3229.2438	3234.4051
3234.7715	3246.1872	3250.0295

M8R

Zero-point correction=0.604384

Thermal correction to Energy=0.639839

Thermal correction to Enthalpy=0.640784

Thermal correction to Gibbs Free Energy=0.532263

Sum of electronic and zero-point Energies=-2294.229908

Sum of electronic and thermal Energies=-2294.194453

Sum of electronic and thermal Enthalpies=-2294.193509

Sum of electronic and thermal Free Energies=-2294.302030

Cartesian coordinate

N	-4.54490800	-0.16183400	-0.36382500
C	-3.63191800	-0.62611000	-1.22982200
C	-2.45936300	0.08580200	-1.51673000
C	-2.22284700	1.31029800	-0.89623300
C	-3.18568300	1.79013300	-0.00924100
C	-4.32011000	1.01700900	0.21648500
C	-0.91226100	2.05073600	-1.13436200
C	0.15600000	1.50780200	-0.16854000
C	0.76070900	0.20804900	-0.63200200
O	0.79886200	-0.18221200	-1.77306800
C	-3.89855500	-1.95779200	-1.83736200

C	-3.27730500	-2.35894200	-3.02531800
C	-3.52166200	-3.61965700	-3.55944400
C	-4.38928000	-4.49713500	-2.91428900
C	-5.02233900	-4.10114400	-1.73818500
C	-4.78320000	-2.83947500	-1.20564200
H	-1.72571400	-0.31761300	-2.20716800
H	-3.06562800	2.74669600	0.48811200
H	-5.08730600	1.36316000	0.90540700
H	-0.57555600	1.81298300	-2.14940000
H	-2.62226700	-1.67748000	-3.55899300
H	-3.04073100	-3.91292000	-4.48696200
H	-4.57817100	-5.48072500	-3.33188000
H	-5.70723700	-4.77632100	-1.23553300
H	-5.28383800	-2.51715800	-0.29894100
C	-1.07360600	3.55675100	-1.03740800
C	-1.57794300	4.24426400	-2.14468400
C	-0.78628200	4.27314600	0.12569100
C	-1.78340800	5.61804500	-2.09440000
H	-1.81343300	3.69304100	-3.05149100
C	-0.99248200	5.65105600	0.17903200
H	-0.40512600	3.76393100	1.00697100
C	-1.48971900	6.32617400	-0.93030000
H	-2.17145100	6.13714100	-2.96460800
H	-0.76413400	6.19422200	1.09016000
H	-1.64879400	7.39845200	-0.88982800
H	-0.22829600	1.41037100	0.85183100
C	6.02971000	-0.47069100	-0.78018400
C	4.74391800	0.03578200	-0.61099100
C	4.52859700	1.35799900	-0.23781200
C	5.63256700	2.17918700	-0.03137600
C	6.92557700	1.67716800	-0.20028100
C	7.13326900	0.35287700	-0.57636900
C	6.00102700	-1.91694800	-1.19938400
C	4.53562500	-2.36683400	-1.01180000
C	3.70747100	-1.02708700	-0.89694500
H	3.52447400	1.75179600	-0.10394000
H	5.48929300	3.21374900	0.26061900
H	7.77715600	2.32834500	-0.03384400
H	8.13949700	-0.03341700	-0.70417500
H	6.66299700	-2.55661700	-0.60847200
H	4.17406500	-2.95580100	-1.85430500
H	6.29894100	-2.02484500	-2.24699300
H	3.13150800	-0.83659300	-1.80439000
N	2.74263600	-1.13855800	0.21112600

O	4.36907600	-3.22053600	0.10855300
C	1.51727300	-0.62368800	0.38848700
C	3.07077400	-1.78814900	1.36862800
N	1.14229100	-0.99223800	1.61283000
N	2.09878800	-1.72414500	2.23712200
C	4.34429000	-2.57172700	1.36411300
H	5.21245800	-1.91764800	1.51926500
H	4.31846400	-3.33434600	2.14204300
C	-0.15337900	-0.82656800	2.20533500
C	-0.24444600	-0.27808900	3.47939800
C	-1.27120700	-1.23684900	1.48555600
C	-1.50344200	-0.10694700	4.03919100
C	-2.52880700	-1.06742500	2.05180900
C	-2.63193600	-0.49324200	3.31614500
H	-1.61388900	0.32502800	5.02670900
H	-3.41898000	-1.37850800	1.51722400
H	-1.16934200	-1.70696400	0.51118000
H	0.65217400	0.00981000	4.01699200
Cl	-4.20203600	-0.25866200	4.00846000
H	1.00457400	2.20821300	-0.11865800

Variable frequencies

12.2343	17.8233	22.2748
23.9889	24.8793	34.9823
39.2505	44.6832	46.9395
52.4093	65.1706	76.2823
81.7010	84.5300	99.3541
114.5426	117.1110	136.2319
147.0282	170.7224	181.6234
205.5721	217.6216	225.9449
229.2490	239.9714	248.7588
263.0693	270.6291	286.9288
305.9770	313.5078	351.9965
360.7458	375.2469	383.4238
410.8368	414.9713	415.8284
417.7199	425.6319	429.6408
438.9411	444.5165	474.5785
480.8925	485.4819	493.8310
519.9059	524.1187	529.3278
546.1251	566.2469	591.3123
602.1730	608.3746	625.6918
626.7193	630.7510	644.3550
648.4784	649.9269	671.0190
706.7369	714.7624	720.1346

723.7987	724.4467	730.8006
742.9264	754.0044	759.2665
764.3474	767.8748	787.6811
797.0811	808.9669	811.6515
836.8656	851.0915	858.1229
863.1512	868.4402	874.3750
874.8323	875.2840	882.3949
886.3660	903.8082	909.6700
938.8411	948.5148	950.4395
960.2968	979.0165	983.6801
989.2807	1001.1338	1005.0248
1006.4501	1007.4705	1015.6675
1016.1944	1019.6674	1022.9120
1025.5296	1028.2607	1029.3171
1032.0572	1036.6251	1047.5209
1052.9773	1064.1122	1068.8644
1069.3655	1080.6252	1099.1234
1114.9956	1118.3780	1123.4197
1132.9207	1138.0822	1143.9495
1154.9369	1156.7850	1165.1594
1177.2745	1181.7914	1185.4851
1192.9567	1198.3819	1200.4457
1203.9833	1218.9885	1220.7468
1222.4813	1236.3238	1241.0980
1250.3387	1266.8757	1276.1083
1288.7081	1299.3567	1306.5555
1309.1276	1317.2324	1324.8205
1332.1054	1333.5611	1335.4118
1344.3268	1348.0792	1353.4806
1359.1678	1361.2972	1368.9330
1372.5824	1375.1506	1378.3610
1408.3923	1416.1290	1445.6468
1458.4693	1461.1630	1464.3867
1481.4647	1484.9647	1499.8937
1508.4071	1519.2155	1534.0277
1536.5707	1538.9949	1544.4476
1558.5716	1559.3722	1590.4307
1652.0850	1669.8130	1675.0800
1678.0271	1681.8662	1682.1453
1685.5695	1690.6201	1694.5990
1703.3398	1704.0617	1864.2429
3045.8233	3086.3284	3091.9435
3098.0443	3131.0052	3143.7610
3160.0832	3176.4601	3191.8706

3196.5083	3197.5111	3199.8353
3200.0194	3200.1136	3208.6246
3212.4662	3213.3935	3215.7787
3220.4872	3223.6913	3228.1556
3229.7845	3231.2794	3232.1009
3233.4805	3237.0204	3237.2918
3242.5417	3254.4409	3264.4697

MeOH + PivO⁻

Zero-point correction=0.188957

Thermal correction to Energy=0.201035

Thermal correction to Enthalpy=0.201980

Thermal correction to Gibbs Free Energy=0.150463

Sum of electronic and zero-point Energies=-461.858095

Sum of electronic and thermal Energies=-461.846016

Sum of electronic and thermal Enthalpies=-461.845072

Sum of electronic and thermal Free Energies=-461.896589

Cartesian coordinate

C	3.53102300	0.50145700	-0.26410600
H	4.44847800	0.88146800	0.20756200
H	3.73529900	0.43284300	-1.34845800
H	2.72931600	1.23611900	-0.12006000
O	3.19599700	-0.73662100	0.30113000
H	2.20855600	-0.82727700	0.18333600
C	-1.60754900	-0.01425900	-0.02204300
C	-1.94360800	-0.64898200	-1.37491900
H	-3.02104800	-0.83991200	-1.46397500
H	-1.64694900	0.01030800	-2.19853000
H	-1.40212000	-1.59138300	-1.48332900
C	-2.31438800	1.32959700	0.12232700
H	-3.40346500	1.20544700	0.06016300
H	-2.06599900	1.79403700	1.08005800
H	-1.99303800	2.01877300	-0.66313300
C	-2.04180100	-0.96397000	1.09913900
H	-1.49345700	-1.90520900	1.01778100
H	-1.82737000	-0.52818800	2.08140600
H	-3.11903400	-1.16904100	1.04625600
C	-0.05879800	0.15662900	0.06409500
O	0.59090000	-0.92223700	-0.07774700
O	0.39579600	1.29875700	0.25836300

Variable frequencies

41.2981	68.6449	72.9266
78.1849	143.0322	176.6884
216.0993	223.7582	262.2403
281.5371	299.9481	305.6613
360.4145	385.4872	386.3466
541.9488	597.6110	800.4548
809.4450	886.3023	934.5644
949.2362	956.7863	967.5278
1049.1137	1055.7010	1148.3986
1175.7971	1208.3558	1258.0467
1262.8456	1285.0515	1385.2018
1396.4479	1409.3578	1458.3140
1483.7204	1488.5889	1497.0053
1500.0527	1506.4498	1511.9936
1518.3753	1534.7297	1549.4120
1573.7424	1748.7123	2961.4632
3035.1368	3035.5463	3039.0204
3046.2070	3106.9509	3107.8609
3113.2109	3127.9876	3150.5032
3151.7582	3153.5192	3161.6833

M09R

Zero-point correction=0.796872

Thermal correction to Energy=0.844544

Thermal correction to Enthalpy=0.845488

Thermal correction to Gibbs Free Energy=0.711834

Sum of electronic and zero-point Energies=-2756.195904

Sum of electronic and thermal Energies=-2756.148233

Sum of electronic and thermal Enthalpies=-2756.147289

Sum of electronic and thermal Free Energies=-2756.280942

Cartesian coordinate

N	5.93856700	-1.15340000	-0.54798200
C	5.78658900	-0.17155400	0.35655100
C	4.54049900	0.39623400	0.62933000
C	3.40473000	-0.03917100	-0.05337900
C	3.57867400	-1.04713100	-1.00144400
C	4.85630300	-1.56546900	-1.20063000
C	2.06148900	0.60917300	0.24115600
C	0.88227500	-0.27481400	-0.18690500
C	-0.41168800	0.08880800	0.59420800
O	-0.49592000	1.27385100	1.05502400
C	7.01601300	0.26319400	1.07369500

C	7.12133200	1.53563700	1.64516000
C	8.27799800	1.91415100	2.31966700
C	9.34558000	1.02743000	2.43147200
C	9.25306500	-0.23806700	1.85558400
C	8.09938600	-0.61591400	1.17886300
H	4.43994400	1.16502700	1.38967600
H	2.74382200	-1.44338100	-1.57128800
H	5.01041900	-2.35989000	-1.92834400
H	1.99367000	0.76284900	1.32375300
H	6.30919500	2.24844500	1.54095400
H	8.34826100	2.90758400	2.75120100
H	10.24660900	1.32290900	2.95955900
H	10.08235900	-0.93387000	1.93551400
H	8.01714500	-1.59564600	0.72152800
C	2.00837300	1.98696900	-0.41024200
C	1.74196100	3.12859200	0.34689300
C	2.22807700	2.12633600	-1.78252400
C	1.69911400	4.38342400	-0.25357100
H	1.52469200	3.01666300	1.40411400
C	2.18039100	3.37909600	-2.38854000
H	2.45437800	1.24670100	-2.38196100
C	1.92226500	4.51368800	-1.62289400
H	1.48069500	5.26075000	0.34735000
H	2.35736800	3.47017300	-3.45584600
H	1.89144500	5.49326400	-2.09070400
H	0.71281800	-0.14102700	-1.26400600
C	-4.09263900	3.65089100	-0.53978300
C	-2.93994400	2.87963600	-0.40941000
C	-1.73850100	3.26232200	-1.00206600
C	-1.72223500	4.43181600	-1.75892300
C	-2.87798900	5.20290400	-1.90532900
C	-4.06833400	4.82347300	-1.29053200
C	-5.24306600	3.06073000	0.23398900
C	-4.75255100	1.67315000	0.70739400
C	-3.20012800	1.65928100	0.44584500
H	-0.83744000	2.67361800	-0.84489500
H	-0.79477500	4.74720900	-2.22618200
H	-2.84630100	6.11165200	-2.49845900
H	-4.96316100	5.43042200	-1.39506200
H	-6.15690200	2.95254000	-0.35995400
H	-4.93119500	1.49717600	1.76672100
H	-5.49619500	3.68706600	1.09541400
H	-2.62766100	1.66155600	1.37079700
N	-2.81408400	0.42461200	-0.26678600

O	-5.46088500	0.61791500	0.06258200
C	-1.67269900	-0.27931600	-0.26485400
C	-3.66078100	-0.17333800	-1.15836100
N	-1.87938500	-1.27079200	-1.13776500
N	-3.12094500	-1.22222600	-1.70515700
C	-5.04416400	0.37236300	-1.26457900
H	-5.05994700	1.28564400	-1.87593000
H	-5.71172700	-0.36841600	-1.70595100
C	-0.98780900	-2.33692000	-1.49024000
C	-0.47001700	-2.36747800	-2.78002300
C	-0.66012900	-3.29829700	-0.54276800
C	0.42505700	-3.37176400	-3.12678500
C	0.24303200	-4.29860300	-0.88671400
C	0.77929000	-4.31995500	-2.17021700
H	0.84996600	-3.41879100	-4.12252100
H	0.52810500	-5.05647300	-0.16641500
H	-1.09368900	-3.25242900	0.44912600
H	-0.75934100	-1.60563100	-3.49624100
Cl	1.92205400	-5.56403600	-2.59487000
H	1.11763500	-1.32931100	-0.02318200
C	-0.11822400	-0.62638500	2.95060300
H	-0.32910600	0.43322900	3.11031800
H	-0.65900100	-1.22685000	3.68690200
H	0.95770200	-0.81140000	3.05683400
O	-0.56717400	-1.02101400	1.66405900
H	-1.95835700	-1.64736400	1.75828100
C	-5.14322000	-2.22987800	2.26073000
C	-5.47565300	-2.73836300	0.85129400
H	-6.39447200	-3.33233200	0.88301500
H	-5.63762900	-1.89528600	0.17361700
H	-4.66898300	-3.35918900	0.45431800
C	-6.25103600	-1.31211900	2.77142100
H	-7.18786100	-1.87301900	2.84584100
H	-6.00335800	-0.91144300	3.75748600
H	-6.40000000	-0.47523100	2.08411400
C	-4.95298900	-3.42415400	3.21015900
H	-4.16140500	-4.08587700	2.85090600
H	-4.69409700	-3.08701400	4.21878200
H	-5.88529000	-3.99418100	3.27087700
C	-3.82638100	-1.46347500	2.21749800
O	-2.82830300	-2.17902000	1.70727600
O	-3.67274300	-0.32822900	2.62753100

Variable frequencies

10.2159	18.9225	24.2200
26.4613	30.9796	33.6209
37.4666	42.7576	43.7548
50.0427	52.7567	59.7920
60.0261	66.7306	72.8616
80.2623	82.6780	85.5365
87.0979	94.2241	101.1795
101.6181	109.8316	125.0351
129.9490	139.2916	142.3896
153.9334	168.1249	190.3253
198.8189	202.9991	211.0643
224.9346	231.5050	238.0671
251.1303	256.5947	257.6718
260.8098	270.1337	282.4831
292.1154	300.9317	305.0366
309.1636	330.9683	333.7677
349.1422	356.0770	362.6058
366.4317	373.3049	380.7064
394.5702	402.7043	416.4721
417.8449	420.0360	424.9024
427.9543	447.7976	458.7310
466.7337	476.0828	487.6022
493.1712	510.1364	511.7052
529.4337	535.6698	541.2581
559.4310	570.2412	579.4525
600.0020	600.5392	604.7496
611.4855	630.1781	632.3630
640.4250	641.8839	652.3417
665.5279	693.6473	707.1489
716.2183	720.6154	721.7641
729.3274	734.4617	753.3151
763.4323	769.2628	774.0558
779.5793	783.2328	789.5657
793.8534	800.7081	809.0922
818.6431	830.7441	841.8546
847.1579	860.1939	865.9043
874.3618	877.2146	877.7616
884.2275	894.5229	898.0345
912.2503	923.7053	931.8815
948.2597	956.6090	957.3361
959.2142	965.0829	968.1298
975.8911	986.2167	990.0654
993.2354	996.5713	1001.1577
1005.3350	1012.7296	1014.6904

1017.1050	1017.8518	1020.7529
1023.6616	1024.1081	1027.6139
1035.5347	1052.1101	1055.4557
1059.8292	1063.5777	1065.2230
1068.6720	1071.8370	1084.6157
1100.1970	1109.6929	1114.7204
1120.8475	1123.5551	1125.0115
1131.1491	1136.1581	1144.7437
1154.0357	1164.5055	1176.3924
1177.4538	1184.9635	1188.2008
1197.7962	1198.1676	1203.4869
1203.8427	1207.2885	1210.0562
1218.9198	1224.5254	1225.9529
1228.1858	1242.0842	1243.7056
1247.3222	1256.1154	1261.5527
1276.3190	1276.7488	1276.8401
1298.8673	1308.9960	1312.4145
1318.8173	1327.9890	1329.8970
1332.7751	1339.7123	1342.8754
1351.0954	1358.2282	1359.5880
1360.8765	1364.7714	1370.0301
1372.6993	1375.1426	1381.9503
1396.8798	1399.9434	1406.2762
1426.3498	1429.6933	1439.0762
1461.5424	1461.9213	1473.1078
1474.4450	1477.2628	1485.6776
1486.2473	1496.5756	1497.5567
1499.4935	1502.6485	1504.7444
1507.0652	1509.7176	1511.5508
1514.2636	1517.3785	1527.6703
1530.8195	1533.8097	1535.9376
1540.9287	1543.1466	1550.7063
1564.4992	1578.7650	1651.7803
1677.5049	1680.3844	1680.6142
1682.9452	1689.9806	1692.6185
1697.1648	1699.5886	1700.1696
1701.9433	1825.1454	2793.4040
3049.9567	3059.6471	3061.5668
3062.5981	3066.7309	3070.2962
3082.1903	3098.7420	3124.3102
3129.0156	3141.0339	3141.1107
3148.7743	3150.8547	3158.6219
3162.2485	3164.1886	3167.3889
3178.4057	3183.4350	3187.4728

3189.3789	3195.2093	3196.0378
3196.3225	3200.7550	3200.8885
3207.0070	3209.9081	3212.9863
3214.0617	3215.6230	3217.1126
3220.9614	3223.1583	3227.7989
3228.5058	3229.1351	3232.4561
3241.1870	3243.8249	3263.2627

TS9R

Zero-point correction=0.793536

Thermal correction to Energy=0.840668

Thermal correction to Enthalpy=0.841612

Thermal correction to Gibbs Free Energy=0.710202

Sum of electronic and zero-point Energies=-2756.193519

Sum of electronic and thermal Energies=-2756.146387

Sum of electronic and thermal Enthalpies=-2756.145443

Sum of electronic and thermal Free Energies=-2756.276853

Cartesian coordinate

N	5.94355300	-1.23866500	-0.47202200
C	5.81128000	-0.20291100	0.37379200
C	4.56955400	0.37339500	0.64699600
C	3.41916100	-0.10888900	0.02257800
C	3.57149700	-1.17238100	-0.86546200
C	4.84714500	-1.69711600	-1.06584600
C	2.08304700	0.55544200	0.31556400
C	0.90321700	-0.30359400	-0.14829700
C	-0.41353600	0.17836500	0.45972100
O	-0.48994300	1.24953200	1.06541700
C	7.05838700	0.28561900	1.02190200
C	7.16874700	1.59222600	1.50869800
C	8.34306500	2.02259700	2.11828000
C	9.42348200	1.15409600	2.24827000
C	9.32541500	-0.14591900	1.75635000
C	8.15403600	-0.57580100	1.14433600
H	4.48550500	1.18739900	1.36086800
H	2.72707100	-1.60983600	-1.38901700
H	4.98572400	-2.53583700	-1.74550800
H	2.00111500	0.68544700	1.40082100
H	6.34599700	2.29018300	1.38827200
H	8.41647700	3.04164000	2.48443800
H	10.33907000	1.49044500	2.72437300
H	10.16463300	-0.82788300	1.85033000

H	8.06739800	-1.58274600	0.75160800
C	2.04348800	1.94107600	-0.32112300
C	1.78912800	3.08004600	0.44371600
C	2.25128800	2.08497900	-1.69532300
C	1.73923500	4.33748100	-0.15235500
H	1.59438000	2.96965900	1.50592700
C	2.19770700	3.33951600	-2.29601700
H	2.47472400	1.20714500	-2.29866800
C	1.94499700	4.47124800	-1.52355800
H	1.53049200	5.21296900	0.45440900
H	2.36537600	3.43497700	-3.36429400
H	1.90899200	5.45227000	-1.98767200
H	0.82260500	-0.23617200	-1.24123800
C	-4.12038800	3.68562200	-0.51450800
C	-2.96386800	2.91821300	-0.39415800
C	-1.76073800	3.32874100	-0.96528000
C	-1.74133800	4.52406100	-1.67942700
C	-2.89966500	5.29379200	-1.80985200
C	-4.09413600	4.88361300	-1.22412900
C	-5.28048300	3.05983400	0.21526200
C	-4.78199700	1.66978000	0.67459300
C	-3.22736700	1.67288600	0.42355800
H	-0.85300300	2.74320000	-0.84165900
H	-0.81130800	4.85910000	-2.12737500
H	-2.86691000	6.22319000	-2.36973100
H	-4.99239600	5.48676900	-1.31974700
H	-6.17330200	2.95022800	-0.40960000
H	-4.95401400	1.47790100	1.73217800
H	-5.57036800	3.66423200	1.08049800
H	-2.68612500	1.64930900	1.36626200
N	-2.82053000	0.45924400	-0.31045400
O	-5.48117500	0.61669400	0.02170300
C	-1.66642100	-0.21849600	-0.32554900
C	-3.66372600	-0.16612600	-1.18421700
N	-1.85147700	-1.21550700	-1.19549600
N	-3.10209700	-1.20250200	-1.73483800
C	-5.05272500	0.36276600	-1.29760000
H	-5.07141100	1.26992500	-1.91896200
H	-5.70971800	-0.38818600	-1.73732600
C	-0.95596300	-2.29364400	-1.51270500
C	-0.24728700	-2.24846700	-2.70794100
C	-0.82452200	-3.34417400	-0.61302100
C	0.65588000	-3.26421100	-2.99628400
C	0.08369700	-4.35824000	-0.90084700

C	0.81968200	-4.30113400	-2.07986400
H	1.23095700	-3.25335400	-3.91468400
H	0.22044800	-5.18550000	-0.21441900
H	-1.42326600	-3.35782900	0.29113600
H	-0.39184000	-1.42095000	-3.39492700
Cl	1.97266900	-5.55808900	-2.42671200
H	1.05621400	-1.35429900	0.10506600
C	-0.52103900	-0.76483500	3.02727700
H	-0.55841800	0.33315400	3.03258900
H	-1.33578100	-1.13238000	3.65911700
H	0.44080000	-1.09454600	3.43459400
O	-0.67606900	-1.24590800	1.71046600
H	-1.74585500	-1.65581700	1.61060700
C	-5.15496400	-2.21975200	2.15287100
C	-5.57943800	-2.72454700	0.76890900
H	-6.48971300	-3.32820600	0.85192400
H	-5.79215100	-1.88004000	0.10637900
H	-4.79042000	-3.33254100	0.32024100
C	-6.22016500	-1.29344000	2.73290800
H	-7.15751300	-1.84271700	2.87229600
H	-5.90045100	-0.89287800	3.69795900
H	-6.40731100	-0.45474100	2.05682900
C	-4.92960600	-3.41965100	3.08632600
H	-4.16737000	-4.08660000	2.67666500
H	-4.60297900	-3.08756900	4.07733900
H	-5.86235200	-3.98098500	3.20594000
C	-3.81187500	-1.48558600	2.03520100
O	-2.87448300	-2.17765600	1.46139000
O	-3.64543500	-0.35227400	2.49070500

Variable frequencies

-322.3484	11.6996	19.7171
23.9655	27.8598	32.8655
34.1349	41.3929	46.2208
47.0558	57.1375	58.7248
63.8599	64.2897	75.0495
77.5113	83.3725	85.8310
90.8210	93.2955	101.6519
106.9463	112.2244	122.6291
130.5492	132.6560	149.3883
154.9705	157.5939	182.3369
196.0591	198.2310	201.1780
222.6301	227.0308	236.8114
248.3926	249.6296	256.1294

260.3984	264.7598	267.6192
282.9326	287.6493	303.4485
305.4485	308.7445	331.7347
336.0107	345.3267	354.8743
357.9793	365.4568	371.8487
380.8869	405.7705	413.4025
418.8133	419.2820	424.3438
429.0254	444.2233	455.1956
462.7716	475.3519	479.8176
487.1107	491.2108	505.2058
510.5200	528.6692	536.6563
559.4121	571.3499	580.9613
586.5630	602.7385	606.9574
613.3864	629.6638	632.9371
638.2085	645.5528	651.5317
659.6008	681.4328	704.9586
716.1487	719.4254	722.5723
726.7869	732.1648	740.6847
748.4339	764.3685	766.0061
774.7937	788.5891	792.6593
801.4826	803.6612	809.0682
817.1491	824.2176	831.7296
849.6549	853.7990	867.7498
871.1523	876.5627	876.7607
878.5158	888.2372	896.4350
909.8832	913.8747	923.2333
933.5357	952.8148	953.8399
957.4372	959.3324	961.6702
963.5662	983.7839	985.0253
999.0813	1000.3322	1004.6620
1005.0444	1007.7641	1012.7788
1014.9187	1017.0004	1018.7773
1020.7938	1023.2319	1025.0563
1033.6098	1039.8029	1050.6212
1052.8269	1060.2289	1068.0264
1068.9743	1069.4119	1071.7164
1091.9553	1107.9482	1116.5837
1121.4256	1124.0432	1125.6359
1127.6621	1135.7840	1142.4500
1153.1073	1162.3146	1169.7192
1177.5904	1179.3086	1183.3783
1191.5435	1196.4748	1199.8040
1204.2238	1206.2091	1206.4843
1207.2535	1217.8784	1219.4755

1228.4991	1244.3624	1247.7312
1255.3110	1263.4446	1270.9871
1279.2030	1280.9751	1282.9732
1306.2789	1307.5709	1313.0095
1324.6712	1325.7803	1329.2417
1335.1267	1341.4329	1342.2599
1345.2288	1356.7926	1362.3671
1367.3512	1368.5664	1371.8955
1373.5345	1385.2293	1386.0951
1391.0671	1396.2603	1413.2891
1419.7494	1432.1743	1461.9678
1463.4912	1466.8227	1473.9339
1480.8940	1483.2915	1485.6421
1486.2901	1494.8057	1499.7654
1502.4682	1504.0105	1505.1950
1507.6800	1509.9446	1512.5793
1518.2961	1520.6728	1536.2952
1538.6651	1539.3131	1542.4928
1550.4566	1551.2795	1563.1442
1589.6694	1654.9081	1677.6954
1677.7418	1680.3380	1681.9701
1683.9745	1690.1573	1693.2652
1697.0768	1698.8530	1700.4770
1702.4341	1707.8867	1793.8159
3038.3396	3055.4328	3055.5049
3060.5028	3064.7917	3074.2651
3084.5267	3100.5477	3107.7549
3129.2096	3131.7400	3134.9861
3140.8148	3143.2180	3156.9873
3159.6374	3163.9701	3164.8108
3177.5597	3179.2335	3187.4025
3189.6013	3197.5043	3197.5232
3197.9868	3203.1727	3203.7047
3204.9998	3210.7488	3211.8097
3213.7808	3215.9020	3216.3623
3218.0401	3219.1308	3224.2886
3226.4262	3227.2708	3235.2864
3239.1686	3246.9761	3263.5385

M9R

Zero-point correction=0.648622

Thermal correction to Energy=0.686082

Thermal correction to Enthalpy=0.687026

Thermal correction to Gibbs Free Energy=0.577283
 Sum of electronic and zero-point Energies=-2409.433637
 Sum of electronic and thermal Energies=-2409.396176
 Sum of electronic and thermal Enthalpies=-2409.395232
 Sum of electronic and thermal Free Energies=-2409.504975

Cartesian coordinate

N	-3.80722000	-3.42720900	-1.13615300
C	-3.88807400	-2.25018900	-0.49452200
C	-2.76472900	-1.45397200	-0.27289900
C	-1.51433500	-1.85423800	-0.73930700
C	-1.43751500	-3.08125600	-1.39390100
C	-2.60776500	-3.82021000	-1.55785900
C	-0.32906600	-0.93954700	-0.49104800
C	0.79072100	-1.03297700	-1.54210200
C	1.22849800	0.38020200	-1.99716100
O	0.33426400	1.11028200	-2.56209700
C	-5.24368800	-1.80648700	-0.06775900
C	-5.41961500	-0.81917300	0.90947300
C	-6.69607000	-0.39806700	1.26912000
C	-7.81638100	-0.95815600	0.66037700
C	-7.65064700	-1.94910000	-0.30501200
C	-6.37574500	-2.37147500	-0.66451200
H	-2.85448600	-0.49543800	0.22697900
H	-0.49803500	-3.45654000	-1.78708000
H	-2.57368300	-4.78080800	-2.06808700
H	-0.72793200	0.07707200	-0.56734600
H	-4.55932500	-0.38881800	1.41312400
H	-6.81554300	0.36247900	2.03470500
H	-8.81180400	-0.62896200	0.94085500
H	-8.51866100	-2.39338200	-0.78192200
H	-6.23357800	-3.14143900	-1.41437700
C	0.14764400	-1.11959900	0.94396300
C	0.13167800	-0.04342000	1.83530300
C	0.56579800	-2.36940200	1.41305700
C	0.53188100	-0.20652900	3.16185100
H	-0.21843700	0.92744000	1.48621500
C	0.95394400	-2.53984500	2.73783100
H	0.57188100	-3.21888500	0.73420900
C	0.94087900	-1.45731000	3.61805800
H	0.51008200	0.64076200	3.84046100
H	1.26592300	-3.51962500	3.08637900
H	1.24145100	-1.59053000	4.65232900
H	1.64284500	-1.62387700	-1.18597200

C	-1.54406500	3.52285800	0.67783300
C	-1.09308100	2.85376900	-0.46684600
C	-1.97106700	2.05030900	-1.19585100
C	-3.27512600	1.88611500	-0.72778500
C	-3.70378800	2.51194300	0.44342300
C	-2.83995000	3.34568800	1.14962600
C	-0.48859700	4.44744700	1.21533900
C	0.40941200	4.63464900	-0.02411600
C	0.32281100	3.29476500	-0.81722000
H	-1.61298100	1.55103100	-2.08873300
H	-3.96554400	1.25623300	-1.28166400
H	-4.72267400	2.36453400	0.78991300
H	-3.17710000	3.87007100	2.03897300
H	0.04717600	3.97473500	2.04683600
H	-0.04003700	5.39635000	-0.66567800
H	-0.88288600	5.39886600	1.57919900
H	0.47343200	3.39450100	-1.89022500
N	1.44299100	2.41773700	-0.33471600
O	1.71956100	5.08531000	0.23562300
C	1.82615900	1.18220200	-0.73553700
C	2.36861200	2.83728500	0.59350200
N	2.90875600	0.90421400	-0.00498900
N	3.25982200	1.92218600	0.82796700
C	2.42192300	4.24072500	1.11378000
H	2.04260400	4.30009200	2.14062500
H	3.46378100	4.56466600	1.11844100
C	3.67416300	-0.31100100	0.06721400
C	3.57488400	-1.05074300	1.23824000
C	4.52505400	-0.68459500	-0.96626600
C	4.32167800	-2.21461300	1.37366600
C	5.27220100	-1.84869300	-0.83195600
C	5.15954700	-2.60098000	0.33357400
H	4.24958200	-2.81547800	2.27289900
H	5.93872500	-2.17026200	-1.62346600
H	4.58010700	-0.08774600	-1.86605400
H	2.90889700	-0.72033100	2.02885900
Cl	6.09656400	-4.06321700	0.49499900
H	0.42041700	-1.49089100	-2.46387000
O	2.42777000	0.13201100	-2.78270000
C	2.81470900	1.25181000	-3.54741800
H	3.16769200	2.08080000	-2.90867600
H	3.64168400	0.93260600	-4.18603500
H	1.98428500	1.61699300	-4.15508400

Variable frequencies

13.6914	19.1538	23.7358
28.6156	34.3646	38.8497
52.9591	57.7841	61.4918
78.5814	83.6841	90.0037
91.2306	99.2881	114.1658
117.2952	121.1694	129.6734
155.7828	158.4708	177.6947
180.5420	196.2515	203.7985
216.5389	223.6121	239.8056
241.4007	252.4344	259.4330
261.7540	286.0344	294.1639
300.7909	311.1371	326.5549
349.1038	364.6743	370.8042
377.6764	391.8144	412.4482
415.3293	418.2328	421.0360
431.3995	453.0828	457.6861
469.4440	473.9846	495.5225
497.7148	507.3831	512.3682
542.1517	553.5003	570.6681
579.3301	592.9649	600.0493
608.5520	622.7275	629.8630
631.6285	638.6404	650.7344
652.1700	661.8352	668.1026
689.1112	715.0388	719.2900
721.7230	725.4564	731.7338
754.8428	763.4373	768.0790
778.2951	795.5496	797.0008
805.4991	811.1765	816.6817
836.6336	848.9325	850.3823
865.5037	877.4002	881.4038
884.5410	886.1539	887.6642
902.2157	922.4975	929.7562
935.7605	944.6434	962.0444
975.0956	985.6883	996.5709
997.2704	997.7905	1007.8669
1012.4199	1014.6529	1015.2031
1017.2479	1018.8544	1019.5553
1025.1378	1031.9737	1040.8091
1045.3627	1052.7141	1061.4500
1067.2943	1070.1966	1071.7639
1074.4816	1090.8469	1096.3640
1110.9471	1118.6823	1121.1082
1127.0566	1131.2543	1133.9301

1136.4989	1146.5911	1155.9783
1160.5644	1173.2318	1178.3120
1179.9297	1186.0478	1187.2242
1196.7888	1204.1208	1205.4304
1208.3377	1212.4356	1217.6963
1224.7931	1233.5987	1239.6782
1243.8196	1261.2241	1276.4064
1278.6920	1295.4780	1310.2429
1313.0087	1315.6555	1321.8209
1323.6303	1326.1053	1339.9790
1340.5295	1352.1195	1352.3971
1354.7399	1359.9558	1367.8684
1373.0348	1375.3992	1382.0399
1389.4056	1419.1481	1424.9245
1443.8350	1457.9063	1463.5930
1472.6686	1480.2257	1492.6309
1498.6577	1501.9339	1502.8890
1505.0900	1514.0393	1520.6732
1526.4640	1527.6915	1532.1882
1538.6435	1548.1829	1563.3800
1568.0869	1656.0594	1672.1312
1672.7771	1675.3837	1677.1300
1683.4124	1690.8752	1692.4451
1698.4189	1698.8068	1701.9794
2992.1213	3078.2153	3078.3862
3093.4794	3111.2735	3116.1110
3139.0827	3141.5275	3154.7087
3169.9373	3172.3571	3182.3470
3183.1367	3192.5380	3195.1151
3201.0900	3201.5416	3202.7267
3206.0068	3206.4112	3212.5357
3215.7381	3216.6445	3221.9036
3230.2038	3231.8045	3233.4116
3235.3216	3236.0779	3242.9713
3254.9428	3255.7051	3280.9690

TS10R

Zero-point correction=0.647233

Thermal correction to Energy=0.684586

Thermal correction to Enthalpy=0.685530

Thermal correction to Gibbs Free Energy=0.575293

Sum of electronic and zero-point Energies=-2409.432773

Sum of electronic and thermal Energies=-2409.395420

Sum of electronic and thermal Enthalpies=-2409.394476

Sum of electronic and thermal Free Energies=-2409.504714

Cartesian coordinate

N	-4.10171900	-3.15067800	-1.31990400
C	-4.08918300	-2.00270500	-0.62205100
C	-2.91012200	-1.29386500	-0.39747400
C	-1.69856200	-1.75536400	-0.90918800
C	-1.71910000	-2.95359800	-1.61794800
C	-2.94169000	-3.60215100	-1.78893700
C	-0.44995700	-0.94005600	-0.62009200
C	0.69152300	-1.10752000	-1.63490400
C	1.21299700	0.25227800	-2.11233800
O	0.43634100	1.07885000	-2.64298500
C	-5.40059700	-1.50222600	-0.12459000
C	-5.48356900	-0.52988800	0.87963500
C	-6.72039300	-0.06253600	1.31255700
C	-7.89365900	-0.56037900	0.75130700
C	-7.82074200	-1.53510500	-0.24140200
C	-6.58548000	-2.00390100	-0.67407000
H	-2.91800400	-0.36275500	0.15850400
H	-0.81633000	-3.38181700	-2.04115900
H	-2.98371700	-4.53833400	-2.34200900
H	-0.76072700	0.10665100	-0.68240800
H	-4.58143700	-0.14710600	1.34746200
H	-6.76785400	0.68541700	2.09819700
H	-8.85794400	-0.19547100	1.09029400
H	-8.73065400	-1.93142800	-0.68101800
H	-6.51470600	-2.76425100	-1.44376500
C	-0.04527200	-1.18962700	0.82643900
C	-0.07115400	-0.14875200	1.75795100
C	0.29271200	-2.47382800	1.26386600
C	0.24205400	-0.38294800	3.09709800
H	-0.35198100	0.85078500	1.42811300
C	0.59842700	-2.71316200	2.59964600
H	0.30163100	-3.29491700	0.55048200
C	0.57646200	-1.66678100	3.52206200
H	0.21348500	0.43637900	3.80897400
H	0.85021200	-3.71857400	2.92338100
H	0.81050300	-1.85382200	4.56523000
H	1.51344500	-1.71386800	-1.24060800
C	-1.06265700	3.66751000	0.81997000
C	-0.75023500	2.99225300	-0.36687600
C	-1.72599700	2.26229200	-1.04149000

C	-2.99940500	2.16895600	-0.47591400
C	-3.29091300	2.79023400	0.73857200
C	-2.32513800	3.55633600	1.39035600
C	0.09295100	4.52181600	1.26673400
C	0.87102800	4.68050000	-0.05857200
C	0.66461100	3.33134800	-0.80197300
H	-1.47534900	1.76936500	-1.97432200
H	-3.77447300	1.60629200	-0.98863200
H	-4.28716000	2.69980100	1.16178800
H	-2.56278200	4.08055600	2.31118300
H	0.68702800	4.00077600	2.02758700
H	0.37973000	5.44931200	-0.65984800
H	-0.20915300	5.48461600	1.68498400
H	0.77684100	3.38797000	-1.88479000
N	1.72064800	2.39988900	-0.31149100
O	2.21488400	5.08805200	0.05067700
C	1.89355800	1.08022300	-0.58598100
C	2.78195800	2.81433200	0.46358300
N	3.02003500	0.77625200	0.06563100
N	3.58968700	1.83233500	0.72344100
C	2.98979300	4.24157800	0.86591800
H	2.76281900	4.38001100	1.93056000
H	4.03706600	4.50424300	0.70688700
C	3.63649800	-0.51362600	0.17812100
C	3.35095000	-1.27527700	1.30270900
C	4.51873000	-0.95891100	-0.79987200
C	3.94532700	-2.52347500	1.45165900
C	5.11604300	-2.20533800	-0.65390800
C	4.81981000	-2.97313800	0.46941600
H	3.72378200	-3.13972200	2.31541200
H	5.80339400	-2.58174000	-1.40215000
H	4.71766200	-0.34384200	-1.66853100
H	2.65641000	-0.89776400	2.04638300
Cl	5.56526400	-4.53959100	0.64581100
H	0.33125600	-1.58692900	-2.55124700
O	2.45586700	0.00479700	-2.73866600
C	2.96140700	1.11528700	-3.45107400
H	3.24812100	1.92909300	-2.76589700
H	3.85109100	0.77045700	-3.98124400
H	2.22290400	1.50076900	-4.15618500

Variable frequencies

-191.3862	11.4119	17.0524
24.5757	28.9725	31.5284

34.0747	49.5630	55.5564
58.8507	81.2026	83.1801
87.9317	91.9021	103.8170
108.7863	117.4206	119.7115
127.2021	152.3586	158.6899
165.8961	171.4648	191.2733
196.3373	216.7583	223.7920
231.2208	240.5551	254.1589
257.0125	260.1472	288.7475
296.2191	299.6095	315.3333
333.8183	349.4347	360.0919
362.0722	386.6104	407.1470
415.0649	417.8080	422.5481
430.7842	440.3897	453.2896
458.2858	463.0301	490.8535
499.3496	502.6388	503.1689
542.0085	544.9648	565.2113
572.8522	588.4648	597.7311
607.7710	609.1718	627.8875
628.6384	634.3649	643.2067
651.4166	652.7407	673.9541
695.4120	708.4857	717.1416
721.7667	727.6286	732.7735
736.6729	762.8082	764.5726
773.0270	794.6988	798.6630
806.9456	808.4476	818.3288
824.6877	847.8301	857.2218
867.4253	871.8653	878.5400
879.0902	884.3199	888.1059
900.0779	919.7586	926.5651
936.5032	947.8039	960.7599
981.2817	983.8374	994.0008
996.2350	1005.4018	1007.2347
1007.3143	1010.8112	1012.9112
1016.7015	1017.1805	1020.4094
1025.2231	1029.8461	1037.0931
1044.4514	1049.6347	1058.1557
1061.7481	1069.4717	1071.2332
1075.7937	1089.4281	1095.8817
1110.9282	1120.1530	1124.2612
1124.9650	1129.3702	1135.1816
1138.4472	1147.2565	1155.1813
1160.3831	1177.7163	1178.6307
1179.8367	1188.4220	1189.3029

1200.1731	1202.1243	1203.8257
1207.9120	1211.2731	1219.3238
1223.0357	1232.0820	1240.8299
1240.8667	1261.7694	1274.9165
1281.4639	1296.1056	1307.6740
1318.6545	1318.8634	1320.5995
1322.9584	1323.2193	1336.2003
1341.1945	1342.5965	1352.7231
1353.6842	1359.1696	1365.7037
1369.3178	1375.2252	1380.5435
1392.8753	1398.3342	1424.7722
1457.2429	1461.8321	1462.6674
1469.0585	1473.0961	1491.0888
1495.9633	1501.1728	1503.1677
1504.5547	1520.1707	1520.8488
1524.9526	1532.0380	1538.3507
1547.3665	1560.8694	1569.5198
1608.1882	1656.4364	1674.2044
1674.8711	1676.5322	1679.5196
1683.5201	1690.6227	1693.7330
1696.1578	1698.6146	1699.2751
3018.1662	3067.1722	3077.7325
3080.3259	3129.4114	3131.4402
3136.0003	3137.1742	3147.6832
3160.5626	3178.2156	3178.9358
3180.9038	3183.5090	3184.6409
3197.8496	3202.0649	3203.5573
3210.4135	3210.7499	3211.4490
3214.3012	3222.4169	3224.4215
3228.7912	3231.3868	3233.5812
3236.9975	3242.8278	3243.3113
3247.8674	3253.2926	3261.2771

PR

Zero-point correction=0.354422

Thermal correction to Energy=0.374798

Thermal correction to Enthalpy=0.375742

Thermal correction to Gibbs Free Energy=0.302189

Sum of electronic and zero-point Energies=-1016.144558

Sum of electronic and thermal Energies=-1016.124181

Sum of electronic and thermal Enthalpies=-1016.123237

Sum of electronic and thermal Free Energies=-1016.196790

Cartesian coordinate

C	-6.11810800	0.85745900	-1.05082700
C	-6.03500100	0.20368200	0.17703000
H	-6.90994200	0.13463400	0.81573600
C	-4.83350700	-0.35999700	0.58983900
H	-4.75722200	-0.87620900	1.54044200
C	-3.69315900	-0.27048000	-0.21576000
C	-3.78794600	0.37860500	-1.45121900
H	-2.92553900	0.42546300	-2.10884900
C	-4.99187600	0.93918100	-1.86523500
H	-5.05207900	1.43306600	-2.82982600
C	-1.18008400	-0.41484100	-0.21597600
H	-1.12615000	0.42222600	-0.90561700
C	-2.41403300	-0.86883800	0.25211800
N	-2.51009000	-1.85547100	1.15981000
C	-1.38367600	-2.41205500	1.59119500
H	-1.49454700	-3.20559000	2.32728000
C	-0.11135900	-2.04193100	1.15640700
H	0.75969600	-2.55201000	1.55302100
C	0.00098600	-1.01064000	0.22726300
C	1.32547900	-0.48321400	-0.29298800
H	1.24832800	-0.41520100	-1.38396700
C	1.60022300	0.92044500	0.23205400
C	1.45371100	1.21257700	1.59115700
H	1.09720400	0.44129500	2.27018500
C	1.74351700	2.48312300	2.07662200
H	1.62159000	2.69701700	3.13379000
C	2.18104900	3.48074200	1.20711800
C	2.32797900	3.19822300	-0.14747600
H	2.66743900	3.96996500	-0.83116800
C	2.03947500	1.92428800	-0.63230600
H	2.16942600	1.69631400	-1.68612000
C	2.50798600	-1.40930300	0.00968400
H	2.77565500	-1.39728000	1.06988100
H	2.26293500	-2.44560200	-0.25538700
C	3.72257100	-1.02701700	-0.80649600
O	3.69058100	-0.48189600	-1.88448400
O	4.85733500	-1.40151400	-0.20391900
C	6.05352000	-1.11578200	-0.93439100
H	6.87266500	-1.48031300	-0.31796700
H	6.14545700	-0.04094500	-1.10123400
H	6.04017700	-1.62560800	-1.89967500
H	2.40284300	4.47360100	1.58528000
H	-7.05712600	1.29539800	-1.37412100

Variable frequencies

15.5957	29.9060	36.1370
40.6252	47.2455	71.8086
90.6335	96.3491	127.1269
134.5903	168.2822	193.0600
209.4267	214.5331	234.6035
257.0898	293.7935	306.5888
344.7018	366.0513	409.9909
417.6476	417.8264	463.0899
485.2923	506.4923	550.7223
581.0713	606.4825	628.3496
630.2592	636.2747	651.5229
678.4304	715.0980	723.0516
732.0292	764.0801	776.9639
792.2496	799.8097	809.3233
871.8563	878.0260	879.8672
910.0981	928.1724	948.6147
957.3871	958.9376	994.8188
1002.7974	1003.6876	1008.8230
1017.3154	1019.5972	1022.9152
1024.1346	1024.6972	1059.0747
1071.7538	1072.6770	1096.6661
1112.0007	1121.3618	1123.3002
1159.2450	1179.4079	1181.5215
1191.0119	1198.0278	1209.4653
1210.0073	1220.1604	1226.5718
1230.9549	1256.9303	1298.1732
1310.2827	1323.7094	1332.7164
1342.3443	1357.5417	1362.6343
1366.9971	1375.4850	1415.9199
1460.2377	1476.7226	1493.3807
1501.1887	1503.6023	1507.5245
1513.4646	1538.9309	1552.3307
1562.1539	1655.2758	1677.1377
1680.8404	1693.6812	1699.6581
1701.7457	1865.1177	3083.1688
3091.8931	3101.3743	3150.9699
3177.7882	3191.1583	3192.8467
3201.0237	3201.5457	3206.2386
3207.5688	3209.3604	3212.4992
3216.8881	3221.2255	3223.9775
3225.3514	3227.5743	3235.7992

²M10

Zero-point correction=0.170944

Thermal correction to Energy=0.179871

Thermal correction to Enthalpy=0.180815

Thermal correction to Gibbs Free Energy=0.135747

Sum of electronic and zero-point Energies=-478.711731

Sum of electronic and thermal Energies=-478.702804

Sum of electronic and thermal Enthalpies=-478.701860

Sum of electronic and thermal Free Energies=-478.746928

Cartesian coordinate

N	1.33084700	-1.18499900	-0.03289600
C	2.64042500	-1.24614000	-0.04141200
H	3.08446600	-2.23735100	-0.07382700
C	0.73963700	0.04030800	0.00311000
C	1.50335100	1.23755800	0.04638700
H	1.02384300	2.20676100	0.09351900
C	3.47504900	-0.09922000	-0.00952000
H	4.55247400	-0.21856500	-0.01909400
C	2.88747000	1.15722600	0.03881900
H	3.49236100	2.05568500	0.07021200
C	-0.70052100	0.04365500	-0.00204100
C	-1.39278500	-1.21080800	0.03163400
C	-1.46305200	1.25295600	-0.04160400
C	-2.76517500	-1.24630200	0.03839900
H	-0.80175200	-2.11727200	0.05583100
C	-2.83364600	1.20371700	-0.03845300
H	-0.97028000	2.21584200	-0.08646000
C	-3.49331700	-0.04332600	0.00479800
H	-3.28929600	-2.19406500	0.07008000
H	-3.41446600	2.11775800	-0.07057700
H	-4.57789700	-0.07154100	0.00987500

Variable frequencies

74.8748	84.7847	186.1204
202.9146	345.9436	370.1257
394.4149	402.3005	435.8228
495.5770	578.0326	611.3906
632.8098	642.4905	714.1991
765.9140	785.2886	831.3314
847.4378	907.1306	989.4771
992.7321	1004.2330	1014.8112
1018.3008	1033.3775	1038.9545

1047.5826	1051.1891	1071.8815
1133.8607	1143.9972	1185.1404
1191.1727	1232.9714	1302.4797
1345.1629	1363.3582	1410.1628
1412.8309	1466.3690	1475.3082
1504.0606	1530.4116	1574.4993
1589.7997	1633.2043	1701.8784
3222.5062	3232.8279	3243.2822
3245.6144	3250.0861	3257.2992
3264.1540	3271.0297	3280.8523

²M14R

Zero-point correction=0.605709

Thermal correction to Energy=0.640822

Thermal correction to Enthalpy=0.641766

Thermal correction to Gibbs Free Energy=0.537001

Sum of electronic and zero-point Energies=-2293.926787

Sum of electronic and thermal Energies=-2293.891674

Sum of electronic and thermal Enthalpies=-2293.890730

Sum of electronic and thermal Free Energies=-2293.995495

Cartesian coordinate

N	4.53412400	-1.34411600	-0.01700700
C	4.52964700	0.00823300	0.11161800
C	3.35154900	0.72989100	0.42235700
C	2.15124300	0.04798900	0.60609800
C	2.18377600	-1.33681300	0.47318600
C	3.40167200	-1.98350800	0.16102900
C	0.86176800	0.78219000	0.97420300
C	-0.33472000	0.04602600	0.42690100
C	-1.46034400	-0.20010800	1.10234500
O	-1.79640200	0.15176100	2.36631100
C	5.79966500	0.66426900	-0.09453000
C	5.94877800	2.08534000	-0.00630900
C	7.17283900	2.66310000	-0.21519600
C	8.29311400	1.85309400	-0.51674900
C	8.17089500	0.45240700	-0.60780800
C	6.95004100	-0.13742000	-0.40166700
H	3.36180200	1.80890100	0.51514800
H	1.28528400	-1.93277000	0.60934000
H	3.42644400	-3.06585700	0.05656400
H	0.82182500	0.76445300	2.07319700
H	5.10022000	2.71712600	0.22303500

H	7.29105500	3.73825400	-0.15037700
H	9.25919700	2.31982100	-0.67829200
H	9.04044200	-0.15056300	-0.84074400
H	6.82092300	-1.21048900	-0.46498800
C	0.88079400	2.24116200	0.53834400
C	0.93305000	3.25584200	1.49327000
C	0.89825600	2.57569400	-0.81985500
C	1.01467800	4.59220300	1.10055600
H	0.92871300	3.00401700	2.55116600
C	0.98118600	3.90712900	-1.21205700
H	0.85529500	1.79409100	-1.57467300
C	1.04606600	4.91817300	-0.25239500
H	1.06053000	5.37328500	1.85205000
H	0.99496100	4.15780200	-2.26751700
H	1.11444700	5.95602200	-0.56049500
H	-0.28910400	-0.29302200	-0.60451200
C	-4.65533000	2.20489600	-0.95997100
C	-3.90649200	1.86847400	0.17229400
C	-2.81376200	2.63513200	0.56399000
C	-2.45030600	3.72853500	-0.21732600
C	-3.18034800	4.05122500	-1.36238600
C	-4.29355900	3.29998500	-1.73590900
C	-5.82836800	1.27491900	-1.13639300
C	-5.95034700	0.64300500	0.26733500
C	-4.50987700	0.66124500	0.84660900
H	-2.26540300	2.40551800	1.47086600
H	-1.60265200	4.33811900	0.07709200
H	-2.89105200	4.91184000	-1.95663400
H	-4.87661600	3.57479000	-2.60900700
H	-5.61388700	0.52607800	-1.90805700
H	-6.54813500	1.30022700	0.90168000
H	-6.74788300	1.78566500	-1.42858800
H	-4.47759900	0.66910800	1.93704400
N	-3.85330400	-0.61188600	0.40993700
O	-6.56783000	-0.62030000	0.35413400
C	-2.55933900	-0.95992500	0.48268800
C	-4.50147600	-1.64996200	-0.20834700
N	-2.46699900	-2.16371800	-0.08051300
N	-3.66890300	-2.60457800	-0.52415100
C	-5.98297300	-1.62215400	-0.43932000
H	-6.18798400	-1.48657700	-1.50814200
H	-6.41044400	-2.57727900	-0.12918300
C	-1.30772600	-3.01271400	-0.15854000
C	-0.71598700	-3.23370500	-1.39595900

C	-0.83543300	-3.60686600	1.00673700
C	0.39719000	-4.06399400	-1.46883700
C	0.27620300	-4.43898600	0.93221800
C	0.88289300	-4.65637600	-0.30441500
H	0.87935000	-4.25878200	-2.41970100
H	0.66287100	-4.92478700	1.82058300
H	-1.33414700	-3.43462800	1.95516600
H	-1.12304800	-2.77121200	-2.28903800
Cl	2.27459300	-5.68754900	-0.39406400
H	-1.13754400	0.74181500	2.75782800

Variable frequencies

19.6561	27.7637	30.8873
38.5445	45.5829	46.7722
57.7123	58.5090	61.7646
69.3343	79.3464	85.4993
88.8048	94.1211	106.5580
114.9779	140.4401	148.9749
166.9152	175.8893	195.5887
212.4375	213.9220	227.7606
241.0363	244.8318	260.2781
264.4624	291.3309	306.2344
316.2101	330.1586	347.4104
370.4286	370.6884	381.5947
386.8018	399.9844	409.6224
420.6166	423.0178	430.2670
447.5884	451.8021	464.7383
471.9108	481.6987	485.8091
496.8291	515.7716	521.1078
539.5530	552.5464	572.3760
575.7908	590.0350	602.5280
608.9532	626.7803	629.9996
633.6768	637.5646	640.5982
650.0816	663.9185	679.0532
710.5622	726.5777	727.4926
729.9275	733.6923	746.6668
761.4901	779.0699	785.6134
791.7013	801.3225	813.5187
813.8510	832.5316	845.5918
852.2091	859.1774	859.7829
869.5882	875.7836	884.7750
891.1161	903.1472	907.5381
916.4081	923.2440	938.8705
967.9449	985.5844	988.8305

992.8995	994.2833	1003.9947
1006.0389	1009.7132	1012.9963
1019.0395	1023.3220	1024.7878
1030.7850	1032.6016	1037.1213
1037.7469	1038.3188	1047.3631
1053.2983	1054.1186	1070.7571
1071.2936	1074.0263	1093.2968
1109.5123	1120.5371	1126.9762
1132.1467	1135.6804	1137.8477
1138.8809	1157.3168	1171.9027
1181.5503	1182.7292	1185.1030
1189.6845	1199.1022	1209.1940
1209.9772	1213.9398	1216.1316
1225.3930	1229.6008	1239.9542
1248.4380	1270.6335	1274.2003
1283.2099	1293.3052	1306.0181
1306.3015	1317.8658	1327.2046
1330.9125	1332.9706	1342.2008
1347.3178	1353.8158	1358.4175
1361.8113	1364.5760	1370.7600
1377.6529	1387.4200	1401.1200
1413.5503	1424.1083	1430.3421
1436.2491	1455.5952	1461.0211
1461.7919	1496.7401	1498.1234
1506.3928	1509.3230	1524.1612
1526.4175	1530.7926	1544.1281
1549.4467	1551.5164	1568.9648
1610.1932	1623.7843	1627.1438
1664.3287	1675.3831	1677.1375
1681.9344	1683.5240	1694.6683
1704.4352	1705.0461	1787.5327
3056.5453	3082.8436	3095.0438
3148.6903	3160.2023	3165.6544
3176.2316	3194.8505	3208.2665
3211.0935	3216.8024	3220.7181
3226.1151	3227.0617	3228.2630
3228.3711	3231.2949	3233.4095
3241.3673	3241.4822	3243.8049
3246.8278	3250.1573	3252.2073
3253.1590	3258.6180	3265.4003
3275.3845	3276.4071	3871.1749

Nts-

Zero-point correction=0.172058
 Thermal correction to Energy=0.183676
 Thermal correction to Enthalpy=0.184620
 Thermal correction to Gibbs Free Energy=0.133965
 Sum of electronic and zero-point Energies=-913.853911
 Sum of electronic and thermal Energies=-913.842293
 Sum of electronic and thermal Enthalpies=-913.841349
 Sum of electronic and thermal Free Energies=-913.892004

Cartesian coordinate

N	-2.30282500	0.26211600	1.11146000
C	-2.16943000	1.70696300	1.17318900
H	-2.68617000	2.06230600	2.07150000
H	-1.12036800	2.05179000	1.25360000
H	-2.60796200	2.22820300	0.30830800
S	-1.76595500	-0.36442000	-0.21435700
O	-2.01337500	-1.81842100	-0.22127000
O	-2.13155200	0.36118400	-1.45679000
C	0.03750300	-0.22150000	-0.18510400
C	0.79696300	-1.19087000	0.47016700
C	0.66567200	0.89628000	-0.72345100
C	2.17392500	-1.04384900	0.57066400
H	0.29070900	-2.05998100	0.87882600
C	2.04872400	1.04129200	-0.61046600
H	0.06389100	1.63062900	-1.25034700
C	2.82106900	0.07621100	0.03399200
H	2.76419800	-1.80915900	1.07078800
H	2.53627500	1.91483900	-1.03766500
C	4.31860500	0.21659400	0.14591000
H	4.83205900	-0.59289000	-0.38324800
H	4.66050700	1.16402500	-0.27785200
H	4.64315200	0.17731700	1.19064700

Variable frequencies

54.4336	74.6777	99.7352
118.6767	168.7929	180.2149
233.5513	279.2920	292.6031
324.3473	368.6949	400.9067
419.2232	478.7044	534.8870
561.8443	588.2019	647.9904
658.7563	727.3073	821.0220
837.9103	872.1329	882.0606
982.3584	995.5481	1007.3899
1040.0839	1066.4952	1106.0523

1127.1152	1138.4385	1151.9876
1158.6786	1199.1726	1224.7269
1249.2268	1269.5838	1319.5041
1351.9571	1422.3725	1447.7311
1461.4042	1498.5839	1508.3450
1510.6429	1524.1340	1553.5424
1667.6638	1697.6148	2953.2803
3032.1147	3065.8749	3093.5159
3131.8136	3153.9314	3177.3213
3178.2946	3215.6584	3216.6092

^{os}TS11RR

Zero-point correction=0.855960

Thermal correction to Energy=0.908027

Thermal correction to Enthalpy=0.908971

Thermal correction to Gibbs Free Energy=0.765226

Sum of electronic and zero-point Energies=-3630.755273

Sum of electronic and thermal Energies=-3630.703206

Sum of electronic and thermal Enthalpies=-3630.702262

Sum of electronic and thermal Free Energies=-3630.846006

Cartesian coordinate

C	-1.39642300	-0.96146900	0.48945600
C	-2.63239900	-0.31439100	0.31912200
C	-3.70094400	-0.98728200	-0.28596400
O	-3.80019700	-2.20028800	-0.62996700
H	-1.35539300	-1.97041000	0.08343400
C	-0.42679000	-0.65715300	1.53441200
C	0.70263400	-1.48197100	1.65920900
C	-0.52665500	0.44960600	2.39307100
C	1.69420100	-1.22230500	2.59440300
H	0.79709700	-2.32399100	0.98109500
C	0.46825900	0.71411000	3.32830100
H	-1.38904000	1.10601700	2.32646400
C	1.58207900	-0.11749500	3.43863900
H	2.55609300	-1.88190400	2.66404300
H	0.37401700	1.57901200	3.97863000
H	2.35276200	0.09232300	4.17359400
H	-2.77652900	0.71641400	0.63498600
C	-6.66576000	-1.69832500	3.06820100
C	-5.77819200	-2.04380700	2.04561900
C	-4.47350600	-2.44209800	2.32648900
C	-4.06326600	-2.46133600	3.65836300

C	-4.94349300	-2.10774100	4.68183000
C	-6.25447000	-1.73100700	4.39565700
C	-8.01814900	-1.32945600	2.51578000
C	-7.96629900	-1.92544700	1.09242700
C	-6.46464300	-1.94608900	0.69958800
H	-3.80615500	-2.72660200	1.51896200
H	-3.04631100	-2.75376900	3.89866400
H	-4.60577100	-2.13356400	5.71323300
H	-6.94268400	-1.47256000	5.19502900
H	-8.13673400	-0.23959100	2.49503800
H	-8.29735000	-2.96541800	1.13244200
H	-8.85319100	-1.73396100	3.09253900
H	-6.18926700	-2.74447800	0.00969900
N	-6.17235300	-0.67375400	0.00055400
O	-8.80055500	-1.31145700	0.12953300
C	-4.96193900	-0.21610800	-0.38997400
C	-7.09406200	0.27985500	-0.33158000
N	-5.20621500	0.98306700	-0.93825800
N	-6.53766200	1.30854700	-0.90094700
C	-8.55335900	0.06037500	-0.07306400
H	-8.88323700	0.67142800	0.77623300
H	-9.12395900	0.36561800	-0.95156400
C	-4.30810800	1.78678700	-1.70617100
C	-4.28069400	3.15803500	-1.48535700
C	-3.53906900	1.19035700	-2.70420500
C	-3.46285100	3.95850600	-2.27719500
C	-2.72669700	1.99145500	-3.49677000
C	-2.69723300	3.36650500	-3.27507000
H	-3.42144300	5.03034000	-2.12270700
H	-2.12641000	1.55195100	-4.28581200
H	-3.56294900	0.11475300	-2.85560900
H	-4.90042800	3.59122300	-0.70819600
Cl	-1.67312300	4.36780400	-4.26457800
C	-0.17548300	-0.15642000	-1.30108000
C	0.63459100	-1.21399400	-1.73448000
C	0.09934100	-2.13739800	-2.65551900
O	-1.08495800	-2.15292000	-3.10811900
H	-1.13491900	-0.08468900	-1.80653300
C	0.32120500	1.08000200	-0.70360700
C	-0.53572900	2.19089500	-0.62109700
C	1.60386200	1.19994700	-0.14328300
C	-0.12622800	3.37589700	-0.02133500
H	-1.53841900	2.10816300	-1.03198900
C	2.00940200	2.38184200	0.46425000

H	2.28108300	0.35172300	-0.16286700
C	1.15146700	3.47949600	0.52544400
H	-0.80827100	4.22107200	0.01692700
H	3.00257900	2.44646000	0.89899500
H	1.47485500	4.40264200	0.99614800
H	1.67303400	-1.30520700	-1.42803100
C	1.20633400	-0.85290400	-6.91183300
C	0.41970600	-1.10743600	-5.78660900
C	0.03367300	-0.07132900	-4.93798300
C	0.47643200	1.21967000	-5.21805800
C	1.26483500	1.47523800	-6.34126500
C	1.62653900	0.44144500	-7.20173700
C	1.49727500	-2.11558300	-7.67818800
C	0.47565400	-3.11603300	-7.09488500
C	0.09662900	-2.58653800	-5.68092200
H	-0.60095400	-0.28191000	-4.08324300
H	0.20806900	2.03317700	-4.54978000
H	1.59396300	2.48889400	-6.54774000
H	2.22817500	0.64193600	-8.08351000
H	2.52957000	-2.43843700	-7.50212800
H	-0.43448300	-3.08592900	-7.69719200
H	1.37750600	-2.00583900	-8.75880700
H	-0.93402800	-2.78501500	-5.39039200
N	0.95291100	-3.27718100	-4.68950200
O	0.87564900	-4.47256800	-7.10703100
C	1.05232200	-3.01076900	-3.35633600
C	1.94405800	-4.16202300	-5.00510200
N	2.11313000	-3.74345200	-2.94748700
N	2.67464500	-4.46100700	-3.97522100
C	2.05636500	-4.73426800	-6.38580900
H	2.94918800	-4.34421600	-6.88972400
H	2.15700600	-5.81881900	-6.31446100
C	2.62559400	-3.93906900	-1.63388100
C	4.00629500	-3.92830000	-1.45848400
C	1.76356500	-4.19679000	-0.57162800
C	4.53764800	-4.16720300	-0.19725600
C	2.29520400	-4.43344600	0.69069200
C	3.67588700	-4.41119100	0.86639400
H	5.60945500	-4.15840100	-0.03811000
H	1.64286500	-4.63389400	1.53352300
H	0.68978400	-4.20916200	-0.73021800
H	4.65263700	-3.73934400	-2.30798700
Cl	4.33889200	-4.69802300	2.45260400

Variable frequencies

-665.1611	8.7109	10.2642
18.6032	19.5920	25.2346
28.3282	30.0406	36.5403
42.2797	46.2134	48.4570
52.9718	59.6245	60.8987
63.8677	68.4694	73.1045
75.0418	77.5024	85.8139
89.8942	96.3638	106.4688
120.8444	136.0145	143.4705
149.3092	168.4607	171.3779
174.7705	178.5129	179.4373
207.2903	212.1459	217.9880
225.6403	230.6858	234.1222
244.0237	250.2108	255.1901
256.3235	265.6427	275.7721
277.1497	287.2009	298.7372
306.6207	325.7574	335.3433
347.0292	355.1048	363.7512
365.4618	378.1174	384.2492
387.4872	408.6106	414.8263
415.2578	420.9425	423.2776
424.7478	434.3587	438.8531
456.3693	461.0794	465.3990
469.1063	475.0156	485.2242
496.0037	496.3005	512.2354
520.3583	525.0663	535.3379
537.3505	539.1400	556.5053
557.7361	579.7300	586.0919
593.9368	598.9119	607.4330
608.2312	623.4956	624.3560
631.3918	633.1901	641.8197
644.3210	650.3391	652.9370
661.9459	675.4826	692.4014
694.9007	700.2266	706.0996
724.3478	727.1899	727.6870
728.7759	730.5027	744.6322
751.9059	760.1911	763.0797
766.1597	768.2726	776.5409
778.7666	788.4322	789.9674
803.0281	817.5106	820.1092
841.2318	845.8069	847.6222
848.2376	849.9696	850.3546
853.6012	856.6930	859.7850

871.6729	880.9885	886.6154
893.6684	901.3629	905.8747
908.3751	919.1843	919.5635
922.3559	923.1915	934.4834
969.8085	975.5201	976.3497
985.2206	985.7761	990.4146
991.2003	995.6044	1003.4980
1004.9302	1006.7895	1009.3997
1009.9849	1012.9707	1017.8337
1024.9685	1025.5827	1030.6702
1032.3883	1040.3388	1043.3648
1051.7585	1054.2508	1063.8272
1067.7088	1068.8342	1071.9612
1074.5925	1081.0493	1096.1668
1097.0317	1103.2964	1113.0102
1124.0760	1126.8376	1127.8450
1130.3662	1133.2537	1134.5556
1136.7170	1143.0895	1145.8386
1147.4749	1165.4655	1167.6950
1177.7647	1179.4755	1181.0889
1182.6499	1189.7988	1196.4955
1198.7592	1199.7814	1200.2668
1200.9454	1202.5063	1204.9515
1207.4378	1224.9131	1235.1281
1240.4924	1241.0637	1245.2415
1250.9337	1258.0507	1260.3566
1263.6831	1278.0758	1278.5456
1300.2820	1302.0530	1318.0047
1319.0378	1324.2868	1326.7397
1331.1150	1331.8011	1340.2705
1342.2740	1342.3666	1344.6213
1347.2414	1349.1106	1352.0471
1354.9533	1364.9247	1367.5045
1373.6389	1374.1320	1376.0229
1377.5339	1383.7049	1384.1710
1412.0345	1418.8211	1424.8580
1446.9173	1461.5578	1464.2802
1467.2775	1476.1305	1490.7109
1490.8591	1495.3694	1500.1293
1504.3476	1512.6571	1516.5606
1519.0349	1519.2210	1519.7176
1533.1616	1535.9005	1537.1010
1540.0526	1551.1515	1551.7480
1565.0255	1569.6168	1602.5312

1632.3154	1663.3393	1663.9648
1670.8472	1675.5930	1679.8322
1680.3233	1681.2199	1682.1248
1684.1071	1688.4255	1689.7700
1690.8263	1699.5803	1701.7599
3073.2644	3077.2591	3088.1332
3091.4629	3134.0033	3136.5398
3148.9474	3149.4119	3167.6471
3167.8016	3170.5544	3177.9674
3184.3002	3186.7618	3188.8626
3190.4812	3193.3185	3195.2620
3195.7976	3197.6822	3200.2721
3204.7020	3206.9836	3210.2390
3212.0782	3212.5812	3213.3686
3217.6710	3218.7683	3219.2265
3219.9223	3220.9407	3226.0151
3227.2367	3228.2649	3231.4374
3231.5229	3236.3491	3239.1131
3241.4064	3243.4505	3251.8366

M11RR

Zero-point correction=0.861949

Thermal correction to Energy=0.913692

Thermal correction to Enthalpy=0.914636

Thermal correction to Gibbs Free Energy=0.771478

Sum of electronic and zero-point Energies=-3630.800497

Sum of electronic and thermal Energies=-3630.748755

Sum of electronic and thermal Enthalpies=-3630.747811

Sum of electronic and thermal Free Energies=-3630.890969

Cartesian coordinate

C	0.78695900	0.73521400	0.44175100
C	1.97415400	-0.15438500	0.23146300
C	2.74065700	-0.03088200	-0.88552100
O	2.81073100	0.86010400	-1.79426000
H	0.65171800	1.29788100	-0.49101200
C	0.90081600	1.74577100	1.56573200
C	0.17752000	2.94301900	1.51452200
C	1.69925700	1.50383400	2.68647500
C	0.24226000	3.86720700	2.55388800
H	-0.43544900	3.15311300	0.64085500
C	1.76475900	2.42296000	3.73097400
H	2.28485600	0.58956600	2.72642400

C	1.03577200	3.60876200	3.66970100
H	-0.31931700	4.79485000	2.48549500
H	2.39220100	2.21388300	4.59277400
H	1.09215100	4.32873100	4.48039200
H	2.10300900	-1.02919900	0.86389000
C	6.90138900	0.73191300	0.61801400
C	5.73424000	1.01233000	-0.09795400
C	4.75823200	1.86791000	0.40691600
C	4.96873200	2.43204500	1.66473200
C	6.12880400	2.14901900	2.38739000
C	7.10768200	1.30186700	1.86876800
C	7.80024200	-0.20095000	-0.15460900
C	7.25863400	-0.05093100	-1.59241400
C	5.75730300	0.29531000	-1.42830900
H	3.86614300	2.08040700	-0.17522600
H	4.21662600	3.09278200	2.08412700
H	6.27527800	2.60139000	3.36351900
H	8.01523700	1.09615700	2.42861700
H	7.68860700	-1.22861700	0.21249000
H	7.73462900	0.81399400	-2.05963300
H	8.86058400	0.05388000	-0.09110400
H	5.32669600	0.87172800	-2.24805500
N	5.01647900	-0.98739500	-1.39581300
O	7.50580300	-1.12667600	-2.47712200
C	3.71214100	-1.15649300	-1.11879200
C	5.53344000	-2.21465200	-1.70294400
N	3.48959700	-2.46453900	-1.27746600
N	4.62280300	-3.14304200	-1.63184600
C	6.97664000	-2.36817300	-2.07156900
H	7.53334000	-2.79703700	-1.22817800
H	7.06447300	-3.05099400	-2.91825900
C	2.23938100	-3.15607200	-1.16361800
C	2.21322800	-4.38105100	-0.50875200
C	1.08480200	-2.58546800	-1.69385800
C	0.99821500	-5.04317200	-0.36172700
C	-0.13544800	-3.23035000	-1.52315300
C	-0.16069700	-4.45179500	-0.85539800
H	0.94742600	-5.99675400	0.15078500
H	-1.04972800	-2.74260200	-1.85435700
H	1.12549300	-1.62719800	-2.20165900
H	3.13083000	-4.80377600	-0.11538500
Cl	-1.69103900	-5.24572400	-0.59722800
C	-0.49037800	-0.17503100	0.57659400
C	-1.75027200	0.54050100	0.20565300

C	-2.45733500	0.12642200	-0.88256900
O	-2.29931400	-0.84897100	-1.69608900
H	-0.36453500	-0.94255500	-0.19227500
C	-0.56307700	-0.89870700	1.90772000
C	-0.07093600	-2.20281600	2.02469900
C	-1.12535700	-0.30166500	3.04173900
C	-0.14167800	-2.89602600	3.23247100
H	0.36795300	-2.67994700	1.15161000
C	-1.20340100	-0.99004700	4.24789900
H	-1.50678000	0.71378300	2.97406800
C	-0.71390600	-2.29220600	4.34882200
H	0.24206500	-3.91049100	3.29467000
H	-1.64821600	-0.50942500	5.11412900
H	-0.77817000	-2.82923800	5.29026300
H	-2.08587800	1.40893000	0.76566400
C	-6.11357500	-1.71852800	0.94992400
C	-4.94812700	-1.68946300	0.17835500
C	-3.73696100	-2.16012100	0.68059400
C	-3.70648900	-2.63711800	1.98962500
C	-4.86574600	-2.65628100	2.76662500
C	-6.08066700	-2.20635400	2.25100500
C	-7.29184500	-1.18169500	0.17714400
C	-6.78907500	-1.26037500	-1.28067600
C	-5.24630300	-1.12984600	-1.19544900
H	-2.84679200	-2.15258900	0.05814400
H	-2.76784500	-2.99268200	2.40434400
H	-4.82093100	-3.03339700	3.78383500
H	-6.98418200	-2.23805500	2.85285100
H	-7.50636200	-0.14859400	0.47712800
H	-7.00069000	-2.25711800	-1.67379600
H	-8.21041700	-1.75582600	0.31930100
H	-4.70139000	-1.62282400	-2.00072300
N	-4.92442200	0.31381000	-1.30352700
O	-7.38864700	-0.36837300	-2.20094800
C	-3.72154800	0.88932100	-1.12806600
C	-5.81572500	1.31051700	-1.58981800
N	-3.92931200	2.19526800	-1.31328600
N	-5.23798700	2.47760300	-1.59437200
C	-7.25192200	0.99606400	-1.87843200
H	-7.87833300	1.28463700	-1.02515500
H	-7.57858000	1.56887100	-2.74797400
C	-2.95232600	3.24038400	-1.28760700
C	-3.24194900	4.40648200	-0.59264900
C	-1.74268400	3.06514500	-1.95608300

C	-2.29465100	5.42493500	-0.55309700
C	-0.79360200	4.07731800	-1.90786000
C	-1.07947700	5.24613400	-1.20458000
H	-2.49418300	6.34445800	-0.01550600
H	0.16459900	3.95520400	-2.39941700
H	-1.53963100	2.14321100	-2.49036300
H	-4.19649500	4.51292700	-0.08968300
Cl	0.11931600	6.50687300	-1.12972600

Variable frequencies

5.2257	11.7820	21.9965
24.5699	27.1790	28.6092
31.9562	36.0737	41.1681
45.7210	48.0534	51.0279
55.1179	61.8708	63.4584
69.2891	75.4086	79.0882
82.6126	85.9094	90.9635
97.0193	108.8378	126.1930
136.2501	143.9881	146.3343
154.1619	157.9787	176.2038
182.3354	185.8502	190.4790
206.4544	213.6215	218.1056
223.3540	233.9394	237.0564
250.3127	251.4298	253.4386
266.4844	269.7014	284.1942
287.3113	306.3280	315.1745
319.4476	344.7365	346.1464
364.8720	370.7536	373.4770
377.1584	383.2323	405.3491
412.6578	417.2799	420.4803
424.8255	428.3031	437.0007
446.1371	452.5086	459.9314
461.8675	465.0750	467.4974
472.8515	494.5094	496.3099
499.8654	524.8749	531.1945
535.5008	539.2658	548.0444
550.7947	576.1702	579.5848
581.8460	588.5159	594.9711
608.6330	610.2046	624.2241
628.4690	630.7302	633.1259
642.3767	645.4450	651.2774
652.6349	669.4474	686.2726
689.9625	706.2508	710.5936
716.2261	721.4724	727.9256

728.5438	732.0561	734.6599
739.3888	744.9026	759.3733
761.1294	763.4852	776.1599
779.7747	788.9267	791.3068
795.9309	799.2698	812.3811
814.9843	817.0915	833.4754
849.3232	851.0211	852.2584
853.5174	857.3769	868.6968
873.6599	875.2139	876.8391
887.9866	890.8500	894.3701
905.6119	909.1956	923.8210
924.8270	929.6807	937.6612
961.0769	978.7808	980.4057
990.6554	991.5721	992.3880
994.4615	995.6370	1004.0679
1008.8388	1010.2226	1011.7301
1012.4404	1013.0321	1018.5047
1020.4518	1026.7139	1027.4444
1031.1242	1035.5873	1047.0265
1053.3304	1053.6770	1062.7111
1067.2029	1069.6262	1072.7099
1074.5830	1077.6361	1081.3858
1095.6612	1098.4452	1105.8296
1110.4486	1126.0231	1130.7275
1131.4727	1132.7333	1135.0111
1137.3267	1139.8894	1141.1083
1154.5670	1155.4025	1165.6753
1166.6781	1174.2201	1176.7735
1178.8805	1182.6050	1185.7563
1188.9363	1197.8201	1199.6309
1201.4310	1202.7594	1203.2046
1206.1522	1209.3006	1212.1041
1217.3224	1229.7966	1239.2334
1240.5839	1252.3087	1255.1955
1260.6043	1261.3417	1263.4087
1275.1204	1277.1723	1278.1289
1301.2634	1301.4766	1315.5757
1323.4732	1324.3967	1327.5694
1327.7942	1334.7099	1340.7225
1341.5126	1343.3328	1347.9085
1353.7173	1354.2126	1358.4107
1362.2518	1363.6149	1364.7045
1367.8999	1376.4835	1376.6060
1383.8430	1384.4795	1391.2515

1417.8271	1418.5589	1459.1267
1461.9052	1467.2966	1468.4807
1478.0119	1484.8817	1492.1378
1494.4177	1506.9776	1508.3735
1509.0260	1509.2847	1515.8041
1518.8638	1520.4553	1525.7575
1537.6439	1538.0468	1541.8191
1544.2529	1548.2692	1553.5414
1574.2087	1579.0012	1670.3930
1672.5219	1673.3149	1673.9335
1677.4648	1681.9205	1683.8384
1685.7461	1686.9578	1691.2648
1695.4504	1699.5410	1700.1150
1701.4653	1714.6338	1741.0081
3068.1843	3069.3691	3071.1811
3081.6347	3083.4042	3131.1059
3135.7546	3135.8372	3146.7204
3151.5286	3164.0806	3168.0881
3169.5713	3182.0764	3184.3489
3188.6747	3189.0222	3195.9579
3197.4173	3202.5339	3202.8846
3204.9340	3205.1822	3206.8957
3209.9468	3213.5952	3213.8326
3217.2937	3218.4825	3220.3705
3221.4641	3226.5910	3228.5241
3230.6444	3232.0685	3232.0741
3234.0507	3235.1794	3237.0727
3246.1505	3250.6263	3252.4333

^{os}TS12RR

Zero-point correction=0.775226

Thermal correction to Energy=0.823169

Thermal correction to Enthalpy=0.824113

Thermal correction to Gibbs Free Energy=0.688998

Sum of electronic and zero-point Energies=-3208.074928

Sum of electronic and thermal Energies=-3208.026985

Sum of electronic and thermal Enthalpies=-3208.026041

Sum of electronic and thermal Free Energies=-3208.161155

Cartesian coordinate

N	2.79980000	-0.99736800	-1.58411800
N	4.09709700	-1.46157000	-1.58171500
C	4.58083400	-2.00716400	-2.85150100

C	1.74669800	-1.89472800	-1.75617300
C	0.46029500	-1.48492400	-1.71587200
C	0.14040000	-0.11752800	-1.41423300
C	1.23859400	0.76207500	-1.23525500
C	2.54017300	0.34155800	-1.25916700
C	-0.84082700	-0.26830400	0.74311300
C	-2.12492400	0.23524800	0.51978800
C	-2.98244500	-0.43124900	-0.37352900
O	-2.69973100	-1.49723300	-1.02209500
S	4.56093400	-2.36817100	-0.20032100
O	3.64197400	-1.97225400	0.85246900
C	6.16639600	-1.70209100	0.13408300
O	4.71162100	-3.76840100	-0.58176500
C	7.29549100	-2.45790100	-0.15668500
C	8.54892300	-1.91388900	0.11062700
C	8.67503300	-0.63562700	0.65839100
C	7.51510300	0.09845200	0.93970000
C	6.25611600	-0.42359800	0.68466000
C	10.02944300	-0.04944200	0.95729400
H	4.39283500	-1.26241800	-3.62612200
H	5.65820000	-2.16808300	-2.76583400
H	4.09943900	-2.95282300	-3.11995600
H	-0.34522700	-2.19607100	-1.85777600
H	-0.83736200	0.25820000	-1.68161400
H	1.06296900	1.81385600	-1.03246200
H	-0.69219700	-1.31909300	0.51231100
H	7.18498800	-3.45389200	-0.57276000
H	9.44118600	-2.49269800	-0.10838100
H	7.59986600	1.09728200	1.35910200
H	5.35774500	0.14690200	0.90746900
H	10.16470600	0.07797600	2.03563900
H	10.83142400	-0.69176800	0.58890100
H	10.13843100	0.93623200	0.49639800
C	0.15268000	0.35101900	1.60607300
C	1.31644700	-0.36679700	1.93303600
C	0.04520000	1.67200300	2.08279800
C	2.30060100	0.18185200	2.74715000
H	1.44651400	-1.36930600	1.53608100
C	1.02248000	2.21534600	2.90900500
H	-0.81437900	2.27722200	1.80645000
C	2.15188000	1.47106600	3.25746400
H	3.18655400	-0.40402200	2.97273400
H	0.90573300	3.22939900	3.28067300
H	2.91218900	1.89921300	3.90345100

H	-2.45126400	1.15793300	0.98830400
C	-6.45759800	-3.15660200	1.10228400
C	-5.24628200	-2.78080700	0.51616600
C	-4.03559300	-3.01475300	1.16577400
C	-4.06394800	-3.61236100	2.42442900
C	-5.27325900	-3.97855800	3.01618300
C	-6.47965200	-3.75950500	2.35488700
C	-7.62616500	-2.83121500	0.21137100
C	-6.95277400	-2.58499800	-1.15591900
C	-5.48150600	-2.17316700	-0.85529300
H	-3.10327000	-2.74544300	0.67958700
H	-3.13117700	-3.80128100	2.94595700
H	-5.27371500	-4.44848900	3.99493100
H	-7.42066100	-4.06066700	2.80619800
H	-8.14853700	-1.93951800	0.57602000
H	-6.91012000	-3.52893600	-1.70349700
H	-8.36598600	-3.63335100	0.15361800
H	-4.76219000	-2.51497100	-1.59790500
N	-5.41042300	-0.69589900	-0.85239600
O	-7.63249400	-1.69295500	-2.01781700
C	-4.33732100	0.08439100	-0.52514700
C	-6.48489400	0.13231700	-1.01801200
N	-4.84270900	1.34711600	-0.49806600
N	-6.18316000	1.37445600	-0.80123600
C	-7.80475100	-0.40001700	-1.48715500
H	-8.54029700	-0.37756600	-0.67382700
H	-8.17664100	0.23345400	-2.29446400
C	-4.16738100	2.58966100	-0.33902300
C	-4.72558400	3.54399400	0.50439200
C	-2.99568500	2.85297000	-1.04692800
C	-4.09840900	4.77606600	0.65820700
C	-2.36192500	4.07674000	-0.88586400
C	-2.91868200	5.02670400	-0.03173000
H	-4.51663500	5.53041200	1.31431700
H	-1.44889300	4.29982100	-1.42552900
H	-2.57972200	2.09901200	-1.70600100
H	-5.64533900	3.31916900	1.03222000
Cl	-2.12150500	6.56405900	0.16774500
H	2.05075300	-2.91967100	-1.93673400
C	3.65939800	1.26234100	-0.97866200
C	4.80983000	1.33663500	-1.77718200
C	3.54760200	2.11622000	0.12597100
C	5.82769600	2.22814500	-1.46480700
H	4.90489600	0.70171200	-2.65074200

C	4.57208900	3.00648500	0.43782400
H	2.66438200	2.05293500	0.75402800
C	5.71840400	3.06086100	-0.35121800
H	6.71304200	2.27078800	-2.09134800
H	4.47304300	3.64914100	1.30745700
H	6.52095000	3.74919000	-0.10491600

Variable frequencies

-541.1759	10.2799	12.3826
14.5682	20.1904	23.4113
29.4818	32.7078	34.2525
46.3092	47.6514	50.2282
57.4021	63.8554	70.8186
74.2616	82.1466	88.3022
93.8656	95.0721	104.4117
108.6364	120.0030	126.1043
135.5912	145.8988	151.3771
164.6089	174.6042	180.1420
191.7461	196.4937	204.3925
207.1100	211.1774	224.6936
239.5310	253.7338	263.2317
263.9229	266.4465	272.6165
283.6377	293.9522	308.6254
312.3127	324.8071	338.0030
346.9244	351.5742	358.1106
363.1788	378.7221	381.1587
399.5000	411.9421	420.4505
422.7637	423.7601	426.5555
431.5956	442.9515	453.0139
470.6546	480.9739	487.4128
495.2890	497.1938	502.5852
519.5216	528.4060	536.3473
550.8461	556.0953	561.1522
575.5720	579.4602	582.2121
594.8516	607.9368	617.7573
628.2831	630.2026	632.0120
640.6511	643.2141	651.2926
657.3711	658.8191	660.3331
686.2967	698.4823	712.2024
716.3095	719.6641	721.7347
726.7381	728.2773	750.9797
760.3360	766.1580	772.9862
774.7545	780.2019	783.7930
790.9293	820.2534	830.1117

839.0070	842.1458	847.1602
848.7199	852.4060	852.7964
858.4113	871.5448	874.5595
879.1216	885.6161	892.2818
902.5299	916.8384	921.5597
928.6717	949.6501	961.6336
971.8839	985.2438	986.0006
987.4218	992.7372	999.6850
1000.4773	1006.6445	1010.4570
1011.6328	1012.6875	1013.3507
1015.6527	1025.5211	1026.2016
1027.0913	1032.6360	1036.4759
1043.1599	1046.8459	1052.4028
1063.4497	1067.8615	1070.5960
1072.3014	1074.0977	1091.9360
1096.8106	1115.3769	1117.9500
1122.5507	1123.3878	1124.7402
1134.6368	1137.5285	1139.8209
1144.6577	1146.9160	1152.5257
1157.6487	1167.1569	1175.9823
1177.4045	1181.3345	1184.2566
1196.6137	1199.7170	1205.4270
1206.9231	1210.0838	1212.7812
1220.9363	1223.8732	1234.1143
1238.8948	1244.9454	1253.3490
1257.3768	1270.3635	1275.5338
1299.2421	1316.1765	1320.4884
1323.3722	1326.2948	1331.1980
1331.7280	1337.3654	1340.6027
1341.6901	1349.3712	1354.5938
1356.2036	1361.0744	1369.5666
1371.4543	1378.2988	1381.8365
1383.5113	1384.2879	1413.9489
1421.4612	1424.1953	1436.8314
1456.1191	1461.7700	1465.8077
1468.5099	1470.6023	1489.6928
1493.7608	1496.0918	1496.6056
1498.3571	1498.5796	1508.3318
1510.7664	1515.8746	1517.3426
1534.4475	1535.6742	1545.8000
1550.2228	1552.7712	1562.3509
1576.6732	1595.9186	1658.3632
1664.0760	1669.4093	1677.6860
1680.2165	1683.3727	1684.9878

1691.7550	1693.2557	1694.5189
1703.0894	1705.7836	3072.0568
3075.3498	3076.8429	3090.9402
3131.6426	3143.8607	3147.5462
3156.2382	3158.7549	3165.8618
3184.1887	3187.3048	3192.2261
3192.4105	3196.2283	3199.7207
3205.3112	3206.1888	3209.7477
3210.7544	3212.3654	3215.0084
3216.4831	3217.6536	3219.3652
3220.4343	3222.1859	3222.8939
3225.5157	3230.4794	3231.1666
3232.1907	3234.1162	3234.9541
3238.6838	3242.7228	3244.7841
3245.2853	3246.0843	3251.1625

M12RR

Zero-point correction=0.779819

Thermal correction to Energy=0.827487

Thermal correction to Enthalpy=0.828431

Thermal correction to Gibbs Free Energy=0.694584

Sum of electronic and zero-point Energies=-3208.114217

Sum of electronic and thermal Energies=-3208.066548

Sum of electronic and thermal Enthalpies=-3208.065604

Sum of electronic and thermal Free Energies=-3208.199451

Cartesian coordinate

N	-2.93739100	1.75183500	-0.55332600
N	-3.93719400	1.56065700	0.40090700
C	-4.57155700	2.78734000	0.87723300
C	-1.73401500	2.35605900	-0.13010500
C	-0.54547300	2.05091200	-0.64725200
C	-0.34873900	0.91206400	-1.60853000
C	-1.68358100	0.45663500	-2.13396000
C	-2.86020400	0.78117100	-1.58245000
C	0.43990900	-0.24301300	-0.89547800
C	1.83233700	0.20109500	-0.54750300
C	2.37135000	-0.03636100	0.68481900
O	1.91474200	-0.60744000	1.72220600
S	-3.53133900	0.45586400	1.64637200
O	-2.72265600	-0.56626700	0.99919700
C	-5.14637900	-0.18058200	2.02013000
O	-3.03486900	1.15666700	2.82735200

C	-5.64875500	-0.05020400	3.30799800
C	-6.91467300	-0.56062900	3.58587800
C	-7.67073900	-1.18655500	2.59369300
C	-7.13456700	-1.29798200	1.30309400
C	-5.87445800	-0.80277700	1.00569800
C	-9.03819300	-1.74139200	2.89357100
H	-4.91500500	3.34112600	0.00289000
H	-5.43469200	2.51384700	1.48835500
H	-3.90265000	3.41437000	1.47684200
H	0.32877600	2.60133700	-0.31756900
H	0.28101900	1.23614300	-2.45221600
H	-1.69648500	-0.20533300	-2.99375800
H	-0.09229200	-0.46037900	0.03840500
H	-5.05459300	0.44474700	4.06891600
H	-7.32142900	-0.46672900	4.58840100
H	-7.71493400	-1.77862000	0.52000100
H	-5.46073000	-0.88837500	0.00496200
H	-9.04122100	-2.83163600	2.80088500
H	-9.35764000	-1.48636300	3.90578400
H	-9.77969600	-1.35189900	2.19051800
C	0.39810700	-1.49253600	-1.75941900
C	-0.55781300	-2.48467300	-1.51616100
C	1.24856400	-1.64298300	-2.85761300
C	-0.66838200	-3.59129900	-2.35838100
H	-1.22541000	-2.37093300	-0.66439400
C	1.14249800	-2.74561200	-3.70058500
H	2.01045300	-0.89096000	-3.04508200
C	0.17952000	-3.72338100	-3.45682700
H	-1.41690900	-4.35175900	-2.15450500
H	1.81489400	-2.84445400	-4.54766200
H	0.09530600	-4.58391600	-4.11332900
H	2.42927800	0.71697100	-1.29703600
C	5.24173800	-3.51588100	0.24137800
C	4.13033400	-2.81995300	0.72583900
C	2.85380800	-3.05890600	0.22493800
C	2.71311300	-3.99196700	-0.80083700
C	3.82185000	-4.67682700	-1.29874500
C	5.09468800	-4.45175300	-0.77555100
C	6.49751600	-3.11235900	0.97040900
C	5.93260900	-2.44230200	2.24121500
C	4.54296800	-1.88241000	1.83864400
H	2.00104600	-2.52782700	0.63705900
H	1.72746600	-4.17906500	-1.21570800
H	3.68933200	-5.40210700	-2.09592800

H	5.95351300	-5.00164700	-1.14963700
H	7.08327500	-2.40980800	0.36548100
H	5.75382900	-3.21224600	2.99475300
H	7.15244600	-3.95197100	1.21475900
H	3.81972500	-1.82292200	2.65158100
N	4.74522700	-0.48666900	1.37135100
O	6.77214700	-1.49665600	2.87514400
C	3.82842800	0.33742800	0.82443700
C	5.92514900	0.20069800	1.44190100
N	4.49096300	1.47439100	0.58439000
N	5.80492800	1.40259400	0.95943300
C	7.14448600	-0.40970600	2.06187700
H	7.86055600	-0.70041800	1.28291900
H	7.62541200	0.32883800	2.70554600
C	3.97853600	2.71528900	0.09401000
C	4.70382000	3.39902300	-0.87307000
C	2.80154500	3.23160800	0.62738100
C	4.23784800	4.62713200	-1.33029200
C	2.33427700	4.45573400	0.16646800
C	3.05556800	5.13998300	-0.80876800
H	4.78439300	5.17851600	-2.08618000
H	1.42081000	4.88112900	0.56599800
H	2.25812800	2.68178100	1.38886200
H	5.62486900	2.97577800	-1.25734400
Cl	2.46823000	6.67620900	-1.37954000
H	-1.86549100	3.12955500	0.61930800
C	-4.14374900	0.19241700	-2.02977500
C	-5.30718700	0.96294800	-2.13726200
C	-4.20772200	-1.17479300	-2.31454000
C	-6.50911900	0.37751500	-2.51500000
H	-5.25997900	2.02544900	-1.91896300
C	-5.41190900	-1.76064000	-2.69961400
H	-3.31073800	-1.77763900	-2.20133600
C	-6.56695300	-0.98862800	-2.79294800
H	-7.40510000	0.98570700	-2.59024600
H	-5.44900000	-2.82481200	-2.91012200
H	-7.50806000	-1.44661100	-3.08115300

Variable frequencies

11.7994	13.2484	18.7498
20.9933	27.3968	31.9032
37.2041	38.1722	42.8585
52.7698	54.2821	58.7660
69.4659	72.5377	75.7292

79.3428	82.2751	84.9387
92.1941	96.2767	100.0773
107.3233	123.4902	139.7837
143.0346	158.5359	167.4129
174.2840	182.9403	189.2037
200.4337	210.2423	215.2721
221.8088	230.4864	236.9817
251.5695	253.8649	263.7978
266.8986	282.8855	290.3491
303.4945	312.3556	312.9691
322.9970	330.4716	348.6345
356.3335	363.7251	371.6495
373.4025	387.6798	410.0796
417.4318	418.2673	420.7116
424.0426	426.9973	435.9267
452.4616	457.8461	469.1774
476.1318	490.7157	496.1713
500.5019	521.9867	526.3412
538.0497	538.4215	553.1691
554.0282	572.9464	585.3062
589.1907	593.5350	609.1924
620.3946	626.4202	629.4193
632.4463	635.0926	644.1166
648.0353	652.4255	659.8586
676.0831	686.1258	703.9646
707.0866	712.8676	717.8406
724.1485	724.4800	725.9716
731.3138	756.4553	760.9058
767.5701	776.4572	787.4625
787.8413	792.2498	805.3654
814.1310	818.1072	838.8024
842.2885	848.6341	849.5640
854.7009	861.1885	873.6891
875.3904	879.1389	880.3691
880.5424	892.4834	906.2988
924.2449	933.7607	951.3646
962.1138	971.3857	979.6403
990.8875	991.4242	994.7588
996.1660	1002.2966	1004.3506
1008.2261	1010.5265	1012.9786
1013.5096	1016.9949	1019.1352
1025.1998	1031.8338	1033.4401
1037.2695	1042.1068	1048.2561
1056.6747	1066.1228	1066.5892

1069.1773	1072.7753	1073.7376
1083.7086	1097.2140	1103.2931
1111.0212	1116.0701	1123.5668
1125.5109	1131.4736	1132.5505
1141.1443	1144.8012	1148.2054
1155.6418	1164.5300	1166.7745
1178.1713	1179.2256	1181.9870
1182.7291	1184.1521	1198.8101
1198.9658	1202.5712	1207.9115
1209.3883	1213.1982	1222.0918
1236.1915	1238.0188	1239.4507
1250.8275	1254.9627	1260.7049
1277.1464	1282.4922	1293.2909
1297.8997	1300.2380	1311.5522
1325.2636	1329.3548	1333.5478
1335.9275	1339.5744	1341.8775
1349.2506	1354.7966	1355.7225
1358.1998	1360.8769	1362.4729
1364.6037	1372.7957	1378.0199
1384.4184	1385.8235	1419.7575
1424.2609	1428.5119	1444.8213
1453.8751	1456.5222	1463.3976
1466.8201	1483.2636	1494.1864
1494.6749	1495.7397	1497.5618
1503.1997	1508.0513	1508.9334
1513.2031	1519.0792	1521.0219
1535.8879	1541.1451	1548.1013
1550.7177	1554.9379	1576.3999
1668.7052	1670.7237	1673.9066
1674.5625	1680.4322	1687.4658
1692.4689	1693.8561	1695.7626
1698.1366	1700.2402	1726.5464
1743.2889	1787.0716	3013.3609
3071.3330	3072.4912	3075.1860
3085.1433	3094.0856	3136.5207
3146.2167	3151.6648	3153.8566
3165.6861	3167.8374	3172.5822
3179.7481	3183.3070	3189.0851
3192.5104	3196.1468	3196.4543
3202.8046	3203.8012	3205.3985
3208.6998	3212.9405	3214.6970
3215.3444	3217.8097	3220.1719
3220.3716	3222.8033	3225.0247
3229.8867	3232.7862	3234.1304

3236.6239	3238.7797	3240.1499
3246.9967	3248.8000	3253.7168

²TS13RR

Zero-point correction=0.599837

Thermal correction to Energy=0.635084

Thermal correction to Enthalpy=0.636028

Thermal correction to Gibbs Free Energy=0.528167

Sum of electronic and zero-point Energies=-2294.315487

Sum of electronic and thermal Energies=-2294.280241

Sum of electronic and thermal Enthalpies=-2294.279296

Sum of electronic and thermal Free Energies=-2294.387157

Cartesian coordinate

N	3.96574000	1.41902700	-1.97847300
C	2.76211000	2.02247400	-1.97185300
C	1.89461200	2.03016500	-0.90643800
C	2.21980400	1.27631600	0.27987500
C	3.58749100	0.82378500	0.32199400
C	4.36546800	0.83954500	-0.82233000
C	1.10288000	-0.26877400	0.17765000
C	-0.28339700	0.14436200	0.25066600
C	-1.07114000	0.06121900	-0.87905100
O	-0.79734000	-0.32119100	-2.05037500
H	0.92923700	2.51711300	-0.98445300
H	1.79609800	1.62196500	1.22394000
H	3.98274400	0.41355100	1.24469100
H	1.36360600	-0.58917900	-0.83259000
C	1.62583000	-1.20656000	1.20672200
C	1.14845000	-1.23692200	2.52193100
C	2.64345500	-2.10269800	0.84930500
C	1.66002000	-2.14513000	3.44470700
H	0.35715600	-0.55802100	2.82519900
C	3.15540400	-3.01244300	1.76983900
H	3.02950600	-2.08192900	-0.16738200
C	2.66182800	-3.03946100	3.07334300
H	1.27051900	-2.15791800	4.45808500
H	3.93749000	-3.70227000	1.46629600
H	3.05554900	-3.74975800	3.79320900
H	-0.73585000	0.45275900	1.18865100
C	-3.34460000	-3.62339900	0.22488300
C	-2.45933500	-2.86430000	-0.54612700
C	-1.08150000	-2.96212400	-0.36993400

C	-0.60214800	-3.81031000	0.62789600
C	-1.48479400	-4.55412800	1.41201200
C	-2.86207500	-4.47650100	1.21006600
C	-4.77404500	-3.37184500	-0.18190700
C	-4.60560200	-2.72820100	-1.57507800
C	-3.22908200	-2.01611200	-1.53463200
H	-0.40916400	-2.38671500	-0.99949100
H	0.46771300	-3.88522900	0.79902800
H	-1.09146000	-5.21024400	2.18223600
H	-3.54355300	-5.07418700	1.80816400
H	-5.25626300	-2.68637100	0.52555700
H	-4.53055200	-3.51855600	-2.32493800
H	-5.38491300	-4.27629500	-0.22376400
H	-2.74504600	-1.90355800	-2.50498900
N	-3.47101300	-0.64006000	-1.02768200
O	-5.66133800	-1.89814200	-2.01641900
C	-2.54833200	0.27431000	-0.67262800
C	-4.70103300	-0.08016400	-0.81726600
N	-3.24858200	1.33232800	-0.25817400
N	-4.59732600	1.12528800	-0.33675600
C	-5.95834300	-0.81975600	-1.16151400
H	-6.46631200	-1.14484300	-0.24484100
H	-6.63029100	-0.15188200	-1.70330800
C	-2.74823700	2.60057100	0.16917700
C	-3.32642600	3.20496000	1.27792000
C	-1.72204700	3.20804300	-0.54711900
C	-2.85592900	4.44505900	1.69366900
C	-1.24280000	4.44061100	-0.12225800
C	-1.81356400	5.04539200	0.99502500
H	-3.28908100	4.93924000	2.55519600
H	-0.44051000	4.93429400	-0.65839500
H	-1.31218900	2.72512500	-1.42867000
H	-4.13618200	2.71083400	1.80254100
Cl	-1.21635900	6.59225700	1.52167000
H	2.49039500	2.53424900	-2.89327500
C	5.73220000	0.24588700	-0.83145900
C	6.68159700	0.71144000	-1.74808700
C	6.09420400	-0.78089900	0.04767200
C	7.96420700	0.17655600	-1.77354700
H	6.38899000	1.49673800	-2.43625800
C	7.37829800	-1.31728100	0.02051500
H	5.36089000	-1.18195600	0.74200900
C	8.31919900	-0.83915100	-0.88804000
H	8.69067000	0.55375000	-2.48687300

H	7.64086600	-2.11856100	0.70455900
H	9.31996700	-1.25915900	-0.91016300

Variable frequencies

-538.9426	11.7463	13.6020
22.1609	26.5904	32.8829
37.7608	45.3822	51.2713
54.2422	61.8464	78.1942
79.6335	82.7576	98.1649
108.8212	119.9390	127.9569
135.3148	144.9896	172.1227
187.2053	205.4857	215.6025
227.9962	239.6624	254.3093
264.9340	270.2614	274.4061
288.0722	313.3047	327.8812
344.7271	357.8650	373.0940
378.8669	402.0770	413.5659
414.9612	423.5401	424.6440
426.5268	445.1962	460.6443
466.7573	479.0202	486.4700
496.5936	525.8446	536.3343
538.9834	555.2688	574.7604
590.8445	595.4306	606.7285
619.4768	626.5581	630.8199
631.9226	642.7108	645.9262
652.4436	687.0606	708.3153
710.6044	718.0775	723.6414
726.9582	731.7196	739.8472
757.7389	765.7493	773.4075
777.1021	789.2294	789.8821
798.6427	804.4301	815.6538
848.0337	852.9817	853.9044
863.2548	865.5446	873.5979
885.8000	887.5252	902.6752
913.3364	932.2239	933.9176
959.6047	979.7512	982.0539
986.9740	989.4727	991.5920
1003.0906	1008.9514	1009.2744
1010.7296	1015.6509	1017.4269
1018.8525	1024.7210	1028.0934
1032.3951	1046.3989	1054.4931
1063.4172	1067.0032	1069.2244
1077.7673	1079.1642	1083.1414
1099.5892	1110.1896	1114.7375

1118.3389	1127.6567	1131.6146
1133.7554	1140.4495	1148.2114
1155.6014	1163.8768	1169.3938
1178.9344	1182.3016	1183.4383
1188.5702	1199.5641	1201.2628
1206.3563	1207.7444	1214.4462
1240.3598	1241.9832	1250.0302
1258.6160	1261.3950	1276.0171
1301.2672	1305.9163	1315.9443
1318.5139	1326.1535	1328.3786
1341.3064	1343.5634	1344.6098
1353.6884	1359.7826	1365.4932
1365.8080	1370.1319	1376.6356
1383.6616	1419.8899	1432.9793
1465.0408	1467.1932	1488.2253
1493.9541	1500.7460	1503.6741
1504.7642	1514.0094	1519.9820
1520.6067	1535.0583	1536.2831
1542.6562	1553.1664	1564.3054
1579.0071	1638.0738	1667.4278
1671.9618	1676.3763	1678.2880
1680.0123	1688.2632	1689.4215
1691.7685	1701.4370	1702.6234
3072.7933	3087.3861	3131.8305
3142.6713	3153.7576	3153.8737
3167.3798	3173.0615	3179.8290
3187.0130	3192.3296	3193.2695
3200.6684	3203.0399	3204.4766
3206.7838	3212.8492	3214.3895
3218.1624	3219.6562	3222.4389
3222.8073	3230.2897	3233.5453
3236.1176	3237.2486	3238.0595
3238.2865	3257.1099	3261.2132

²M13RR

Zero-point correction=0.601075

Thermal correction to Energy=0.636346

Thermal correction to Enthalpy=0.637290

Thermal correction to Gibbs Free Energy=0.530547

Sum of electronic and zero-point Energies=-2294.322271

Sum of electronic and thermal Energies=-2294.287000

Sum of electronic and thermal Enthalpies=-2294.286056

Sum of electronic and thermal Free Energies=-2294.392799

Cartesian coordinate

N	4.37464900	1.69594000	-0.99043500
C	3.19151600	2.32648700	-0.78728300
C	2.16271500	1.84358100	-0.03300300
C	2.25822500	0.52347600	0.63909000
C	3.62172700	-0.04833900	0.48721500
C	4.56062000	0.51042000	-0.34401900
C	1.14385800	-0.47294100	0.08950100
C	-0.23127300	0.10715900	0.23294500
C	-1.09690100	0.08395400	-0.82387200
O	-0.98202200	-0.36734500	-2.00494400
H	1.23697000	2.40044700	0.05784200
H	2.01389800	0.62722200	1.71198600
H	3.85669800	-0.95157200	1.03948600
H	1.33284700	-0.60048200	-0.98232700
C	1.32917800	-1.81911700	0.76945000
C	0.88879300	-2.03290100	2.07807200
C	2.02049700	-2.84882500	0.12392800
C	1.14196300	-3.23618700	2.73046500
H	0.33340900	-1.24981900	2.58779600
C	2.27837600	-4.05609100	0.77296600
H	2.36971200	-2.69394100	-0.89453100
C	1.84274900	-4.25185200	2.08177100
H	0.79023600	-3.38262000	3.74718900
H	2.81760300	-4.84297300	0.25425700
H	2.04312600	-5.18945400	2.59045700
H	-0.54701700	0.53651200	1.18092700
C	-4.06573800	-3.16574600	0.21332500
C	-3.07439700	-2.53216000	-0.54211400
C	-1.74239600	-2.92689900	-0.46610400
C	-1.41246300	-3.96044000	0.40838000
C	-2.39529200	-4.58458700	1.17718100
C	-3.73169900	-4.19857300	1.08072200
C	-5.42548400	-2.58631700	-0.08260000
C	-5.18439000	-1.87971500	-1.43380400
C	-3.68814200	-1.47140800	-1.42528900
H	-0.99277800	-2.43549900	-1.08017900
H	-0.37805200	-4.27821700	0.49010600
H	-2.11595700	-5.38942800	1.85043700
H	-4.49760600	-4.70102400	1.66424500
H	-5.71772600	-1.87587900	0.70036300
H	-5.30571300	-2.60887200	-2.23771700
H	-6.21771100	-3.33503000	-0.15367400

H	-3.22827000	-1.39902500	-2.41115600
N	-3.60501900	-0.10913600	-0.83912700
O	-6.06767700	-0.82411000	-1.75713800
C	-2.49217800	0.58964000	-0.54127400
C	-4.67783700	0.69479800	-0.56859200
N	-2.93427700	1.77405300	-0.11031100
N	-4.29965000	1.85323500	-0.11297900
C	-6.07879200	0.23380800	-0.82841100
H	-6.56235500	-0.04944800	0.11510300
H	-6.64920100	1.05175900	-1.27134100
C	-2.17157100	2.94080100	0.20651200
C	-2.52764500	3.68739400	1.32237400
C	-1.13846400	3.33243400	-0.63918100
C	-1.82289400	4.84992700	1.61280600
C	-0.43098300	4.49132200	-0.34406700
C	-0.77798900	5.23652400	0.78019100
H	-2.07969800	5.44927500	2.47817400
H	0.37973400	4.81814000	-0.98542200
H	-0.88839800	2.73661900	-1.51142500
H	-3.35118700	3.36405700	1.94876100
Cl	0.11078000	6.68685300	1.14613500
H	3.08986700	3.28821900	-1.28691500
C	5.87753300	-0.15003000	-0.56651700
C	6.98705900	0.61416000	-0.94240400
C	6.03081900	-1.53301600	-0.41916600
C	8.22506000	0.01246100	-1.14161000
H	6.85727100	1.68245200	-1.07711900
C	7.26939600	-2.13424500	-0.61883800
H	5.17083100	-2.14874200	-0.17012600
C	8.37245900	-1.36299600	-0.97657400
H	9.07888700	0.61933400	-1.42669100
H	7.37030400	-3.20919700	-0.50537000
H	9.33861200	-1.83207400	-1.13383000

Variable frequencies

16.3337	21.4709	21.8756
29.6139	34.4085	40.8772
41.7646	53.1996	57.1721
75.2824	81.6231	84.0036
89.3384	98.8752	110.3731
118.8822	126.2204	138.6133
149.5299	169.0044	185.0377
208.2103	218.5228	220.7261
237.6452	253.7765	264.1423

268.1781	281.4336	287.6542
311.4631	323.3098	346.1942
356.0777	370.6582	375.3705
400.6810	410.3134	414.8383
418.9897	422.1221	425.7303
440.4001	457.5989	466.8586
478.2289	482.0402	497.8426
521.4583	538.2167	540.1947
551.5131	571.9511	591.3151
599.6544	609.3682	625.5060
627.2467	629.0017	632.0888
634.5009	645.6346	652.3228
669.1959	689.1000	708.4705
710.7506	720.6340	722.8861
726.8624	731.9742	749.5214
761.0920	770.8301	781.8357
790.2267	792.3525	793.3200
804.6231	815.7748	847.6255
851.2378	853.5592	856.1368
862.2405	873.9281	877.3667
885.9991	892.5442	906.3134
926.9435	930.6464	948.5078
956.6308	964.7525	980.9768
988.6276	996.4664	997.0506
999.0473	1006.2351	1008.1892
1009.4458	1016.2240	1016.8794
1018.0180	1028.5528	1028.9944
1033.0047	1048.0758	1053.6425
1055.3897	1067.2693	1072.7537
1073.7948	1077.2963	1088.4210
1098.0409	1107.5207	1109.1910
1120.9598	1124.7109	1131.1059
1137.0794	1141.8946	1154.8573
1160.3546	1166.4265	1171.3858
1180.6214	1181.7836	1182.2778
1194.0698	1201.0121	1202.9943
1206.1489	1206.5159	1208.2640
1236.0142	1240.1612	1251.8494
1262.4737	1267.0471	1275.7734
1293.4309	1300.2990	1301.7079
1309.6115	1324.3026	1329.1840
1339.5401	1340.8424	1345.7159
1353.5204	1360.8835	1361.8486
1362.2980	1368.3723	1375.2946

1381.8601	1385.5263	1419.7324
1457.6845	1463.0240	1469.7065
1482.9848	1494.9989	1502.6102
1503.6292	1509.5292	1510.1318
1520.9053	1531.5233	1537.7040
1544.5569	1549.5568	1563.5567
1580.5054	1638.9269	1674.3836
1675.2738	1675.7273	1680.3912
1688.0531	1695.2081	1695.4333
1697.9753	1704.2739	1720.9977
2976.5059	3071.7720	3085.6428
3101.9099	3137.0321	3148.3937
3173.1164	3180.9639	3182.3371
3183.7118	3187.8825	3196.9364
3197.5086	3203.7409	3209.5175
3212.8187	3215.0083	3217.9721
3220.0425	3220.7233	3230.2280
3230.6712	3231.4826	3232.7847
3234.9695	3237.8867	3239.0483
3240.5226	3244.1022	3261.8144

²TS5^{C2}

Zero-point correction=0.778552

Thermal correction to Energy=0.826223

Thermal correction to Enthalpy=0.827167

Thermal correction to Gibbs Free Energy=0.692565

Sum of electronic and zero-point Energies=-3207.925863

Sum of electronic and thermal Energies=-3207.878192

Sum of electronic and thermal Enthalpies=-3207.877248

Sum of electronic and thermal Free Energies=-3208.011850

Cartesian coordinate

N	-2.07884000	0.66028500	0.97154200
N	-2.92555300	-0.29124500	0.37999800
C	-3.25759300	-1.38219700	1.31010600
C	-0.75490700	0.28629400	1.27418300
C	-0.28037700	0.68224300	2.57475900
C	-0.91929600	1.66969900	3.25268500
C	-2.09818400	2.26568800	2.70799900
C	-2.69923900	1.73277200	1.60264500
C	0.47180000	1.20189300	-0.02433400
C	1.70417000	0.53889800	0.18457600

C	2.13941200	-0.41290000	-0.75353500
O	1.66220000	-0.69816200	-1.86342000
S	-2.39014100	-0.80193600	-1.16519200
O	-2.07057100	0.42556200	-1.87987000
C	-3.86300500	-1.54421900	-1.79092200
O	-1.37056600	-1.83935800	-1.01207700
C	-3.81219900	-2.86680900	-2.21958500
C	-4.96504700	-3.43510700	-2.74909200
C	-6.15023600	-2.70073600	-2.85017400
C	-6.16516600	-1.37303700	-2.40302500
C	-5.02633100	-0.78091200	-1.87711700
C	-7.38394500	-3.31683000	-3.45183200
H	-3.78028600	-0.93477000	2.15734000
H	-3.93204600	-2.07745000	0.80822400
H	-2.36625900	-1.91554900	1.65966900
H	0.62290100	0.21112200	2.94919000
H	-0.54648000	2.01190100	4.21206500
H	-2.53712000	3.14279100	3.16619100
H	-0.02189000	0.88267000	-0.94311100
H	-2.88863500	-3.42950200	-2.13718400
H	-4.94504100	-4.46634600	-3.08801800
H	-7.08416900	-0.79838400	-2.46777200
H	-5.04028200	0.24493300	-1.52111100
H	-7.39685600	-4.39888200	-3.30763000
H	-8.29093500	-2.89490200	-3.01417900
H	-7.41462900	-3.12394100	-4.52898000
C	0.25583700	2.63123100	0.28524700
C	0.97937700	3.32110700	1.26581800
C	-0.73865000	3.31388400	-0.42729300
C	0.68998800	4.65205600	1.54642500
H	1.77124900	2.81774200	1.81321900
C	-1.03115000	4.64325000	-0.14355600
H	-1.27830000	2.78215600	-1.20675700
C	-0.32251100	5.31315700	0.85183800
H	1.25512000	5.17681300	2.31024800
H	-1.81294000	5.15399900	-0.69658600
H	-0.54873400	6.35010900	1.07798800
H	2.34627500	0.75822600	1.03383400
C	5.82379700	1.91970900	-0.90595600
C	4.72671300	1.35987000	-1.56834200
C	3.56722600	2.09139900	-1.80566000
C	3.50059800	3.39687200	-1.32191000
C	4.58330100	3.95257500	-0.63810400
C	5.75681700	3.22603100	-0.43558900

C	6.96964600	0.93792400	-0.83496200
C	6.58955800	-0.06939900	-1.94294000
C	5.04300900	-0.06121100	-1.95988200
H	2.73184600	1.65342500	-2.34445700
H	2.59992500	3.98216700	-1.47755100
H	4.51511900	4.97169300	-0.27126300
H	6.60376000	3.67699400	0.07201400
H	7.00483400	0.45857500	0.15165200
H	6.92041400	0.32270100	-2.90682700
H	7.94718100	1.39047600	-1.01206900
H	4.60718000	-0.39593000	-2.90301800
N	4.61015800	-1.03383300	-0.91664400
O	7.13978400	-1.36605600	-1.86145400
C	3.38980400	-1.17966600	-0.38487000
C	5.41441300	-1.97723700	-0.33062600
N	3.48281400	-2.19251000	0.47043600
N	4.74541200	-2.69924600	0.52543200
C	6.87248800	-2.06509300	-0.66921500
H	7.46376700	-1.68531600	0.17374400
H	7.14616400	-3.10830700	-0.83525200
C	2.40525300	-2.76940500	1.21707600
C	2.62384600	-3.15413500	2.53455600
C	1.16906800	-2.92735700	0.59489100
C	1.56691700	-3.68885000	3.26193800
C	0.11376000	-3.45481700	1.32898200
C	0.31959300	-3.82243700	2.65527300
H	1.70620600	-3.99516200	4.29210100
H	-0.85335500	-3.58652100	0.85651600
H	1.01492400	-2.64900600	-0.44363400
H	3.60471900	-3.03576200	2.98111900
Cl	-1.01018100	-4.47044100	3.57006200
H	-0.53224100	-0.72174100	0.93536400
C	-3.97805700	2.24756600	1.07141400
C	-4.98523600	2.62735400	1.96333800
C	-4.17468900	2.42187200	-0.30404200
C	-6.17162700	3.17965600	1.48994200
H	-4.84349000	2.47177700	3.02851600
C	-5.35948900	2.97909800	-0.77153400
H	-3.39764800	2.12189900	-1.00033900
C	-6.36036200	3.35814000	0.12264700
H	-6.94943100	3.46509300	2.19023400
H	-5.50022300	3.12150800	-1.83845800
H	-7.28454200	3.78981500	-0.24721500

Variable frequencies

-195.3512	10.7690	17.8980
21.9220	22.5672	27.0161
30.1713	30.4676	35.8856
43.2059	44.7226	47.0164
57.2016	60.2302	64.9586
73.9846	81.8470	86.4718
91.6953	93.8933	99.3814
104.7468	106.4288	127.3885
134.3714	139.6424	150.0976
162.2996	173.4224	187.7793
191.1392	199.9653	212.3103
216.6691	219.5937	232.8586
237.3281	249.8159	253.5065
258.4235	269.0834	271.3979
276.3497	281.9426	306.6368
313.7878	322.1669	339.4476
341.5981	344.9442	364.0376
377.7117	380.6845	395.9493
407.4874	414.6324	416.3727
418.5894	427.4170	431.7981
449.4931	457.5504	461.8734
462.8980	484.9947	493.5264
497.0943	513.1565	523.6433
524.6449	534.7026	540.4610
542.8696	552.9809	571.4032
583.3255	587.7636	593.4427
602.0558	607.0543	618.1897
625.9803	630.4761	636.3424
639.3511	643.3340	653.0111
663.1351	689.4300	692.4197
709.1295	716.7206	718.1443
722.9266	729.6297	734.1215
741.4776	756.7025	762.5281
766.5951	770.5099	780.1996
783.5672	792.3247	803.8462
808.1979	814.2839	829.9313
842.7194	845.4282	855.3386
857.6172	859.9250	873.2824
874.7300	878.7674	885.0394
887.8845	889.3780	900.3343
910.1434	921.0319	950.4801
966.9118	988.1956	989.4815
990.7185	994.4211	999.7172

1003.3466	1009.3879	1009.9257
1010.7445	1015.0076	1017.7208
1018.1313	1020.2500	1026.7792
1028.0437	1028.5854	1032.5883
1033.2861	1035.5648	1046.3463
1052.4270	1053.7407	1065.3798
1067.6600	1069.7901	1074.3451
1075.8272	1086.8676	1092.0789
1097.6141	1113.5070	1120.9840
1124.7000	1133.4082	1135.7203
1137.5436	1141.4008	1147.3815
1150.9370	1152.4023	1165.3907
1172.1493	1177.2634	1183.8117
1185.0367	1186.6014	1189.1310
1204.5939	1205.8131	1209.3464
1212.2998	1212.5473	1213.2472
1215.0677	1218.8838	1241.2922
1251.7955	1253.4972	1256.0495
1267.4321	1273.3105	1276.5513
1281.5148	1304.6247	1323.2215
1325.3665	1326.0983	1328.6782
1330.6104	1340.6861	1341.3742
1343.0404	1345.4749	1355.6323
1356.6531	1361.6268	1362.0346
1364.8635	1366.9529	1377.2094
1378.1086	1386.5064	1422.4986
1423.4972	1451.4960	1452.4185
1454.0153	1455.5848	1468.0881
1490.4880	1495.4301	1498.1346
1500.0068	1502.0691	1503.0968
1504.6194	1504.7487	1509.6933
1520.2100	1528.4144	1537.6362
1542.7928	1548.5767	1549.2348
1550.5062	1573.6835	1594.8704
1612.3499	1662.2292	1667.0302
1670.0283	1671.7585	1678.4493
1679.4689	1684.5364	1689.7137
1690.4720	1690.7359	1691.8288
1698.9469	1703.9169	3071.1535
3072.1184	3074.5878	3085.1786
3145.6829	3151.1836	3160.3365
3163.8048	3167.0749	3171.0769
3172.7113	3181.5685	3191.2074
3201.7317	3204.0795	3206.5879

3208.7419	3212.1353	3212.7623
3212.9576	3214.1476	3215.8515
3218.9863	3219.3459	3219.9547
3221.4209	3222.4514	3225.9070
3226.1570	3227.2293	3229.1870
3230.9801	3233.4236	3236.4285
3237.8629	3239.2100	3241.1523
3249.5153	3254.4946	3260.2539

²M5C₂

Zero-point correction=0.780199

Thermal correction to Energy=0.827878

Thermal correction to Enthalpy=0.828823

Thermal correction to Gibbs Free Energy=0.694327

Sum of electronic and zero-point Energies=-3207.933059

Sum of electronic and thermal Energies=-3207.885380

Sum of electronic and thermal Enthalpies=-3207.884435

Sum of electronic and thermal Free Energies=-3208.018931

Cartesian coordinate

N	-2.12158100	0.76350100	0.86709600
N	-3.04024800	-0.20851000	0.45624600
C	-3.40963400	-1.17979700	1.49435700
C	-0.78826600	0.29406500	1.26664800
C	-0.53464100	0.48322800	2.73263000
C	-1.18326900	1.45960400	3.38633600
C	-2.18561400	2.26322700	2.71396000
C	-2.69948100	1.86178700	1.52703100
C	0.26734400	0.97046700	0.31023000
C	1.54050200	0.22464400	0.38937600
C	2.09763600	-0.36573600	-0.77771000
O	1.69428400	-0.22560900	-1.93272900
S	-2.61088300	-0.90266800	-1.04021400
O	-2.14091200	0.18923900	-1.88116200
C	-4.17646000	-1.50437800	-1.59007200
O	-1.72114500	-2.05126100	-0.82340200
C	-4.30885900	-2.85032700	-1.91051400
C	-5.53803000	-3.30266000	-2.37979100
C	-6.61780900	-2.42877500	-2.52805300
C	-6.44912300	-1.07917200	-2.18988300
C	-5.23280700	-0.60362800	-1.72341800
C	-7.93794400	-2.91693500	-3.06085100
H	-3.81390300	-0.60929700	2.33276200

H	-4.18723200	-1.84014600	1.10567300
H	-2.55494900	-1.77915200	1.83165100
H	0.14667900	-0.19612500	3.23822700
H	-1.00105600	1.63415100	4.44255100
H	-2.55001500	3.17589000	3.16932200
H	-0.13164800	0.84072200	-0.70093500
H	-3.46582100	-3.52174400	-1.78842700
H	-5.66058200	-4.35150000	-2.63214500
H	-7.28600100	-0.39468900	-2.29207200
H	-5.10282500	0.44008700	-1.45001700
H	-8.03985000	-3.99726400	-2.94263700
H	-8.77205300	-2.43010500	-2.55051300
H	-8.02491400	-2.68676800	-4.12749500
C	0.45411300	2.45798000	0.55469200
C	1.19743500	2.95297600	1.62934900
C	-0.14732400	3.35597800	-0.32988700
C	1.31404300	4.32541500	1.83001600
H	1.67800500	2.26870300	2.32205700
C	-0.03282300	4.72894300	-0.12835300
H	-0.71475900	2.97000000	-1.17302900
C	0.69642300	5.21622800	0.95448900
H	1.88978800	4.69927100	2.67082200
H	-0.51438600	5.41656400	-0.81588500
H	0.78623100	6.28594500	1.11328300
H	2.05301100	0.08654500	1.33891000
C	5.86812500	1.78058300	-0.72112400
C	4.70452200	1.40786700	-1.40330500
C	3.58278300	2.23397400	-1.42679200
C	3.62262500	3.42732200	-0.70804800
C	4.77099900	3.78736500	-0.00138000
C	5.90621600	2.97657100	-0.01416500
C	6.96097600	0.75584400	-0.90958700
C	6.46472100	-0.01115700	-2.15516300
C	4.92109800	0.07299100	-2.07505300
H	2.69686600	1.96572000	-1.99367700
H	2.75105300	4.07551600	-0.69840700
H	4.78492000	4.72036400	0.55288400
H	6.80559200	3.27869100	0.51328700
H	7.03179700	0.10186100	-0.03118300
H	6.76571300	0.53229900	-3.05313700
H	7.94810300	1.19401400	-1.06848200
H	4.41764400	-0.06313400	-3.03319600
N	4.49494800	-1.05840600	-1.19517700
O	6.93772300	-1.32766500	-2.33937300

C	3.31204300	-1.23486900	-0.59546500
C	5.29106400	-2.09978700	-0.79920100
N	3.41430700	-2.35106300	0.11776400
N	4.64951500	-2.90296700	0.00718500
C	6.71264800	-2.20598300	-1.26402400
H	7.38629500	-2.01215400	-0.42004100
H	6.90136800	-3.21827900	-1.62572900
C	2.38743200	-2.95475600	0.91750300
C	2.73051400	-3.45859200	2.16732900
C	1.07984300	-2.98981800	0.43832800
C	1.73103800	-3.99017300	2.97183300
C	0.08095100	-3.51095000	1.25297200
C	0.41458100	-3.99775400	2.51348600
H	1.96682200	-4.38754800	3.95198000
H	-0.94052800	-3.53738400	0.88987400
H	0.81711800	-2.63486400	-0.55396900
H	3.76105100	-3.43030900	2.50281300
Cl	-0.83570700	-4.63323500	3.53662000
H	-0.75475300	-0.77428100	1.02643900
C	-3.83139800	2.53580000	0.85702200
C	-4.86198700	3.09720400	1.61677000
C	-3.86947700	2.64928700	-0.53829200
C	-5.90565500	3.77654100	0.99599500
H	-4.85311300	2.98156100	2.69634300
C	-4.91585700	3.32724400	-1.15547300
H	-3.07795000	2.19826500	-1.12958900
C	-5.93528300	3.89369900	-0.39119100
H	-6.70176700	4.20495300	1.59612700
H	-4.93360500	3.41623100	-2.23728500
H	-6.75096800	4.42003900	-0.87611700

Variable frequencies

11.8231	14.2277	20.4210
21.9191	28.7811	32.2979
33.1293	39.4545	43.4668
46.7277	48.7961	56.4391
61.7677	63.8090	69.5846
77.2726	85.4809	92.7691
96.9065	102.5348	106.7864
112.4030	127.9573	131.5260
135.5292	149.7271	160.7337
173.0911	188.5060	190.6741
203.1291	214.5769	215.5634
227.0297	236.8848	240.9623

243.8442	257.7133	259.0251
268.5924	275.5592	276.8434
281.5874	299.3067	313.0239
322.4240	339.0329	343.6117
347.2927	360.2088	384.9914
387.9379	397.9066	405.4882
414.4871	418.5070	423.1462
424.3202	430.6090	442.4866
461.5880	464.2280	465.1940
483.3001	491.4765	495.9213
509.6303	514.7631	527.3366
538.6696	543.6907	546.6661
552.7619	570.9063	583.3746
588.1643	594.3418	604.2175
606.2373	608.3227	627.0626
628.9631	635.9757	642.2502
649.9445	653.1725	669.1877
682.3170	691.2653	704.2955
716.5520	718.2175	721.7307
725.8417	728.6107	731.1961
757.5201	758.1385	762.9193
767.9520	773.4738	792.5584
796.1052	801.3833	810.5643
824.4574	829.4575	837.3178
839.8962	851.7904	856.9598
861.1416	866.9377	870.2179
872.4488	877.9320	880.7793
887.4199	891.4490	906.0305
929.7547	943.1089	944.0559
967.7220	988.0732	990.0234
992.2899	993.9273	995.0513
1003.5335	1008.8622	1011.3760
1012.0413	1013.0322	1014.5449
1017.9638	1021.7161	1022.5882
1024.4649	1031.9891	1032.3443
1034.7787	1037.4343	1040.3724
1054.4365	1057.9434	1064.5839
1066.4015	1066.5693	1070.2387
1075.1022	1077.9146	1095.6752
1112.5860	1117.7406	1119.4503
1134.8183	1135.2238	1136.7841
1143.0338	1147.4471	1148.7018
1162.1980	1173.9354	1176.1099
1177.6664	1180.5931	1181.7165

1189.2517	1196.2591	1201.6945
1202.2807	1204.4871	1206.0281
1209.2258	1214.4945	1216.6356
1219.3446	1231.0245	1244.6674
1249.3708	1253.0830	1254.1003
1264.2719	1270.2327	1277.2494
1302.3578	1305.2887	1312.9843
1318.0790	1326.8623	1332.9695
1336.5520	1340.4702	1343.1683
1346.1615	1348.7274	1355.7783
1359.5141	1360.0764	1361.4850
1364.5666	1372.5301	1373.5346
1382.4672	1402.5333	1420.2445
1424.4551	1442.1676	1452.4446
1454.4697	1455.0271	1462.7483
1468.2824	1495.6681	1497.2107
1498.5106	1499.0482	1501.1019
1503.4165	1506.0654	1506.1462
1516.8831	1519.6426	1536.9811
1542.0742	1546.8133	1548.7823
1552.7145	1556.5962	1610.2917
1630.3133	1656.5967	1660.9086
1670.3187	1675.4075	1676.6640
1677.1570	1681.5055	1686.0247
1689.3108	1692.6064	1693.1079
1702.1503	1733.2923	3061.8855
3075.8768	3075.9892	3089.9479
3114.4294	3124.4844	3149.6103
3151.5436	3153.0601	3162.8731
3165.9633	3170.6807	3177.1741
3181.9085	3189.7541	3195.6942
3200.2841	3202.5124	3205.6312
3207.4959	3210.3878	3210.7568
3211.0516	3212.8219	3214.1763
3216.9626	3218.7549	3220.4694
3221.4806	3222.6132	3225.8998
3229.8571	3230.5750	3233.9308
3236.4482	3239.5249	3243.2543
3243.2941	3244.3429	3250.4856

²M5^{C3}

Zero-point correction=0.778552

Thermal correction to Energy=0.826370

Thermal correction to Enthalpy=0.827314
 Thermal correction to Gibbs Free Energy=0.692287
 Sum of electronic and zero-point Energies=-3207.904828
 Sum of electronic and thermal Energies=-3207.857011
 Sum of electronic and thermal Enthalpies=-3207.856067
 Sum of electronic and thermal Free Energies=-3207.991094

Cartesian coordinate

N	-2.38145800	0.90217800	1.21737000
N	-3.21211800	-0.12427800	0.73464900
C	-3.46333400	-1.20388400	1.69152000
C	-1.13637800	0.60968100	1.57356600
C	-0.15459800	1.64435200	1.93002900
C	-0.81023700	2.96683100	2.11990600
C	-2.07654400	3.20874300	1.69357900
C	-2.90528300	2.17866500	1.18792700
C	0.98645700	1.67170500	0.76614400
C	1.78379400	0.41694000	0.77776900
C	2.00696400	-0.25293400	-0.40104900
O	1.61191900	-0.03108100	-1.57614800
S	-2.73694100	-0.59518100	-0.86842400
O	-2.20794100	0.62656400	-1.44082500
C	-4.30364400	-1.00006000	-1.55931100
O	-1.92940600	-1.80218800	-0.75603800
C	-4.63607200	-2.33690100	-1.75119600
C	-5.87844700	-2.63571000	-2.30037800
C	-6.77200600	-1.62132800	-2.65387800
C	-6.40042700	-0.28519100	-2.44601700
C	-5.16794200	0.04011700	-1.90274500
C	-8.10606800	-1.94519800	-3.26896300
H	-3.94821600	-0.77620900	2.57084300
H	-4.15511900	-1.90156900	1.21502200
H	-2.55692700	-1.73922200	1.99011800
H	0.40590100	1.34287600	2.82545000
H	-0.22371000	3.76240800	2.56527300
H	-2.51559400	4.19623200	1.77791700
H	0.45542700	1.72883800	-0.19197000
H	-3.93078600	-3.11842700	-1.48820900
H	-6.15446400	-3.67275500	-2.46281900
H	-7.08746000	0.51093400	-2.71853300
H	-4.87548600	1.07604400	-1.75350000
H	-8.12072500	-1.64795000	-4.32193400
H	-8.32132100	-3.01345300	-3.21559900
H	-8.91043800	-1.40340400	-2.76486300

C	1.76747000	2.95797000	0.96434700
C	2.74906500	3.06960800	1.95237100
C	1.45126900	4.08242200	0.19704600
C	3.39602900	4.28193600	2.17308100
H	3.02066900	2.19833100	2.54228900
C	2.09825400	5.29779800	0.41494200
H	0.69107000	4.00134300	-0.57613100
C	3.06944000	5.40137100	1.40794900
H	4.16037600	4.35403800	2.94033000
H	1.84483000	6.16097600	-0.19226600
H	3.57392300	6.34633600	1.58093800
H	2.27650900	0.08729800	1.68834400
C	6.32932500	0.77860200	-1.27110900
C	4.95784200	0.72934600	-1.53981400
C	4.14029300	1.83727400	-1.34135100
C	4.72223200	3.00097500	-0.84219200
C	6.08678500	3.05000500	-0.55590100
C	6.90410400	1.94182700	-0.77400200
C	6.99553200	-0.52899800	-1.61497900
C	5.96321800	-1.16885500	-2.56709000
C	4.58800000	-0.62155000	-2.10361800
H	3.08119900	1.78667500	-1.57827900
H	4.10561900	3.87815500	-0.67523800
H	6.51809000	3.96825300	-0.16922700
H	7.96958300	1.99009400	-0.57066100
H	7.14198700	-1.13191500	-0.71045400
H	6.12918500	-0.78391200	-3.57546300
H	7.97128700	-0.41483100	-2.09169300
H	3.82921400	-0.58593200	-2.88655600
N	4.06987500	-1.55814600	-1.07126400
O	6.00497800	-2.57428500	-2.69506200
C	2.97195500	-1.41720400	-0.30922100
C	4.61217300	-2.78192600	-0.77922900
N	2.89414300	-2.53981000	0.40416700
N	3.91488800	-3.40408900	0.12718500
C	5.83328700	-3.28073600	-1.48975700
H	6.70889700	-3.20167900	-0.83334100
H	5.69299900	-4.33249500	-1.74440200
C	1.80247900	-2.97361900	1.21926000
C	2.05699800	-3.49148800	2.48190500
C	0.52059600	-2.92853400	0.68164000
C	0.99308100	-3.96270800	3.24481900
C	-0.53751000	-3.41501200	1.43821100
C	-0.29230600	-3.91567500	2.71465000

H	1.15870800	-4.36826800	4.23596900
H	-1.53537500	-3.42811600	1.01637300
H	0.34459400	-2.53226800	-0.31419700
H	3.07315500	-3.52977200	2.85858100
Cl	-1.63306700	-4.49974400	3.66121000
H	-0.83639000	-0.43142000	1.47754300
C	-4.23985100	2.44055000	0.63039600
C	-5.39161800	1.75705900	1.04478100
C	-4.34886700	3.45064600	-0.33452700
C	-6.62507500	2.07268300	0.49183500
H	-5.32325400	0.99084600	1.80911800
C	-5.58614700	3.75312200	-0.89565100
H	-3.45577300	3.97238800	-0.66511100
C	-6.72458200	3.06481000	-0.48401600
H	-7.51225100	1.54312700	0.82215500
H	-5.65850200	4.52472200	-1.65441000
H	-7.69018400	3.30400900	-0.91743100

Variable frequencies

6.2305	9.9375	20.6253
23.7974	27.6166	31.2420
35.1068	45.0352	47.4379
53.8575	58.0262	61.8108
70.3145	72.8597	73.8444
76.6301	81.6945	85.3652
92.2040	96.8929	110.5168
115.8040	123.5007	125.8114
142.1097	148.5553	166.5018
169.8144	174.1803	182.5758
201.8880	213.0924	217.8526
225.9681	240.7125	245.7468
251.0246	256.2883	262.0165
268.0550	279.6565	285.4555
294.7342	306.6487	314.0955
325.1908	335.8081	344.3459
364.8316	366.7121	373.3753
375.4524	378.3773	406.5375
411.1912	413.2295	415.5903
417.9689	430.5209	438.4780
453.0079	460.5595	463.2951
468.2642	480.2127	488.7129
498.3828	502.8280	525.4880
535.4704	538.7996	543.3768
550.5647	572.1018	578.4615

580.0174	592.6339	593.9085
608.7564	620.5739	623.2680
627.1134	634.6482	641.2841
642.4891	651.8053	653.0392
662.2850	690.9549	695.8707
698.5078	712.9251	713.4176
717.3028	724.5073	728.8011
734.8041	738.3781	744.8194
761.5554	777.6321	781.9675
789.4116	797.4993	813.2747
814.6347	826.6322	831.6048
837.2097	846.0757	850.8889
854.1460	860.6855	864.1488
865.6995	874.2520	875.5418
880.9449	890.7789	901.6502
912.9492	923.3861	951.5577
956.8177	962.4777	986.3439
988.4205	991.1175	1000.9891
1003.7260	1004.9618	1006.9065
1009.0512	1009.5880	1014.0959
1014.4661	1017.4858	1026.9400
1029.3720	1029.9375	1032.9530
1033.9874	1036.0101	1046.2404
1052.3651	1065.7202	1068.9777
1071.7628	1072.8223	1076.5425
1083.6008	1093.8327	1100.0234
1105.8702	1118.0908	1124.1958
1126.3929	1128.7603	1133.4471
1137.6577	1143.7028	1149.0150
1156.2165	1165.3043	1172.4276
1176.4533	1178.5951	1182.7925
1183.5520	1183.8068	1194.9887
1197.5112	1202.8428	1203.5618
1212.0495	1212.6759	1215.1168
1224.9939	1232.4585	1238.6241
1241.8733	1251.7274	1254.5718
1263.6808	1269.2233	1272.0435
1275.7694	1294.7309	1302.5450
1317.8834	1324.2980	1324.6588
1328.3515	1334.9741	1343.7097
1345.4898	1352.2395	1352.5721
1358.7997	1359.1495	1362.5515
1363.4576	1370.5109	1374.9206
1384.1008	1390.5338	1418.3494

1418.8061	1427.0043	1456.7544
1456.8528	1460.5852	1464.8809
1480.0807	1492.4114	1494.0246
1495.4424	1498.9648	1499.7859
1504.5471	1504.7791	1510.0496
1516.3152	1518.1753	1521.6863
1536.3345	1540.2135	1543.8891
1547.2519	1548.4400	1554.6097
1587.0226	1638.8206	1664.6551
1668.6529	1671.4563	1673.4010
1681.5703	1685.4816	1688.7731
1689.1115	1690.2045	1691.4335
1701.1885	1709.1719	3054.7465
3069.7678	3078.3767	3081.4879
3085.8960	3100.3367	3143.8592
3154.9416	3155.1059	3164.3606
3166.8886	3174.3409	3174.5139
3185.8813	3190.3874	3200.9350
3202.7829	3204.1655	3210.6182
3211.1189	3213.2284	3215.9702
3216.7937	3220.0855	3220.1832
3220.3367	3222.3938	3225.6311
3229.7953	3230.0585	3230.8086
3232.6071	3233.6902	3237.3277
3237.6457	3238.5653	3241.5965
3241.6527	3251.8551	3253.5505

²M5C5

Zero-point correction=0.779468

Thermal correction to Energy=0.827113

Thermal correction to Enthalpy=0.828058

Thermal correction to Gibbs Free Energy=0.694615

Sum of electronic and zero-point Energies=-3207.904630

Sum of electronic and thermal Energies=-3207.856984

Sum of electronic and thermal Enthalpies=-3207.856040

Sum of electronic and thermal Free Energies=-3207.989483

Cartesian coordinate

N	1.86108100	1.06132500	-1.80705200
N	3.08074300	0.43774100	-2.09526700
C	3.59231300	0.62052300	-3.45886600
C	0.80607300	0.84701100	-2.64664300
C	-0.33664400	1.65498300	-2.54017900

C	-0.51859200	2.35993600	-1.39414700
C	0.38747900	2.09784700	-0.23391900
C	1.77400400	1.85362100	-0.70330500
C	-0.17690500	0.74750000	0.54066300
C	-1.64173600	0.54563800	0.37809500
C	-2.08850600	-0.27191100	-0.63118400
O	-1.47175200	-0.80956600	-1.59732300
S	3.18427900	-1.18782300	-1.50688100
O	2.22511500	-1.24805300	-0.41582200
C	4.82952500	-1.19230300	-0.87598100
O	3.09139400	-2.08758500	-2.64284700
C	5.81069400	-1.91136900	-1.54855600
C	7.10426200	-1.90204900	-1.03560000
C	7.41331400	-1.18863500	0.12499900
C	6.39678200	-0.47324200	0.77498000
C	5.09979100	-0.46972600	0.28706700
C	8.80735500	-1.20070900	0.69080900
H	3.52950600	1.68118800	-3.70706300
H	4.64281200	0.32061900	-3.44915500
H	3.06015000	0.02529200	-4.20523800
H	-1.05073100	1.65433300	-3.35394800
H	-1.36538600	3.02147000	-1.24868500
H	0.37285400	2.92713800	0.47352000
H	0.32027200	-0.07693100	0.02028400
H	5.55831900	-2.46942200	-2.44411300
H	7.88432400	-2.45995300	-1.54395400
H	6.62935900	0.08820100	1.67512500
H	4.31101000	0.07946100	0.79570600
H	8.85511500	-1.85554500	1.56647600
H	9.53093400	-1.56409600	-0.04066200
H	9.10870900	-0.20100600	1.01273300
C	0.27262000	0.79661500	1.97859400
C	-0.28592700	1.71977800	2.87046800
C	1.30873200	-0.02717900	2.42413300
C	0.19554500	1.83102800	4.17109100
H	-1.09230500	2.37063300	2.53867900
C	1.78705000	0.07744900	3.72913200
H	1.75463900	-0.73383100	1.73185800
C	1.23887100	1.01166900	4.60292100
H	-0.24113400	2.55702900	4.84947500
H	2.59552800	-0.56743400	4.05935900
H	1.61646200	1.10041500	5.61632100
H	-2.33452600	0.92010500	1.12421800
C	-2.54342200	-4.25915100	1.32846300

C	-2.04005400	-3.39743500	0.34863600
C	-0.73082100	-2.92628400	0.40842100
C	0.05917800	-3.31198800	1.48963800
C	-0.44987700	-4.14584300	2.48599700
C	-1.75353000	-4.63254900	2.40922600
C	-3.94161700	-4.70734200	0.98963200
C	-3.99200200	-4.43508500	-0.52874200
C	-3.06679100	-3.20978000	-0.74778900
H	-0.33979400	-2.28891900	-0.37858300
H	1.08852900	-2.97302100	1.54044100
H	0.18218000	-4.43704400	3.31891100
H	-2.13760000	-5.30773900	3.16780100
H	-4.67977900	-4.10778600	1.53614300
H	-3.52889300	-5.27484000	-1.05138800
H	-4.13601000	-5.75640700	1.22169500
H	-2.63905900	-3.14044100	-1.74773200
N	-3.91458500	-1.99650500	-0.57289200
O	-5.27093000	-4.29485100	-1.10947400
C	-3.52275800	-0.71076600	-0.50802200
C	-5.28081600	-2.00675700	-0.46335100
N	-4.64579600	-0.00670400	-0.36164800
N	-5.75446500	-0.80241400	-0.32534100
C	-6.06316700	-3.28256100	-0.53799700
H	-6.43043400	-3.55619600	0.45899600
H	-6.92629100	-3.13550200	-1.18943800
C	-4.79479800	1.41479900	-0.32306400
C	-5.59698600	1.97591600	0.66132400
C	-4.16607500	2.19240400	-1.29020300
C	-5.76649100	3.35582900	0.69009300
C	-4.33124700	3.57082600	-1.25773500
C	-5.12716200	4.13923800	-0.26492300
H	-6.38794500	3.81994800	1.44675400
H	-3.86501900	4.20234100	-2.00563800
H	-3.56820600	1.71908900	-2.06306500
H	-6.08532200	1.33836800	1.38973400
Cl	-5.33530800	5.86493200	-0.22976100
H	0.94811100	0.09194600	-3.40703500
C	2.96106800	2.37132600	-0.02667900
C	4.16228900	2.64822000	-0.71215400
C	2.90026300	2.65750200	1.35021600
C	5.26818500	3.13320600	-0.03396700
H	4.22668200	2.50796900	-1.78249600
C	4.02186100	3.12118400	2.02754600
H	1.98773700	2.49217600	1.90841400

C	5.21162000	3.34992400	1.34351400
H	6.17925400	3.34560700	-0.58252000
H	3.95547300	3.30680400	3.09403400
H	6.08507200	3.71578700	1.87328300

Variable frequencies

11.0638	15.6610	18.6818
25.2310	28.9041	29.7483
30.7217	45.6622	47.7807
50.5617	56.6260	59.8608
65.9693	72.7678	78.5940
83.7096	86.7565	91.8208
100.6773	110.0673	112.2429
124.0674	138.5830	144.7631
148.6740	153.3658	173.8856
178.6697	183.7001	193.2923
202.9468	210.5129	215.7266
227.4417	236.4054	239.9620
252.6215	254.9877	260.0189
265.1281	279.8944	284.3892
292.2577	304.1265	309.5509
320.5189	323.1080	342.1539
350.8514	359.0076	371.8830
378.6280	384.7983	403.3482
418.0300	421.1934	424.8918
426.8525	432.5433	436.0021
447.2498	460.1108	465.9120
470.0911	485.0295	491.8661
497.6527	509.3541	524.0771
529.3274	535.5807	540.8365
554.8406	563.8785	571.8795
578.5179	591.6636	598.1245
607.2238	610.0331	626.6238
628.2055	633.5067	637.3788
642.9730	646.9752	653.8098
671.7276	686.2252	691.6378
704.1523	710.6419	712.8273
715.9140	724.4187	727.7753
730.0958	732.8185	747.7333
759.0196	767.9531	775.4700
787.5903	792.9357	800.9189
804.5670	815.4329	830.0353
835.5160	848.5362	849.3569
850.9650	857.3739	863.5074

872.6682	875.2979	881.9669
887.1469	890.4497	903.8200
916.2120	924.1960	946.3983
959.5828	966.5596	979.7307
992.9882	993.9295	995.8170
1003.2003	1008.3454	1010.6478
1012.6243	1015.4531	1016.6264
1019.0115	1021.4030	1028.3661
1028.7949	1031.3591	1034.1699
1035.3565	1041.5517	1044.3727
1051.9824	1067.3404	1070.1311
1070.6060	1074.8993	1078.6338
1083.4548	1097.1494	1106.4756
1112.0397	1120.3397	1128.4743
1129.9548	1132.8240	1135.9318
1137.8520	1144.1515	1150.9532
1155.0635	1167.0850	1172.9772
1183.2224	1183.6433	1185.5603
1188.2073	1190.4210	1192.6360
1198.4071	1204.1235	1205.7037
1211.4813	1212.4746	1218.7295
1225.4882	1227.3838	1236.3644
1241.7443	1247.1909	1257.2158
1262.9986	1265.5029	1274.3830
1295.2169	1300.5581	1302.8706
1308.4828	1320.5454	1325.9938
1336.9196	1340.5602	1344.3800
1345.6262	1348.2370	1354.7332
1359.9576	1361.3802	1365.2844
1371.3744	1373.0286	1375.3751
1383.1672	1388.2589	1418.4868
1418.9974	1424.8785	1448.2699
1454.9169	1458.6156	1459.6268
1463.9753	1491.1125	1491.4236
1496.8301	1497.3609	1498.6575
1503.5661	1504.1022	1510.9722
1516.2191	1518.3057	1523.2083
1535.6229	1539.8223	1544.9845
1548.0292	1551.3420	1553.0367
1589.1923	1600.2092	1659.1014
1669.1620	1669.3802	1675.6129
1680.7543	1683.9601	1685.0073
1688.5024	1691.0798	1692.9777
1696.4410	1703.0529	3072.1834

3077.8198	3083.5202	3085.2488
3139.6710	3145.4298	3148.2972
3149.1470	3155.8656	3168.8436
3172.1217	3177.8211	3181.5529
3182.1806	3189.6556	3204.1297
3209.6799	3214.1546	3214.8176
3217.2425	3218.9293	3218.9840
3223.0593	3225.9058	3226.1755
3226.5739	3227.5971	3228.0954
3231.2204	3232.7694	3232.9701
3233.7641	3233.8236	3242.9415
3244.4910	3245.0348	3247.5516
3257.8204	3271.1938	3300.6531

M3-wb97xd

Zero-point correction=0.930837

Thermal correction to Energy=0.988384

Thermal correction to Enthalpy=0.989328

Thermal correction to Gibbs Free Energy=0.834357

Sum of electronic and zero-point Energies=-3555.172975

Sum of electronic and thermal Energies=-3555.115428

Sum of electronic and thermal Enthalpies=-3555.114484

Sum of electronic and thermal Free Energies=-3555.269456

Cartesian coordinate

C	4.78096000	-0.56028200	-0.34788800
C	3.63260600	-0.07004200	-0.84179300
C	2.83862900	0.93574500	-0.15755700
O	3.30834900	1.50139600	0.99229400
H	5.11901800	-0.22480800	0.62865900
C	5.60652600	-1.59796800	-0.97501900
C	6.49228700	-2.31839900	-0.15911400
C	5.54098700	-1.92156100	-2.33763400

C	7.26785600	-3.34519800	-0.68587400
H	6.53903100	-2.06794000	0.89831900
C	6.32017400	-2.94560000	-2.86221300
H	4.88717700	-1.35616500	-2.99546300
C	7.18428900	-3.66532100	-2.03895700
H	7.93951900	-3.89865400	-0.03638800
H	6.25737600	-3.17904600	-3.92101300
H	7.79242500	-4.46448800	-2.45153600
H	3.25567400	-0.41872400	-1.79979000
C	1.92822300	5.96164300	-0.09247500
C	2.36884500	4.64841300	-0.23155300
C	3.51648100	4.34528700	-0.95687400
C	4.20943700	5.38805300	-1.56601200
C	3.76538000	6.70549300	-1.43925700
C	2.62474700	7.00265500	-0.69733500
C	0.69336200	6.03364600	0.76976600
C	0.23006100	4.56928100	0.93040300
C	1.45578200	3.68728700	0.49866100
H	3.86405200	3.32101500	-1.04104000
H	5.10664900	5.17465500	-2.13773100
H	4.31677300	7.50717500	-1.92045100
H	2.28560700	8.02931000	-0.59453400
H	-0.11026400	6.63800900	0.33786900
H	-0.06161900	4.35133500	1.95905400
H	0.92663200	6.46549700	1.74882600
H	1.97019600	3.26040600	1.36010500
N	0.98839700	2.57581900	-0.31773700
O	-0.94954900	4.29009000	0.17334100
C	1.67182300	1.39837600	-0.67626100
C	0.08269300	2.81550900	-1.31321700

N	0.93064000	0.91256500	-1.78219200
N	-0.02741900	1.87666400	-2.18343100
C	-0.70316600	4.07987100	-1.20680900
H	-0.15696200	4.92155900	-1.65281200
H	-1.66437300	3.98477900	-1.71241700
C	0.54471300	-0.42510800	-1.99042400
C	-0.21911900	-0.73785300	-3.12461000
C	0.90972300	-1.45520000	-1.11599900
C	-0.58778300	-2.05063900	-3.38628100
C	0.53520100	-2.76733500	-1.37621500
C	-0.20649000	-3.06250100	-2.51183100
H	-1.16526300	-2.28510900	-4.27360900
H	0.82992400	-3.55355700	-0.68978200
H	1.50327000	-1.24091100	-0.23693000
H	-0.50971400	0.05389700	-3.80358600
Cl	-0.67680400	-4.71686600	-2.84071200
S	-4.44478200	0.91166700	1.53964400
O	-4.49544200	2.35268500	1.73079800
O	-4.17003900	0.02293200	2.65369500
N	-3.21439600	0.53459600	0.37946300
N	-1.99994300	0.22507100	1.00453300
C	-6.75194100	1.33894400	0.14556900
H	-6.57754200	2.39263000	0.33170700
C	-7.85830400	0.90885600	-0.57821300
H	-8.56006900	1.64272300	-0.96167100
C	-5.86393700	0.38674800	0.63294100
C	-6.05737700	-0.97732600	0.41709500
H	-5.35566600	-1.70561000	0.80808400
C	-8.07930700	-0.44952000	-0.81712800
C	-7.16372100	-1.38185100	-0.31102900

H	-7.32038700	-2.44106100	-0.49071100
C	-1.20192700	1.22507900	1.45901900
H	-1.52508700	2.23747800	1.24263300
C	-1.71275000	-1.09459800	1.19527700
C	-0.54890300	-1.40714000	1.87756700
H	-0.30088600	-2.45406400	2.00336600
C	-0.03354000	0.92243500	2.10948800
H	0.62503600	1.71810900	2.42971300
C	0.31303000	-0.41114800	2.31831100
H	1.29862300	-0.64388600	2.73722700
C	-3.11752100	1.43964700	-0.76692600
H	-2.31326800	1.09094700	-1.41781500
H	-4.06455800	1.37883500	-1.30546700
H	-2.93519400	2.47856300	-0.47383100
C	-2.60867800	-2.13553500	0.65327700
C	-2.87977400	-2.20194300	-0.71526200
C	-3.13567300	-3.09257700	1.52151400
C	-3.68167800	-3.22066700	-1.21004200
H	-2.44187800	-1.47499100	-1.39099000
C	-3.95110500	-4.10378300	1.02091100
H	-2.93083800	-3.02724700	2.58490900
C	-4.22265200	-4.16851800	-0.34271600
H	-3.87244600	-3.28290300	-2.27567900
H	-4.36863600	-4.84085700	1.69803200
H	-4.84948400	-4.96365000	-0.73259900
C	4.13541900	-1.33065300	2.76181800
O	5.33885100	-1.04334800	2.74285400
O	3.17256600	-0.49777900	2.60234400
H	3.37675700	0.76683300	1.69018000
C	3.69960900	-2.81081200	2.94534000

C	2.94797000	-3.24039300	1.67413700
H	2.63730600	-4.28980900	1.74519600
H	2.05741200	-2.62248900	1.52770500
H	3.58033300	-3.12878900	0.78686300
C	4.91855500	-3.71311400	3.14629700
H	5.51299800	-3.38027700	4.00072500
H	4.60195200	-4.74847900	3.32082600
H	5.56655200	-3.69699600	2.26646800
C	2.76941300	-2.92985600	4.16169800
H	2.44513200	-3.96878800	4.29512500
H	3.27998900	-2.61723200	5.07851100
H	1.87745500	-2.30747300	4.04846500
C	-9.28610100	-0.91464800	-1.58681900
H	-9.01316500	-1.67590400	-2.32240600
H	-10.02041700	-1.36193800	-0.90901900
H	-9.77181600	-0.08793100	-2.10906900

Variable frequencies

9.4849	15.6815	19.7964
22.0471	26.5994	27.5012
32.2716	33.3601	34.9283
38.7309	42.8778	49.8386
56.4409	63.4276	67.2325
68.9970	70.5128	73.0218
76.1968	84.9913	86.4184
89.3090	91.2922	93.7535
98.2563	103.5730	113.5381
117.2910	126.1385	127.5920
138.2668	148.3758	149.5458
155.4193	169.2637	179.6436

188.5484	191.0200	198.0009
203.1764	213.7148	225.5312
234.9240	242.5909	243.8707
255.6912	261.0229	273.3729
273.9643	278.0163	280.0303
290.3364	291.8855	295.4550
298.5878	306.9193	312.8744
317.9757	328.9914	334.9830
345.4089	354.4643	363.0522
366.7259	373.2254	386.5383
391.1953	392.9767	401.2841
416.1681	418.8616	426.1217
428.1359	429.3962	433.9944
436.0305	449.9770	458.8456
468.7637	488.1704	493.2256
500.4015	506.5063	509.5988
523.3394	526.8661	532.3015
546.4885	548.7054	563.3721
565.0749	571.5428	585.9922
589.9075	590.4085	598.1992
604.7285	610.5500	634.9992
635.2628	637.2317	646.1929
650.1481	651.6712	668.4223
670.6823	685.3283	704.5248
722.8398	724.0937	725.6694
727.2846	728.5388	729.7280
754.7153	755.8865	763.1735
774.6005	776.0389	782.7140
792.4159	802.6740	803.8445
816.1232	826.8730	834.7222

840.2362	849.2773	856.3038
857.4633	860.2216	865.0361
878.6451	881.0541	883.7728
891.3357	893.0717	896.5107
898.3356	905.5266	915.4224
938.1858	952.3736	955.5851
957.5591	958.2559	968.5333
970.9574	974.7131	983.8705
987.2136	994.8180	1003.5739
1007.1076	1011.7165	1016.9177
1017.4507	1021.1081	1022.8715
1024.9882	1026.3744	1028.0453
1031.2212	1033.6580	1038.0998
1045.9790	1048.3703	1050.5449
1051.5328	1054.7009	1057.6150
1057.7542	1064.9377	1071.2178
1072.0775	1076.0720	1077.5938
1081.2398	1093.0142	1105.9705
1122.6490	1123.1747	1124.0047
1125.1673	1128.6847	1133.7020
1141.9530	1152.7987	1160.8982
1170.2695	1172.0108	1181.3745
1184.0730	1191.8568	1192.3755
1193.1172	1198.1134	1209.0850
1218.9095	1222.2189	1226.1549
1226.8026	1228.7011	1239.1450
1246.7728	1249.1435	1251.2405
1255.7011	1259.1803	1261.1200
1269.3770	1273.5099	1288.2733
1292.8941	1302.3623	1317.1187

1328.7273	1330.4630	1330.7232
1334.2711	1338.6456	1342.9648
1346.3258	1351.1208	1356.2476
1360.5058	1360.9683	1362.0700
1368.2758	1374.8511	1376.1933
1376.6231	1383.9727	1388.9506
1391.8283	1397.2092	1400.6154
1408.4633	1414.6175	1417.9119
1433.4013	1433.7332	1449.3209
1464.4496	1468.9454	1474.9690
1484.1800	1487.7100	1488.3165
1490.0642	1494.5940	1501.9075
1503.5965	1504.7946	1506.2906
1507.5579	1510.2296	1512.2151
1515.7656	1518.0682	1520.3794
1525.1645	1534.0718	1536.1772
1544.7695	1547.9108	1553.9732
1556.7839	1561.4564	1585.1427
1651.3455	1651.9669	1660.6598
1662.3518	1669.4011	1677.6799
1681.7836	1689.5735	1690.2433
1690.5202	1695.0897	1700.3702
1728.2901	1732.0967	1737.9335
1760.8471	2847.9103	3051.7187
3054.3205	3059.7642	3061.4229
3071.0371	3072.3105	3079.7788
3085.0172	3129.5332	3130.9115
3131.8785	3139.4122	3140.1152
3146.7939	3153.0448	3159.6950
3160.5752	3164.9299	3166.9187

3169.6289	3171.6386	3194.5395
3201.6955	3204.1688	3207.8922
3210.1396	3217.9003	3218.8433
3223.1621	3223.8640	3224.2596
3224.6028	3225.2419	3230.7760
3233.6214	3233.6864	3237.9710
3238.0559	3244.0777	3245.0531
3252.5248	3252.7584	3254.2522
3254.5616	3255.1338	3264.4431
3265.1114	3269.6864	3289.3373

osTS3-wb97xd

Zero-point correction=0.925974

Thermal correction to Energy=0.983477

Thermal correction to Enthalpy=0.984421

Thermal correction to Gibbs Free Energy=0.829112

Sum of electronic and zero-point Energies=-3555.168252

Sum of electronic and thermal Energies=-3555.110749

Sum of electronic and thermal Enthalpies=-3555.109805

Sum of electronic and thermal Free Energies=-3555.265113

Cartesian coordinate

C	4.68001300	-0.46276100	-0.31529100
C	3.42112700	-0.22965300	-0.72643900
C	2.59579500	0.81253900	-0.11859400
O	3.08490500	1.56384100	0.83427800
H	5.06587200	0.13315100	0.50626400
C	5.58245700	-1.49492200	-0.83252100
C	6.68753300	-1.86323600	-0.04917600

C	5.38533000	-2.15226600	-2.05612000
C	7.55566200	-2.86554200	-0.46779300
H	6.84130700	-1.36089800	0.90263300
C	6.25615000	-3.15015300	-2.47443200
H	4.55110600	-1.87191400	-2.69262200
C	7.34425700	-3.51350000	-1.68214000
H	8.40076400	-3.14042700	0.15618500
H	6.08969700	-3.64391400	-3.42708300
H	8.02473600	-4.29196000	-2.01269100
H	3.00950800	-0.79237900	-1.55707300
C	1.78428900	5.66474800	-0.98056500
C	2.16695900	4.33151800	-0.86164100
C	3.28876400	3.84319000	-1.52422800
C	4.00475300	4.71090400	-2.34418500
C	3.61333200	6.04366600	-2.48250000
C	2.50535800	6.53236200	-1.79464100
C	0.58986700	5.96734700	-0.11219800
C	0.07459400	4.58855000	0.35845300
C	1.24246900	3.57875300	0.07136800
H	3.60735600	2.81624400	-1.38690000
H	4.88155900	4.34930700	-2.87146100
H	4.18473000	6.70722400	-3.12402000
H	2.21218300	7.57361500	-1.89261000
H	-0.20749800	6.50925400	-0.63021900
H	-0.17207500	4.59291100	1.42144000
H	0.88366500	6.57624500	0.74974600
H	1.77633500	3.29762400	0.97867600
N	0.70201300	2.34677900	-0.49463300
O	-1.15297100	4.23443900	-0.27866300
C	1.34416700	1.10622400	-0.65161700

C	-0.25856200	2.42299900	-1.45693000
N	0.53130100	0.45474400	-1.60738400
N	-0.43381300	1.33199300	-2.11875600
C	-0.98395200	3.71996100	-1.58501100
H	-0.41573800	4.41164800	-2.22228500
H	-1.96975100	3.58078500	-2.02857600
C	0.37570100	-0.90038200	-1.92024200
C	-0.34155400	-1.24817400	-3.07396400
C	0.88067200	-1.92406600	-1.10772100
C	-0.58933600	-2.57925100	-3.37684300
C	0.62088800	-3.25315000	-1.40456700
C	-0.12218600	-3.57788100	-2.53304300
H	-1.15233800	-2.83600800	-4.26708100
H	0.99831800	-4.03332300	-0.75333500
H	1.46140500	-1.68036800	-0.22916600
H	-0.72196100	-0.46644900	-3.71810000
Cl	-0.46731300	-5.25721300	-2.89488500
S	-4.57916400	0.87826800	1.87687100
O	-4.89228100	2.25822500	2.22060600
O	-4.02228600	-0.02839000	2.86457600
N	-3.44692500	0.85432800	0.57986700
N	-2.13900000	0.62457400	0.99528200
C	-7.07690500	0.93797100	0.76380900
H	-7.08329300	1.99002400	1.02623700
C	-8.15931000	0.34986000	0.11774000
H	-9.02490800	0.95656400	-0.12929300
C	-5.97601500	0.14866700	1.07512700
C	-5.93627800	-1.20902400	0.75913900
H	-5.07028700	-1.81089800	1.01131600
C	-8.14866300	-1.00580800	-0.21683900

C	-7.02341900	-1.77282400	0.11290800
H	-6.99681700	-2.82790700	-0.14220400
C	-1.44090700	1.62169300	1.62009200
H	-1.92717400	2.58767300	1.64352300
C	-1.66383600	-0.67227400	0.94295000
C	-0.44017600	-0.92649000	1.51816200
H	-0.06640400	-1.94049200	1.47280000
C	-0.20665400	1.37989700	2.15026300
H	0.33820500	2.19011700	2.61627900
C	0.34574000	0.09282400	2.05633800
H	1.33118100	-0.11706400	2.45758500
C	-3.61894400	1.86897800	-0.45595100
H	-2.97167000	1.59414500	-1.29016900
H	-4.65806200	1.83254500	-0.78747000
H	-3.38001000	2.88088600	-0.11277900
C	-2.44065400	-1.72711800	0.26938000
C	-2.93616200	-1.55412300	-1.02584000
C	-2.62719600	-2.95121300	0.91926300
C	-3.61561300	-2.58757400	-1.65552300
H	-2.75335400	-0.62621800	-1.55490300
C	-3.31072900	-3.98328400	0.28541000
H	-2.25481800	-3.08359800	1.93002400
C	-3.80832700	-3.80215100	-1.00230100
H	-3.98417300	-2.44796900	-2.66613300
H	-3.45392300	-4.92836300	0.79799400
H	-4.33379600	-4.61036400	-1.50010000
C	4.52845400	-0.55774400	2.99493300
O	5.61302000	-0.05884000	2.74621000
O	3.37278700	0.01122900	2.71490000
H	3.40494500	0.75621800	1.96507200

C	4.36326900	-1.95006800	3.61401800
C	3.80006000	-2.86454300	2.50847400
H	3.66339400	-3.87908300	2.89763300
H	2.83490900	-2.49282700	2.15184500
H	4.48258000	-2.91271400	1.65369300
C	5.72202900	-2.47453800	4.08090600
H	6.15946800	-1.81483500	4.83521200
H	5.60738000	-3.47209300	4.51773200
H	6.42419900	-2.53852600	3.24622200
C	3.37996100	-1.89179600	4.79232700
H	3.25587700	-2.89040600	5.22458800
H	3.74719700	-1.22624500	5.58009600
H	2.40005900	-1.53008700	4.47134600
C	-9.32435500	-1.64662500	-0.90450600
H	-8.99993500	-2.24074800	-1.76346800
H	-9.84792400	-2.32143000	-0.21977900
H	-10.04099900	-0.90039000	-1.25360700

Variable frequencies

-1702.2961	12.5609	16.2134
21.2913	22.9310	23.5599
27.2246	29.5529	30.0602
33.5246	42.8550	43.5557
46.6314	48.2050	48.5387
50.6148	61.0066	66.1397
70.2077	71.7264	78.0958
83.4369	85.3651	92.1613
96.0900	105.4305	111.3308
116.1653	123.7076	127.4356
129.4984	142.4376	149.4405

156.0591	160.6388	172.1504
181.7853	187.8554	195.5103
211.9929	216.7801	224.7746
225.5505	233.1749	242.1505
256.3845	260.7377	261.6530
271.6221	272.1046	279.3011
281.3835	283.1846	297.8141
299.9113	302.7155	306.0505
313.6816	320.7956	327.5779
339.4884	347.2105	353.9190
360.6665	366.2624	374.7330
386.0776	387.0778	388.8972
400.9305	420.1798	421.0683
424.7775	425.9758	438.5198
444.9354	446.9745	450.3526
464.6695	469.4522	487.6925
496.3485	502.8473	505.6337
510.1329	519.3304	523.9883
532.4481	540.7401	552.9682
562.8878	567.3454	571.1791
580.0231	588.6147	590.8266
601.4094	606.7235	612.6116
633.8749	636.8328	638.1497
647.8978	648.2899	650.2664
665.0231	674.0403	693.6880
707.1007	720.8483	721.1965
723.4847	726.2520	729.0960
729.6895	732.0411	756.5139
770.9567	777.6272	780.6822
786.8370	788.9023	790.1003

793.7534	803.3127	815.9689
831.2737	841.4675	843.8585
844.7226	857.0227	862.0360
871.3649	875.5885	877.4960
880.3778	880.8373	891.6040
895.3101	898.9011	905.6077
914.8375	918.1081	954.5922
955.2450	956.0898	958.9559
965.6165	973.4179	975.7347
979.4037	985.6293	995.3847
1000.4995	1009.5825	1010.1391
1012.0078	1020.5166	1020.7987
1022.2074	1022.8971	1025.4554
1025.5736	1025.7698	1027.8818
1028.2338	1035.3441	1042.6381
1052.1754	1053.7144	1055.8279
1058.0224	1058.8276	1064.3134
1071.7033	1072.0261	1073.8838
1081.8464	1086.5500	1095.2839
1110.3999	1122.9806	1124.6117
1125.1764	1128.6965	1135.1340
1146.0247	1157.3970	1159.7908
1159.9398	1173.8777	1184.9343
1185.0643	1194.1662	1194.3979
1194.9804	1199.2134	1203.7451
1207.8104	1218.5903	1225.0568
1225.7621	1226.8134	1228.2690
1230.6419	1236.4544	1241.4818
1252.9665	1253.9783	1255.5346
1256.8428	1262.6297	1276.0294

1290.7881	1295.1676	1305.0452
1317.3936	1323.7221	1328.3147
1332.5995	1336.1061	1338.8193
1342.5810	1347.0809	1348.1081
1358.4217	1361.6276	1362.9919
1367.8833	1372.3088	1374.3056
1379.6044	1382.9104	1384.4822
1393.5911	1394.3764	1395.4939
1406.2920	1410.9332	1423.9148
1424.6766	1434.1520	1445.5225
1457.1147	1459.9645	1463.9195
1476.3707	1484.1484	1490.6768
1491.4151	1495.2175	1499.2112
1500.8056	1501.4650	1504.0052
1507.0469	1509.0213	1511.1603
1516.3957	1517.6451	1517.8378
1520.4051	1520.9574	1537.5787
1542.6309	1545.7306	1550.0380
1555.1240	1558.9606	1566.6298
1583.1839	1587.3418	1651.0661
1660.8910	1661.3897	1666.1630
1676.2465	1681.5655	1687.2450
1688.5617	1694.1146	1694.9812
1698.7811	1712.6535	1732.4588
1790.5310	2146.7645	3053.5778
3057.6442	3059.9796	3066.7955
3071.1916	3072.4226	3076.2582
3124.3551	3135.8879	3137.4590
3142.1425	3145.1730	3146.9994
3150.6720	3160.5923	3165.9540

3167.3938	3168.1805	3169.9005
3170.5589	3190.7045	3201.6974
3206.6664	3212.6137	3215.6409
3215.9069	3216.5962	3217.7882
3221.8467	3226.2218	3227.4995
3228.5514	3234.4256	3235.0609
3236.2656	3238.3136	3239.7164
3244.8252	3245.2091	3245.6704
3245.9298	3247.0792	3258.7974
3267.2957	3269.6729	3275.0423
3275.9682	3280.8557	3293.6972

Part 15: References

1. C. Y. Legault, CYLview, 1.0b, Université de Sherbrooke, 2009, <http://www.cylview.org>.
2. Chemcraft—graphical software for visualization of quantum chemistry computations, <https://www.chemcraftprog.com>.
3. A. V. Marenich, C. J. Cramer, D. G. Truhlar, Universal solvation model based on solute electron density and on a continuum model of the solvent defined by the bulk dielectric constant and atomic surface tensions. *J. Phy. Chem. B*, 2009, **113**, 6378 – 6396.
4. J.-D. Chai, M. Head-Gordon, Long-range corrected hybrid density functionals with damped atom–atom dispersion corrections. *Phys. Chem. Chem. Phys.*, 2008, **10**, 6615–6620.
5. Liptak, M. D.; Shields, G. C. Accurate PKa Calculations for Carboxylic Acids Using Complete Basis Set and Gaussian-n Models Combined with CPCM Continuum Solvation Methods. *J. Am. Chem. Soc.*, 2001, **123**, 7314–7319.
6. L. R. Domingo, M. Ríos-Gutiérrez, P. Pérez, Applications of the Conceptual Density Functional Theory Indices to Organic Chemistry Reactivity. *Molecules.*, 2016, **21**, 748.
7. L. R. Domingo, E. Chamorro, P. Pérez, Understanding the Reactivity of Captodative Ethylenes in Polar Cycloaddition Reactions. A Theoretical Study. *J. Org. Chem.*, 2008, **73**, 4615 – 4624.
8. T. Lu and Q. Chen, Interaction Region Indicator: A Simple Real Space Function Clearly Revealing Both Chemical Bonds and Weak Interactions**, *Chem. Meth.*, 2021, **1**, 231–239.

9. E. R. Johnson, S. Keinan, P. Mori-Sánchez, J. Contreras-García, A. J. Cohen and W. Yang, Revealing Noncovalent Interactions, *J. Am. Chem. Soc.*, 2010, **132**, 6498-6506.
10. J. Contreras-García, E. R. Johnson, S. Keinan, R. Chaudret, J.-P. Piquemal, D. N. Beratan and W. Yang, NCIPLOT: A Program for Plotting Noncovalent Interaction Regions, *J. Chem. Theory Comput.*, 2011, **7**, 625-632.
11. Q. Shi, W. Zhang, Y. Wang, L. Qu and D. Wei, Insights into the isothioureacatalyzed asymmetric [4 + 2] annulation of phenylacetic acid with alkylidene pyrazolone, *Org. Biomol. Chem.*, 2018, **16**, 2301-2311.
12. Y. Wang, Y. Wang, X. Wang, X. Li, L.-B. Qu and D. Wei, Competing mechanisms and origins of chemo- and stereo-selectivities of NHC-catalyzed reactions of enals with 2-aminoacrylates, *Catal. Sci. Technol.*, 2018, **8**, 4229-4240.