Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

A DFT study on mechanism and regioselectivity of NHC-catalyzed double acylation of aromatic 1,2-diketones with α,β-unsaturated ketones

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Content

Computational Details:

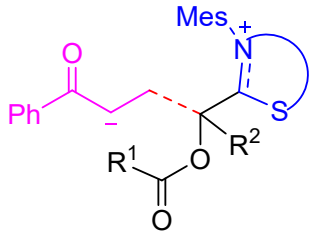
Table S1. Different computational levels.

	Optimization			Single Point Energy		
	Functional	**Basis Set**	**Solvation Model**	**Functional**	**Basis Set**	**Solvation Model**
L1	M06-2X-D3	6-31G(d,p)	SMD	M06-2X-D3	6-311++G(2df,2pd)	SMD
L2	B3LYP-D3	6-31G(d,p)	SMD	B3LYP-D3	6-311++G(2df,2pd)	SMD
L3	ωB97X-D	6-31G(d,p)	SMD	ωB97X-D	6-311++G(2df,2pd)	SMD

Table S2. Comparison of relative Gibbs free energies ($\Delta\Delta G^{\neq}$) of the transition states **TS1** calculated by the different methods (in kcal/mol).

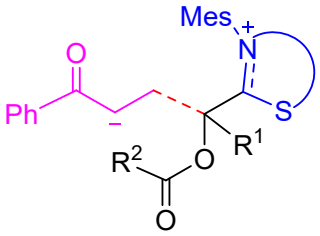
	L1	**L2**	**L3**
TS1	0.0	1.3	3.8

Table S3. The key transition states of other two case of the reaction (in kcal/mol).



TS3^{a} : R^1 = Ph R^2 = Me

TS3$^{a\prime}$: R^1 = Ph R^2 = *p*-ClC_6H_4



TS3^{b} : R^1 = Ph R^2 = Me

TS3$^{b\prime}$: R^1 = Ph R^2 = *p*-ClC_6H_4

	R^1 = Ph, R^2 = Me	R^1 = Ph, R^2 = *p*-ClC_6H_4
$\Delta G^{\neq}$ $_{TS3^a/TS3^{a\prime}}$	26.5	29.5
$\Delta G^{\neq}$ $_{TS3^b/TS3^{b\prime}}$	28.0	29.8
$\Delta\Delta G^{\neq}$	-1.5	-0.3

Fig. S1 IRC analysis of **TS5[a].**

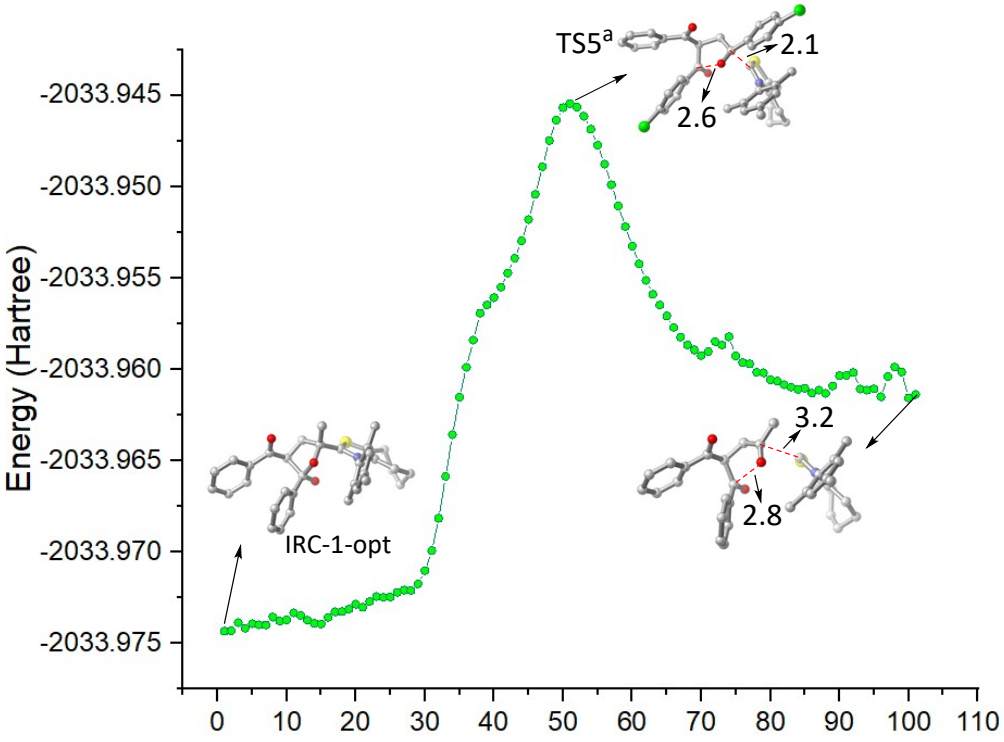


Fig. S2 Other three-dimensional structures of the transition states.

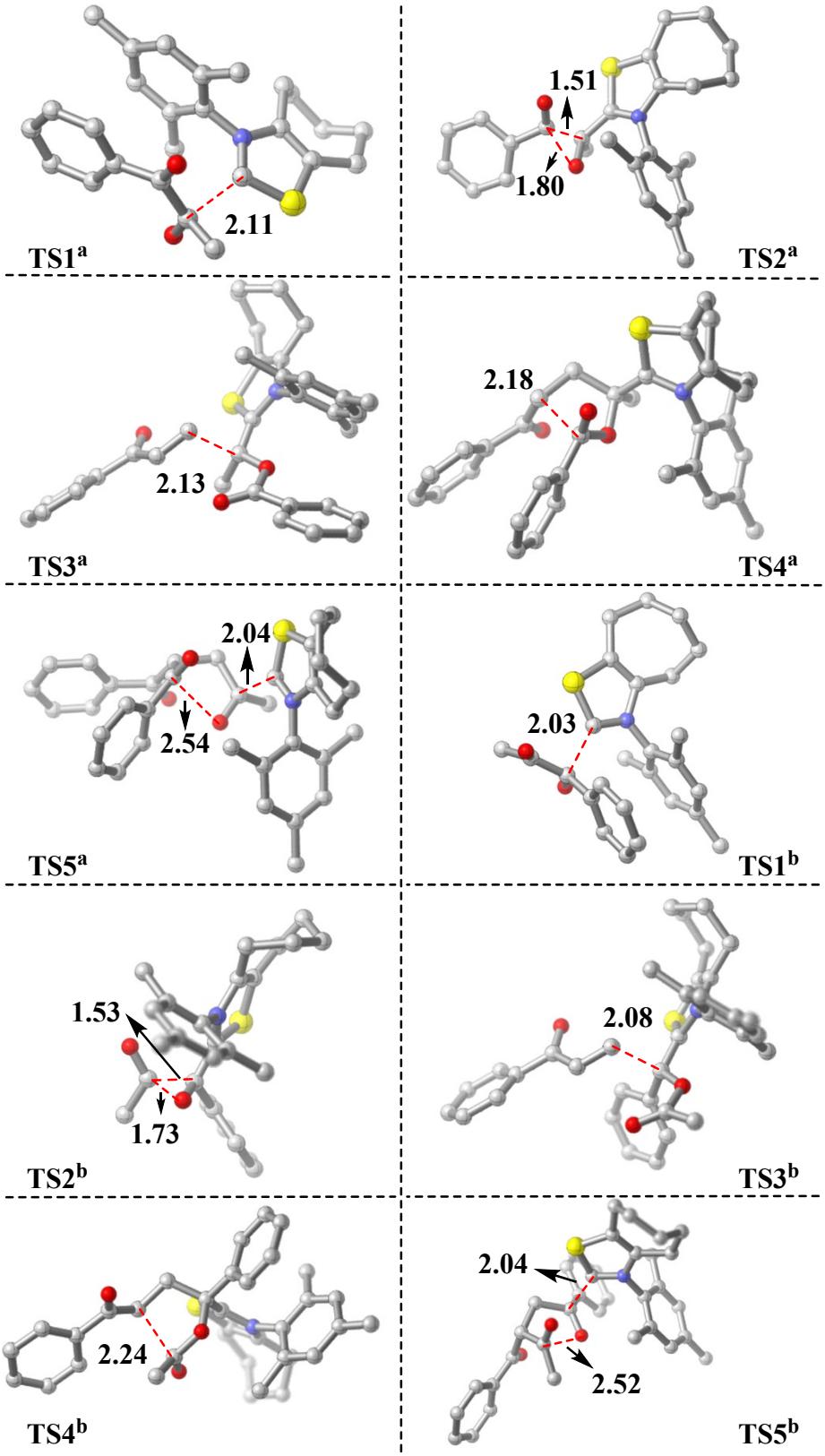
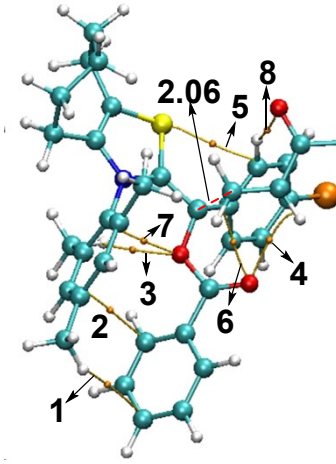


Fig. S3 AIM analyses of the transition states **TS3$^{a\prime}$** and **TS3$^{b\prime}$**, and the summary of Laplacian electron density ($\nabla^2\rho$ in 10^{-1} a.u.). The red, blue, green, yellow, orange and white balls represent oxygen, nitrogen, carbon, sulfur, chlorine and hydrogen atoms in three-dimensional structures, respectively.



TS3$^{a\prime}$ (0.0 kcal/mol)			**TS3$^{b\prime}$** (0.3 kcal/mol)		
type	**$\nabla^2\rho$**	**distance(Å)**	**type**	**$\nabla^2\rho$**	**distance(Å)**
C−H…π	0.059	3.44	C−H…π	0.151	2.92
π…π	0.217	3.26	π…π	0.193	3.34
C−H…O	0.301	2.61	C−H…O	0.353	2.56
C−H…O	0.394	2.52	C−H…O	0.379	2.56
LP…π	0.413	3.11	LP…π	0.407	3.12
C−H…O	0.523	2.50	C−H…O	0.503	2.25
LP…π	0.560	2.75	C−H…O	0.530	2.47
C−H…O	0.604	2.22	LP…π	0.558	2.74

Cartesian Coordinates

NHC

Zero-point correction= 0.343370

Thermal correction to Energy= 0.361837

Thermal correction to Enthalpy= 0.362782

Thermal correction to Gibbs Free Energy= 0.295988

Sum of electronic and zero-point Energies= -1112.717320

Sum of electronic and thermal Energies= -1112.698853

Sum of electronic and thermal Enthalpies= -1112.697908

Sum of electronic and thermal Free Energies= -1112.764702

Cartesian coordinates

C	1.160681	0.040251	0.255926
C	2.358629	0.648685	0.086425
C	3.718786	0.164100	0.504020
C	4.123701	-1.182548	-0.117077
C	3.025767	-2.261618	-0.090645
C	2.083264	-2.178409	1.118602
C	0.850394	-1.308488	0.842538
N	0.109623	0.844558	-0.236022
C	0.377035	2.042113	-0.782844
S	2.090853	2.192930	-0.685647
H	4.468328	0.917903	0.245082
H	3.735547	0.085371	1.596154
H	4.443863	-1.023049	-1.152167
H	5.003051	-1.537971	0.431409
H	2.419992	-2.192528	-1.003176
H	3.507710	-3.243575	-0.123242
H	1.718958	-3.176976	1.377272
H	2.621298	-1.812394	1.999860
H	0.205265	-1.840070	0.130373
H	0.254763	-1.182063	1.756004
C	-1.261879	0.402894	-0.144258

C	-1.988262	0.714053	1.006444
C	-1.810192	-0.316098	-1.210882
C	-3.312139	0.275070	1.077445
C	-3.134852	-0.735202	-1.097081
C	-3.897269	-0.452310	0.040243
H	-3.897593	0.511648	1.962789
H	-3.583497	-1.293931	-1.915707
C	-0.985210	-0.608653	-2.434151
H	-1.563311	-1.178471	-3.164087
H	-0.087992	-1.184369	-2.177998
H	-0.645241	0.320157	-2.904260
C	-1.356912	1.512367	2.114087
H	-2.066169	1.672964	2.928326
H	-1.020597	2.487224	1.745189
H	-0.475907	1.002112	2.519165
C	-5.318191	-0.940653	0.142667
H	-5.849313	-0.444210	0.958036
H	-5.345027	-2.019186	0.331966
H	-5.865236	-0.760693	-0.787221

Vibrational frequencies

24.9534	33.7426	49.4020
53.0470	82.4757	122.1820
137.9565	167.9055	172.6202
187.6400	200.5491	230.2987
241.3541	246.6208	280.5961
291.8436	328.1225	335.8437
343.3715	363.8076	412.8174
458.8933	494.9550	505.7585
525.9676	536.6359	569.2355
574.3641	584.7743	591.4587
611.8683	656.3656	697.2435
740.8117	759.8014	788.4273
804.7486	845.2829	889.9126

907.3602 921.4906 931.6563

958.5933 964.4023 981.4858

986.5126 1017.2663 1035.2311

1042.1023 1054.8839 1063.1640

1064.4135 1070.5138 1071.5554

1090.7552 1114.9177 1135.8820

1180.6836 1203.9139 1214.9581

1243.5239 1256.9516 1273.4313

1280.0148 1297.9187 1312.2339

1337.9851 1347.8010 1356.5496

1368.0538 1388.0017 1390.0177

1406.2412 1411.6979 1413.1665

1419.7543 1429.6880 1456.8823

1459.2901 1473.6439 1475.5990

1477.6420 1479.1401 1480.0309

1484.7372 1485.5155 1497.3585

1501.1361 1517.8474 1548.9971

1684.8756 1693.1010 1697.9858

3052.6102 3059.6524 3063.5418

3065.4288 3068.1979 3070.6840

3074.9739 3083.1754 3095.8524

3107.2604 3117.7464 3124.2204

3129.2027 3129.4203 3130.9829

3136.0393 3166.9301 3167.7393

3170.6225 3195.9810 3209.3669

R1

Zero-point correction= 0.184332

Thermal correction to Energy= 0.199408

Thermal correction to Enthalpy= 0.200353

Thermal correction to Gibbs Free Energy= 0.139424

Sum of electronic and zero-point Energies= -1608.651053

Sum of electronic and thermal Energies= -1608.635977

Sum of electronic and thermal Enthalpies= -1608.635033

Sum of electronic and thermal Free Energies= -1608.695962

Cartesian coordinates

C	3.474761	1.037207	-0.703546
C	4.429839	0.049882	-0.485281
C	4.140490	-1.115240	0.222028
C	2.857360	-1.287961	0.718484
C	1.880215	-0.306478	0.518099
C	2.193905	0.854621	-0.195256
C	0.515025	-0.567886	1.040466
C	-0.515029	0.573046	1.037468
C	-1.880209	0.308952	0.516454
O	0.189603	-1.623197	1.548102
O	-0.189693	1.630953	1.539732
C	-2.857772	1.290709	0.713414
C	-4.140928	1.115525	0.217905
C	-4.429839	-0.052303	-0.485087
C	-3.474319	-1.039967	-0.699936
C	-2.193453	-0.854901	-0.192561
H	3.727271	1.932139	-1.261041
H	4.904397	-1.869282	0.375119
H	2.600607	-2.187243	1.268600
H	1.446901	1.622405	-0.362712
H	-2.601329	2.192143	1.260150
H	-4.905165	1.869733	0.368509
H	-3.726489	-1.937012	-1.254184
H	-1.446082	-1.622882	-0.357447
Cl	6.040535	0.275451	-1.120486
Cl	-6.040515	-0.280938	-1.119254

Vibrational frequencies

21.5867	43.5116	52.8612
88.1830	89.6848	113.6333
141.1123	204.2131	229.6982

241.5044	279.9886	319.5371
321.3123	365.3188	372.7585
409.3724	420.2022	423.3593
495.8082	500.2084	554.8589
556.2416	636.5717	636.6986
701.1151	709.3832	714.1470
752.6115	776.9444	802.0607
861.1221	865.6214	871.7016
878.3456	907.4286	1002.2139
1003.4232	1021.1552	1021.8088
1025.1205	1031.2361	1089.0460
1127.4061	1127.4555	1147.4435
1148.0815	1206.3816	1212.9791
1258.1412	1336.0807	1336.7217
1349.4188	1353.2762	1374.8887
1458.9448	1460.8067	1548.4706
1550.2134	1664.8891	1665.1853
1683.4195	1683.6540	1813.7529
1827.0837	3240.3797	3241.6212
3247.0730	3248.2598	3260.3948
3260.4606	3263.3972	3263.5005

R2

Zero-point correction= 0.144639

Thermal correction to Energy= 0.152331

Thermal correction to Enthalpy= 0.153275

Thermal correction to Gibbs Free Energy= 0.111760

Sum of electronic and zero-point Energies= -422.663771

Sum of electronic and thermal Energies= -422.656079

Sum of electronic and thermal Enthalpies= -422.655135

Sum of electronic and thermal Free Energies= -422.696650

Cartesian coordinates

C	2.412108	1.021510	0.000000

C	2.947698	-0.267165	0.000001
C	2.100269	-1.372084	-0.000001
C	0.718345	-1.196097	-0.000001
C	0.174430	0.093063	0.000000
C	1.035139	1.198371	0.000000
C	-1.300365	0.368557	0.000002
O	-1.703667	1.521044	-0.000001
C	-2.264888	-0.771348	0.000002
C	-3.575788	-0.532362	-0.000001
H	3.069846	1.884929	0.000000
H	4.024070	-0.409173	0.000001
H	2.513415	-2.375692	-0.000002
H	0.081763	-2.073364	-0.000002
H	0.602275	2.193208	0.000001
H	-1.893555	-1.789270	0.000005
H	-4.299822	-1.341071	0.000000
H	-3.950344	0.487408	-0.000004

Vibrational frequencies

-69.6360	66.7668	162.7054
182.7756	336.8126	361.7083
410.2598	432.3277	488.7359
529.1726	626.2862	660.6045
706.4265	751.7845	771.6138
852.1593	880.7516	971.2970
1008.7132	1010.6425	1019.5890
1030.2277	1032.5835	1041.5591
1066.3178	1071.5600	1123.7691
1173.5960	1201.6562	1270.8617
1320.5423	1354.4650	1367.6194
1434.8933	1499.2759	1548.6947
1672.5620	1694.7017	1715.7443
1807.4534	3176.0676	3207.7473
3218.2487	3222.8707	3234.5275

3236.7750 3258.4043 3275.5102

TS1

Zero-point correction= 0.529735

Thermal correction to Energy= 0.563353

Thermal correction to Enthalpy= 0.564297

Thermal correction to Gibbs Free Energy= 0.463415

Sum of electronic and zero-point Energies= -2721.377768

Sum of electronic and thermal Energies= -2721.344150

Sum of electronic and thermal Enthalpies= -2721.343206

Sum of electronic and thermal Free Energies= -2721.444088

Cartesian coordinates

C	4.617360	-2.126888	-0.292410
C	3.842555	-2.173847	0.859030
C	2.457551	-2.066393	0.753558
C	1.852118	-1.921408	-0.500790
C	2.662456	-1.903078	-1.646344
C	0.372045	-1.808879	-0.749159
C	-0.603721	-1.551296	0.432042
O	-0.048330	-1.952791	-1.881572
C	-1.146283	0.465910	-0.366255
N	-0.399605	1.564041	-0.237333
C	-1.012988	2.819713	-0.440464
C	-2.330605	2.680552	-0.725622
S	-2.737755	0.982220	-0.737836
C	-0.236714	4.104600	-0.370645
C	-0.735974	5.077971	0.711773
C	-2.265096	5.227656	0.780774
C	-2.951754	5.163442	-0.590144
C	-3.370998	3.736672	-0.982537
C	3.287250	1.255330	-0.509906
C	1.945017	1.342701	-0.887936
C	0.995264	1.453727	0.126406

C	1.330334	1.491956	1.484306
C	2.679332	1.387971	1.813951
C	3.668484	1.266570	0.830767
C	5.115757	1.134410	1.224321
C	0.260655	1.626492	2.532475
C	1.525298	1.294731	-2.331099
O	-0.149467	-1.358564	1.561678
H	4.310790	-2.291357	1.830495
H	1.854717	-2.094954	1.649727
H	2.192576	-1.802970	-2.619102
H	0.821173	3.887246	-0.206504
H	-0.302793	4.585062	-1.351764
H	-0.356576	4.765525	1.690552
H	-0.282859	6.052092	0.497585
H	-2.686131	4.442887	1.421847
H	-2.495471	6.177481	1.273093
H	-3.860364	5.772369	-0.584975
H	-2.299627	5.593925	-1.357887
H	-4.263021	3.468994	-0.403463
H	-3.670201	3.706202	-2.036841
H	4.046273	1.157638	-1.282599
H	2.967871	1.402326	2.862923
H	5.755843	1.017858	0.346327
H	5.264322	0.265177	1.873832
H	5.454384	2.015296	1.779572
H	0.706178	1.740388	3.523035
H	-0.374163	0.734617	2.533421
H	-0.379245	2.495293	2.341125
H	0.849828	0.450745	-2.514794
H	2.395375	1.191422	-2.982817
H	0.986461	2.205359	-2.617475
C	4.042640	-1.998129	-1.554687
H	4.664047	-1.972298	-2.443329
C	-2.009534	-2.122668	0.304845

C	-2.736339	-2.238866	-0.886411
C	-2.592733	-2.564015	1.494927
C	-4.017143	-2.782881	-0.884675
H	-2.307827	-1.897716	-1.819446
C	-3.871469	-3.110525	1.513895
H	-2.028757	-2.471876	2.416517
C	-4.569584	-3.211580	0.317121
H	-4.580570	-2.865615	-1.807929
H	-4.316634	-3.452530	2.442125
Cl	6.356998	-2.239631	-0.156788
Cl	-6.186470	-3.886913	0.321845

Vibrational frequencies

-72.6462	13.6574	18.6778
30.9399	38.7830	43.7733
55.2734	59.4199	70.8752
78.5034	82.3032	88.9422
101.4820	118.2473	129.6944
132.3017	147.2703	157.9659
162.9574	178.9766	182.4275
198.6061	207.5336	217.5819
232.3588	235.7368	253.6833
258.8909	261.3384	278.5301
282.4017	294.0962	299.9929
335.3829	337.2130	341.2239
344.0951	370.0182	376.7917
381.2746	395.0035	414.8589
419.4369	422.1979	451.8483
458.3802	488.1441	499.5772
504.0993	506.5168	527.6764
530.9462	548.7093	554.8212
572.5986	580.5052	589.9751
592.8139	626.5232	634.3687
639.0236	656.8062	667.1222

695.5290 707.1583 722.7735

734.7495 743.3293 760.3847

764.0340 778.0379 810.0663

844.5358 847.8663 856.1878

859.3416 866.4346 869.2822

882.6208 891.8347 914.9144

925.1362 938.0348 964.5436

973.9830 981.6479 993.4080

994.4579 998.9394 1006.1128

1007.7782 1020.5390 1020.8382

1028.4149 1033.6017 1043.8500

1060.6934 1061.9282 1065.9752

1066.9089 1074.5214 1082.1830

1093.4591 1114.7429 1127.5386

1128.3895 1132.5258 1141.3170

1144.5245 1189.0703 1194.9891

1200.4148 1204.7932 1217.1683

1226.4358 1250.8102 1262.5002

1277.7667 1281.4241 1302.4525

1316.9265 1324.0498 1325.3409

1329.7116 1337.3825 1341.4616

1344.6767 1357.7501 1363.1102

1372.8971 1394.2115 1399.9945

1408.8241 1412.5720 1413.9699

1427.6065 1443.2327 1447.7723

1450.0045 1460.2470 1472.1086

1473.8325 1476.1666 1479.2913

1482.1680 1486.0818 1488.6961

1489.9456 1500.5253 1509.7601

1517.5925 1538.2186 1541.1414

1548.2883 1654.2263 1658.6277

1675.4018 1682.4743 1684.2398

1687.9547 1695.8577 1712.6750

1816.1260 3058.2421 3060.1416

3064.5790	3069.2004	3071.9884
3074.0895	3080.0636	3094.5426
3110.0955	3113.0877	3122.2340
3123.9901	3132.1083	3134.5785
3142.0251	3149.9510	3157.2112
3162.9976	3172.6007	3204.4004
3208.4146	3229.0689	3230.3885
3240.7011	3242.4680	3244.5759
3253.2575	3277.8025	3294.6985

M1

Zero-point correction= 0.530458

Thermal correction to Energy= 0.564277

Thermal correction to Enthalpy= 0.565222

Thermal correction to Gibbs Free Energy= 0.464332

Sum of electronic and zero-point Energies= -2721.391685

Sum of electronic and thermal Energies= -2721.357865

Sum of electronic and thermal Enthalpies= -2721.356921

Sum of electronic and thermal Free Energies= -2721.457811

Cartesian coordinates

C	4.402854	2.256442	-0.481547
C	3.444857	2.214366	-1.488189
C	2.126977	1.911767	-1.157721
C	1.774282	1.656291	0.174041
C	2.759097	1.727301	1.168352
C	0.398006	1.270746	0.628580
C	-0.731661	0.901768	-0.402306
O	0.142102	1.249436	1.821006
C	-1.276804	-0.511132	-0.005739
N	-0.553680	-1.618264	0.161589
C	-1.282437	-2.823295	0.159424
C	-2.607846	-2.610598	-0.035129
S	-2.924571	-0.907906	-0.187077

C	-0.615137	-4.148774	0.394561
C	-0.773313	-5.145965	-0.766510
C	-2.191179	-5.223330	-1.354817
C	-3.299048	-5.061152	-0.305299
C	-3.738513	-3.599480	-0.125470
C	2.765407	-1.530978	1.809759
C	1.380933	-1.578996	1.651790
C	0.885595	-1.600186	0.344239
C	1.706713	-1.669699	-0.786350
C	3.084243	-1.610069	-0.573023
C	3.627561	-1.523117	0.710626
C	5.118369	-1.437457	0.900173
C	1.124929	-1.814140	-2.163248
C	0.453420	-1.630768	2.833202
O	-0.394936	0.795819	-1.676009
H	3.724727	2.410656	-2.517608
H	1.359398	1.848675	-1.918166
H	2.478854	1.531113	2.197952
H	0.446219	-3.994952	0.601094
H	-1.047297	-4.575468	1.304756
H	-0.060920	-4.902366	-1.561402
H	-0.484048	-6.128056	-0.377196
H	-2.316908	-4.448944	-2.121752
H	-2.298242	-6.182640	-1.869750
H	-4.188092	-5.623551	-0.603957
H	-2.976758	-5.482571	0.652916
H	-4.354715	-3.316759	-0.987120
H	-4.377887	-3.499087	0.759197
H	3.177094	-1.485936	2.815148
H	3.747522	-1.631615	-1.434705
H	5.370147	-1.088422	1.904506
H	5.564685	-0.753182	0.172409
H	5.587105	-2.417172	0.757360
H	1.920821	-1.867655	-2.909380

H	0.474506	-0.956397	-2.367125
H	0.525939	-2.730229	-2.234740
H	-0.339631	-0.883019	2.748936
H	1.002937	-1.448889	3.758986
H	-0.019432	-2.617574	2.908086
C	4.077918	2.024362	0.851747
H	4.841642	2.069511	1.621037
C	-1.873581	1.936079	-0.152713
C	-2.534862	2.113198	1.067368
C	-2.247233	2.715748	-1.244489
C	-3.552566	3.054251	1.193664
H	-2.254693	1.517295	1.929644
C	-3.256922	3.668912	-1.135604
H	-1.729456	2.545702	-2.182254
C	-3.898179	3.823413	0.086720
H	-4.069675	3.187798	2.137952
H	-3.544481	4.277015	-1.986885
Cl	6.064112	2.613903	-0.900140
Cl	-5.180528	5.009978	0.237060

Vibrational frequencies

12.6034	22.0086	31.4472
40.2745	46.9234	52.2179
64.4873	73.0840	80.3730
93.2241	110.6285	112.4013
123.6429	125.3143	137.4178
144.4468	146.4055	154.2558
156.9109	173.0823	188.9530
196.8694	202.0296	225.4728
242.7463	248.3362	251.5971
258.0326	276.8741	281.5833
290.5934	309.8453	321.0923
327.3189	333.2428	339.9873
363.7174	369.6756	380.3554

396.4263	414.3281	421.6390
428.2092	432.2680	464.1668
476.5105	496.1337	502.4111
503.8836	520.4404	527.4018
540.3841	546.9685	562.4000
582.1627	589.3338	593.2503
618.8195	633.6390	637.2873
641.8300	672.4865	688.4350
702.6831	728.5419	736.0343
742.1379	744.0050	760.5532
768.3922	814.3704	822.3981
847.2051	858.7827	862.6275
870.6360	881.5608	884.6155
892.9086	918.1209	925.3399
944.6246	962.1856	965.7905
984.8783	985.2048	1002.0340
1007.2219	1008.0117	1019.5907
1022.1086	1023.3083	1027.5694
1037.2723	1043.7693	1051.3967
1060.9319	1063.5898	1069.4587
1069.9468	1075.0098	1093.9036
1112.2585	1116.7807	1119.3958
1128.0223	1128.7211	1133.7693
1143.2893	1168.5353	1185.7066
1190.2814	1197.6970	1205.3874
1216.4191	1252.4752	1264.0219
1275.5497	1278.9499	1279.8765
1293.8411	1305.3530	1313.4170
1323.1248	1338.2895	1341.0563
1342.4692	1345.9883	1358.0074
1366.3815	1371.6695	1397.8705
1403.4192	1405.4568	1414.3584
1417.0400	1427.9524	1443.2684
1446.3693	1456.8379	1461.0604

1466.8641	1474.9777	1475.2949
1481.6185	1483.4983	1486.8900
1494.6504	1501.5711	1503.8155
1514.9848	1519.1337	1532.6628
1533.2215	1538.1221	1653.6250
1664.7680	1671.1178	1676.6066
1678.0992	1684.1866	1691.8075
1796.1468	3049.3958	3065.2515
3070.4650	3072.4872	3072.6906
3075.0661	3088.0526	3097.9445
3112.5862	3116.3353	3126.4375
3127.7439	3137.3569	3141.7276
3144.7270	3154.0030	3160.8572
3161.9431	3172.9769	3195.0960
3202.0191	3227.2641	3228.2598
3235.0888	3236.6403	3244.1258
3245.6972	3251.3536	3257.4579

TS2

Zero-point correction= 0.528867

Thermal correction to Energy= 0.562525

Thermal correction to Enthalpy= 0.563470

Thermal correction to Gibbs Free Energy= 0.460630

Sum of electronic and zero-point Energies= -2721.373435

Sum of electronic and thermal Energies= -2721.339777

Sum of electronic and thermal Enthalpies= -2721.338833

Sum of electronic and thermal Free Energies= -2721.441673

Cartesian coordinates

C	-5.103063	-2.026044	-0.798770
C	-4.547124	-1.644374	0.417964
C	-3.186009	-1.364691	0.479592
C	-2.385718	-1.463180	-0.661850
C	-2.968873	-1.864966	-1.865314

C	-0.908050	-1.152099	-0.709244
C	-0.440808	0.048147	0.092536
O	-0.182123	-1.739741	-1.526868
C	0.891479	0.582397	-0.359501
N	2.082799	-0.012425	-0.298606
C	3.144881	0.732191	-0.845658
C	2.730349	1.915249	-1.363251
S	1.024745	2.101629	-1.129443
C	4.577324	0.288703	-0.770039
C	5.422612	1.189268	0.148389
C	5.227150	2.696969	-0.083723
C	5.018688	3.059853	-1.559343
C	3.538306	3.020277	-1.990063
C	3.008826	-3.569220	0.222065
C	2.669546	-2.388829	-0.441834
C	2.360675	-1.281851	0.352569
C	2.439633	-1.293389	1.746055
C	2.791553	-2.494584	2.359256
C	3.066981	-3.643405	1.614723
C	3.411289	-4.940241	2.297668
C	2.130151	-0.063726	2.551518
C	2.712937	-2.306799	-1.942747
O	-0.407899	-1.026560	0.960479
H	-5.167565	-1.575330	1.305258
H	-2.728441	-1.086481	1.421784
H	-2.339093	-1.959534	-2.743730
H	4.643351	-0.743596	-0.424808
H	4.982806	0.307470	-1.785930
H	5.206106	0.946833	1.194627
H	6.470742	0.924721	-0.028192
H	4.366801	3.055700	0.494932
H	6.101188	3.222770	0.311775
H	5.377041	4.074657	-1.751942
H	5.617635	2.398769	-2.193941

H	3.070980	3.969069	-1.703690
H	3.457279	2.953188	-3.080737
H	3.247191	-4.450250	-0.369679
H	2.854033	-2.530861	3.444234
H	2.538642	-5.601460	2.333414
H	3.742160	-4.770854	3.325204
H	4.201900	-5.472602	1.761934
H	2.448657	-0.190936	3.588115
H	1.049753	0.115211	2.537780
H	2.623985	0.826321	2.145402
H	1.907719	-1.674557	-2.317098
H	2.601015	-3.303694	-2.375844
H	3.677313	-1.907962	-2.280351
C	-4.329704	-2.146208	-1.946564
H	-4.779726	-2.454809	-2.884243
C	-1.391173	1.174348	0.442405
C	-2.110617	1.847869	-0.546773
C	-1.576955	1.520625	1.780467
C	-2.985288	2.878387	-0.211777
H	-2.006008	1.555748	-1.589315
C	-2.446632	2.546729	2.133894
H	-1.053027	0.965297	2.552902
C	-3.136475	3.216101	1.127680
H	-3.548135	3.399412	-0.978639
H	-2.592935	2.819154	3.173636
Cl	-4.237074	4.509101	1.562463
Cl	-6.820694	-2.371518	-0.880840

Vibrational frequencies

-256.4475	11.5254	15.2028
21.1109	28.0352	37.2122
42.8162	49.6377	54.6353
67.4673	89.0283	92.7040
94.4742	106.7172	131.4201

135.5193	138.1346	142.2272
148.8960	161.4932	171.9839
197.8947	201.9214	217.5867
227.9047	238.1475	251.6216
260.5916	269.4435	279.4087
289.8955	300.1067	323.5218
326.1602	340.2230	341.6010
362.6169	377.3748	384.0904
412.7535	420.1322	422.1240
425.8494	440.9668	469.7317
479.7948	485.2625	500.2036
510.6726	511.8817	528.2875
535.2903	548.0437	558.7803
569.8210	577.7210	590.8394
599.7566	626.6854	632.9716
639.3097	647.1849	670.2209
708.8334	732.6911	735.1787
744.9552	747.3718	753.2886
766.4152	804.1065	843.8204
847.3386	851.9957	855.1739
863.1940	880.4451	880.9078
887.6790	920.1844	926.0047
942.3305	964.8610	968.4567
981.7753	982.5874	985.1468
991.1465	999.2987	1002.7672
1005.0006	1018.7551	1030.1859
1037.3696	1049.2219	1050.5921
1059.8860	1064.1857	1065.5435
1067.1112	1075.7742	1091.8036
1114.8187	1117.0517	1119.1685
1125.7446	1126.5806	1133.0942
1139.2857	1175.8659	1187.0607
1189.7368	1197.0809	1209.5130
1216.3953	1252.0988	1256.5666

1273.5079	1278.2916	1282.9757
1302.7486	1305.3844	1316.8100
1320.5426	1335.2792	1338.5224
1342.0461	1344.7259	1356.5572
1362.3787	1367.6789	1393.5106
1395.1579	1398.0828	1409.6427
1414.3949	1425.8402	1444.0734
1450.3805	1457.9957	1465.6819
1470.2958	1472.3558	1473.6396
1478.0414	1484.2349	1486.8598
1495.1050	1504.3208	1507.6349
1510.2446	1517.3511	1533.6703
1540.7618	1544.5665	1636.5918
1666.4587	1670.0734	1680.0052
1683.6157	1687.5708	1689.2359
1694.6616	3058.6243	3067.1210
3070.9305	3071.4785	3076.6955
3077.2189	3087.4193	3102.1784
3115.4273	3119.6893	3129.4657
3132.1245	3136.2044	3142.3417
3148.5777	3162.2602	3164.3901
3169.7676	3195.4317	3195.6227
3199.3507	3206.8559	3222.8764
3222.9741	3229.8108	3234.0457
3234.9047	3241.2467	3243.0355

M2

Zero-point correction= 0.531159

Thermal correction to Energy= 0.565151

Thermal correction to Enthalpy= 0.566096

Thermal correction to Gibbs Free Energy= 0.464432

Sum of electronic and zero-point Energies= -2721.434031

Sum of electronic and thermal Energies= -2721.400038

Sum of electronic and thermal Enthalpies= -2721.399094

Sum of electronic and thermal Free Energies= -2721.500758

Cartesian coordinates

C	4.671067	1.660751	0.697655
C	5.001177	1.529759	-0.648280
C	4.030627	1.418679	-1.639782
C	2.691202	1.418438	-1.267925
C	2.340227	1.539360	0.078081
C	3.328797	1.667467	1.054643
C	0.927631	1.463075	0.534899
O	0.111598	1.013657	-0.450671
O	0.547110	1.744772	1.644250
C	-1.242279	0.838813	-0.130223
C	-1.673761	-0.451031	-0.028307
C	-2.033762	2.063984	-0.095434
C	-3.274280	2.161104	0.557735
C	-4.000728	3.346795	0.557722
C	-3.481473	4.463110	-0.084514
C	-2.241839	4.413912	-0.714025
C	-1.528759	3.223583	-0.714855
N	-0.881803	-1.591967	-0.011789
C	-1.602403	-2.808736	-0.012287
C	-2.935916	-2.652702	-0.036607
S	-3.373440	-0.940290	-0.018927
C	-0.823028	-4.093918	0.037089
C	-1.648204	-5.362522	-0.213034
C	-2.536284	-5.255180	-1.459358
C	-3.943583	-4.693560	-1.183159
C	-4.017260	-3.698585	-0.014624
C	0.513516	-1.596010	0.348471
C	1.480779	-1.722595	-0.654539
C	2.819601	-1.805327	-0.270770
C	3.201037	-1.739959	1.070534
C	2.208722	-1.589811	2.042252

C	0.855729	-1.523844	1.703900
C	1.078560	-1.710354	-2.102653
C	-0.210162	-1.351351	2.751357
C	4.652599	-1.826112	1.463612
H	5.447985	1.747252	1.449347
H	4.317632	1.324398	-2.681273
H	1.922664	1.312982	-2.025933
H	3.039701	1.753268	2.097017
H	-3.671412	1.323449	1.120075
H	-4.953987	3.402605	1.072543
H	-1.838409	5.295121	-1.201667
H	-0.564840	3.190648	-1.212102
H	-0.036454	-4.037428	-0.725506
H	-0.302698	-4.159890	1.001471
H	-0.935054	-6.183307	-0.332963
H	-2.251166	-5.610152	0.666929
H	-2.023130	-4.621580	-2.193549
H	-2.642328	-6.237746	-1.929345
H	-4.325516	-4.216106	-2.091777
H	-4.628782	-5.516068	-0.949348
H	-4.996380	-3.209487	-0.028309
H	-3.967681	-4.238608	0.936778
H	3.583369	-1.895688	-1.040411
H	2.492181	-1.523881	3.090665
H	0.435423	-2.561126	-2.354237
H	0.510784	-0.801402	-2.328936
H	1.958210	-1.742991	-2.749462
H	0.216328	-1.435035	3.753135
H	-0.677947	-0.365010	2.656666
H	-0.999641	-2.104297	2.647507
H	5.303836	-1.502443	0.646857
H	4.861990	-1.207040	2.340398
H	4.926673	-2.856289	1.717571
Cl	6.687440	1.500244	-1.106236

Cl	-4.391479	5.960546	-0.086756

Vibrational frequencies

20.6383	21.8330	29.4401
37.3710	40.4137	52.2351
61.2313	65.7645	84.2533
92.3112	93.6802	100.3191
106.7616	110.2849	126.1528
129.6894	139.7109	149.8296
159.3481	164.1528	181.7993
190.9325	211.8886	215.3675
235.3854	245.3909	251.7761
264.5100	274.8961	278.5170
296.7466	307.9511	320.5334
322.7069	336.1973	342.8711
354.0072	370.7781	400.5213
407.1425	420.8784	422.1730
429.1056	446.2275	457.3161
479.8026	500.6353	505.8001
513.6860	523.3354	538.6691
538.8915	570.1800	573.4785
575.5993	588.5731	590.8815
606.7499	622.7661	636.7067
638.5101	644.5251	670.0879
697.9126	722.9666	730.0851
752.9167	761.9810	773.6985
794.9757	798.4955	841.9068
847.2071	854.7192	863.1185
873.1000	878.0263	884.2962
890.2409	918.2705	926.3627
940.2298	959.2155	968.5226
978.4717	984.1502	987.9487
996.3867	997.7810	1016.6688
1019.2595	1022.2443	1025.4538

1032.3942	1035.2369	1060.9781
1061.2515	1066.5731	1069.1274
1070.2284	1074.5563	1092.9682
1119.5083	1121.7714	1129.9039
1133.4415	1140.5576	1149.4722
1161.9608	1186.4684	1188.9599
1204.6292	1206.6346	1210.7483
1232.4815	1247.4275	1273.9379
1284.6782	1289.4150	1308.5325
1316.6842	1317.2038	1321.6633
1328.6375	1333.3768	1339.0420
1352.1513	1356.2123	1364.5513
1374.4653	1377.5254	1393.6860
1402.7034	1411.9888	1414.3225
1419.6053	1429.0459	1451.7931
1453.5649	1456.3534	1467.7926
1470.5113	1473.1593	1477.9399
1481.2957	1483.4920	1485.8290
1487.4189	1495.9836	1513.4649
1514.3763	1541.6800	1545.3694
1545.8949	1634.3266	1655.5368
1669.6718	1676.1026	1684.7505
1687.3189	1694.3090	1746.7118
1863.0160	3061.5113	3062.8051
3064.3285	3066.6110	3067.1843
3068.3135	3075.1521	3088.0189
3104.5729	3108.8916	3117.9587
3125.8718	3130.7024	3131.4717
3131.7158	3138.2243	3153.4539
3166.6861	3166.8338	3192.2065
3200.6180	3217.3775	3218.9827
3230.1299	3230.6482	3232.1237
3232.9718	3247.3257	3258.1160

TS3

Zero-point correction= 0.677504

Thermal correction to Energy= 0.720406

Thermal correction to Enthalpy= 0.721350

Thermal correction to Gibbs Free Energy= 0.596263

Sum of electronic and zero-point Energies= -3144.072072

Sum of electronic and thermal Energies= -3144.029170

Sum of electronic and thermal Enthalpies= -3144.028226

Sum of electronic and thermal Free Energies= -3144.153313

Cartesian coordinates

O	-3.722811	1.082360	-1.281933
C	-1.043519	0.160565	-1.348078
C	-0.152444	1.339694	0.860857
S	-1.342868	2.295647	1.679659
C	-0.435558	3.754173	1.413002
C	0.703145	3.492611	0.742258
N	0.853655	2.133435	0.420874
C	-0.886942	5.140114	1.757744
C	-1.229205	5.976122	0.497084
C	-0.512673	5.550837	-0.791093
C	1.020038	5.512836	-0.755673
C	1.644358	4.576462	0.314451
C	2.084136	1.669241	-0.186537
C	3.100901	1.244817	0.682407
C	4.296218	0.817281	0.120365
C	4.488330	0.797835	-1.267186
C	3.470454	1.272900	-2.086813
C	2.253873	1.738380	-1.567636
C	5.773733	0.263507	-1.839602
C	1.224119	2.319706	-2.501564
C	2.879021	1.236685	2.169528
H	-0.054407	-0.110264	-1.711660
H	-1.235107	1.232200	-1.319973

H	-1.742003	5.114463	2.437798
H	-0.067195	5.618781	2.305288
H	-2.306256	5.912071	0.312314
H	-1.008791	7.026374	0.716356
H	-0.884542	4.562527	-1.090238
H	-0.815241	6.238035	-1.588595
H	1.366712	5.197301	-1.744837
H	1.412616	6.522170	-0.593075
H	2.583979	4.155841	-0.049130
H	1.885821	5.157063	1.210953
H	5.093249	0.472374	0.775443
H	3.618278	1.298897	-3.164134
H	5.823067	0.416992	-2.919815
H	6.640840	0.747408	-1.380090
H	5.860844	-0.811402	-1.643399
H	0.410983	2.817159	-1.968542
H	1.698944	3.051160	-3.161815
H	0.785442	1.545147	-3.138666
H	3.780835	0.909934	2.691433
H	2.059376	0.560396	2.441203
H	2.609900	2.233433	2.537399
C	-0.345883	-0.055827	0.577772
C	-1.338815	-0.803829	1.391370
C	-2.701478	-0.483006	1.326256
C	-0.937723	-1.865466	2.213953
C	-3.636933	-1.182777	2.085442
H	-3.046265	0.313977	0.674623
C	-1.862608	-2.578136	2.966089
H	0.110677	-2.139510	2.284019
C	-3.206748	-2.225523	2.893371
H	-4.689622	-0.925824	2.030713
H	-1.542102	-3.394305	3.604357
C	-3.452368	-0.064264	-1.695759
C	-4.596909	-0.921948	-2.183248

C	-5.890529	-0.577721	-1.777056
C	-4.425507	-2.025861	-3.025655
C	-6.988134	-1.330507	-2.182258
H	-6.011000	0.290943	-1.137364
C	-5.523971	-2.775370	-3.440622
H	-3.434070	-2.293910	-3.377289
C	-6.806875	-2.433538	-3.016060
H	-7.985845	-1.057514	-1.851134
H	-5.378043	-3.625019	-4.101032
H	-7.661939	-3.021396	-3.336219
O	0.907194	-0.711817	0.485842
C	1.020165	-1.872628	-0.195511
O	0.115620	-2.421504	-0.775091
C	2.414513	-2.394234	-0.142790
C	3.277544	-2.094707	0.911830
C	2.840850	-3.216283	-1.188005
C	4.569339	-2.609827	0.922990
H	2.942387	-1.467449	1.731073
C	4.135056	-3.719678	-1.199978
H	2.157887	-3.448690	-1.998481
C	4.981939	-3.406227	-0.139889
H	5.246762	-2.389835	1.740854
H	4.481065	-4.344496	-2.015824
C	-2.141974	-0.625469	-1.701022
H	-1.999534	-1.675598	-1.920410
Cl	6.616415	-4.028415	-0.146393
Cl	-4.378947	-3.121690	3.839233

Vibrational frequencies

-459.4065	7.4937	14.6118
15.7528	20.2505	21.6570
23.9840	30.9508	34.6855
39.1564	54.1505	63.5574
67.4242	78.9820	79.9420

85.3906 102.3771 112.1891

117.1403 121.0150 128.8253

131.1987 133.3864 141.7014

154.1947 160.2271 166.1950

172.3329 189.0276 204.7698

209.8805 216.6687 230.0813

245.3646 250.3103 259.9233

266.0425 279.8548 282.6919

284.4628 305.8432 315.4159

322.9181 329.6039 340.4105

343.1407 363.3180 372.6142

375.0995 398.7635 408.9723

412.1057 416.0921 422.8907

429.5572 433.7221 441.1632

454.8949 476.4211 489.9896

496.2997 503.5373 525.1116

531.8404 534.2789 541.5434

550.9486 561.8523 571.9046

580.5962 594.7898 611.6338

622.4971 627.2275 637.4698

641.6288 653.5408 665.6461

680.9525 703.1675 707.9205

710.6708 721.7472 728.3363

737.9496 746.4138 752.0804

761.4370 771.5867 776.0864

790.7241 795.8768 811.5683

825.4952 854.9210 860.6909

864.2665 867.5231 876.4556

878.3213 883.4338 892.6131

912.4340 925.2533 926.4000

959.9815 969.2196 971.5449

976.3027 978.7048 993.7785

994.2313 996.8262 1005.8446

1008.1514 1012.2913 1016.3706

1018.1072	1028.5689	1029.8467
1040.2830	1046.2282	1048.7270
1054.9974	1056.5979	1059.4615
1060.3623	1060.8863	1063.3815
1065.0956	1087.0633	1092.5289
1103.6258	1113.7368	1124.6730
1130.2727	1133.3143	1135.3170
1151.4816	1155.6080	1163.9104
1167.9358	1170.3934	1186.1916
1189.0579	1192.8967	1201.3152
1217.1559	1222.4629	1224.0878
1263.5226	1268.5616	1274.2684
1276.8112	1286.5193	1296.1342
1310.6697	1315.2797	1321.5959
1325.7421	1327.7225	1334.2120
1338.6242	1343.1199	1349.3111
1351.4719	1356.4205	1361.4343
1366.1173	1384.5033	1385.6444
1402.4735	1408.3433	1414.1465
1421.8740	1424.2004	1426.8257
1450.1863	1451.1549	1459.4520
1468.9780	1471.1429	1473.9748
1475.1952	1478.2394	1478.4513
1486.2888	1487.5758	1489.7083
1490.6511	1492.1371	1499.0064
1510.0340	1535.6701	1541.2253
1542.7532	1550.4076	1555.7519
1653.3518	1659.8722	1667.2189
1683.5992	1685.6100	1688.0730
1688.1954	1691.8548	1694.1573
1701.6177	1860.2830	3055.8204
3056.7673	3059.6134	3074.4495
3076.8461	3077.9690	3083.1772
3092.7902	3105.0847	3119.8572

3124.3480	3125.7555	3130.1773
3137.1998	3139.6866	3143.3663
3161.7107	3162.3167	3162.5137
3179.6392	3190.2201	3193.1295
3200.8360	3207.0454	3214.0455
3218.0811	3218.5755	3220.8333
3225.4607	3226.5620	3229.3773
3231.1580	3234.1361	3236.3696
3238.5673	3240.0774	3252.5888

M3

Zero-point correction= 0.680766

Thermal correction to Energy= 0.723301

Thermal correction to Enthalpy= 0.724245

Thermal correction to Gibbs Free Energy= 0.602340

Sum of electronic and zero-point Energies= -3144.086215

Sum of electronic and thermal Energies= -3144.043680

Sum of electronic and thermal Enthalpies= -3144.042736

Sum of electronic and thermal Free Energies= -3144.164641

Cartesian coordinates

O	3.565562	-2.047163	-1.871540
C	0.981799	-0.872521	-1.305472
C	-0.783259	-1.597333	0.320343
S	-0.557664	-3.151098	0.991725
C	-2.205383	-3.569972	0.732328
C	-2.876158	-2.535171	0.164284
N	-2.048080	-1.436871	-0.069673
C	-2.839478	-4.895979	1.011843
C	-3.183094	-5.646828	-0.296037
C	-3.550960	-4.747854	-1.482790
C	-4.651941	-3.709539	-1.237890
C	-4.329821	-2.604447	-0.188476
C	-2.579560	-0.236386	-0.686765

C	-3.047057	0.777173	0.160096
C	-3.558633	1.919141	-0.444830
C	-3.629144	2.045018	-1.837768
C	-3.195655	0.986693	-2.630920
C	-2.670320	-0.184858	-2.075307
C	-4.176116	3.307299	-2.448031
C	-2.276110	-1.337739	-2.959676
C	-2.986312	0.632164	1.655226
H	0.157998	-0.653360	-1.990312
H	1.207224	-1.941958	-1.391424
H	-2.200979	-5.511102	1.649880
H	-3.756918	-4.695544	1.577366
H	-2.324632	-6.259755	-0.588535
H	-4.007537	-6.333845	-0.079113
H	-2.649514	-4.232298	-1.836509
H	-3.870918	-5.391971	-2.308567
H	-4.870470	-3.224908	-2.193882
H	-5.570848	-4.216685	-0.926419
H	-4.681358	-1.632382	-0.538993
H	-4.864986	-2.814363	0.743768
H	-3.902229	2.736852	0.185354
H	-3.260000	1.065201	-3.713558
H	-4.011569	3.330619	-3.527381
H	-5.252147	3.393604	-2.264261
H	-3.701274	4.188486	-2.004592
H	-1.593097	-2.034965	-2.468859
H	-3.167648	-1.898656	-3.262825
H	-1.794618	-0.970571	-3.869583
H	-3.388932	1.522822	2.141382
H	-1.957003	0.486850	2.000823
H	-3.568503	-0.235095	1.987751
C	0.415680	-0.660776	0.129548
C	1.419564	-1.000978	1.239518
C	2.555980	-1.772771	0.992350

C	1.142021	-0.584097	2.546535
C	3.410069	-2.112763	2.042146
H	2.813541	-2.107019	-0.015042
C	1.988107	-0.915140	3.597451
H	0.250369	-0.001335	2.758187
C	3.118771	-1.678813	3.327353
H	4.299086	-2.704452	1.850492
H	1.769542	-0.590193	4.608693
C	3.391342	-0.782987	-1.934655
C	4.602241	0.043427	-2.328469
C	5.864631	-0.544273	-2.188784
C	4.533218	1.346807	-2.838002
C	7.025153	0.153116	-2.513733
H	5.902659	-1.564407	-1.820349
C	5.690923	2.046966	-3.169264
H	3.565763	1.814383	-2.996515
C	6.943422	1.455893	-3.003759
H	7.995582	-0.319628	-2.388326
H	5.614649	3.054975	-3.567398
H	7.844900	2.002919	-3.263390
O	-0.006538	0.683055	0.437122
C	-0.213207	1.701816	-0.429366
O	-0.193670	1.635015	-1.631232
C	-0.499569	2.967522	0.313076
C	-0.421514	3.065401	1.702615
C	-0.891487	4.072934	-0.446372
C	-0.746074	4.260633	2.336794
H	-0.104198	2.214017	2.294308
C	-1.219353	5.270544	0.173537
H	-0.947153	3.980712	-1.526335
C	-1.146210	5.343827	1.562517
H	-0.689167	4.347421	3.416168
H	-1.528770	6.132390	-0.407433
C	2.224529	-0.110185	-1.628563

H	2.170586	0.969372	-1.678290
Cl	-1.570835	6.843629	2.355051
Cl	4.195700	-2.100541	4.642786

Vibrational frequencies

12.5033	18.8911	23.2936
24.8751	32.6692	37.6231
39.5120	45.2673	47.3793
55.3110	56.6459	66.6114
70.3979	87.4907	88.4909
98.8678	111.8121	119.4300
122.6730	128.9551	138.2568
144.8931	146.2373	155.2243
159.8352	171.7620	177.7404
182.9107	205.5975	214.4599
221.7357	240.7891	245.9246
253.0213	263.0121	271.3962
282.2979	285.8569	293.1663
303.6960	313.0202	326.8900
334.2762	339.3271	349.5923
373.0731	381.7651	384.6153
398.2470	410.7860	420.8455
422.3281	426.0801	432.1046
441.8053	445.5711	471.6506
480.6549	487.0654	499.6143
514.2563	520.2187	530.6204
544.1380	551.1448	560.7819
566.9835	578.7683	585.5804
593.9850	612.7372	628.9251
638.5210	640.6673	645.0294
658.8366	661.3702	678.2740
687.4595	689.7410	712.0384
723.2455	733.5557	740.7039
749.1920	752.5138	759.5390

768.0812	773.4518	796.4171
815.1513	816.5134	819.7206
844.3194	858.8449	862.5524
872.0076	874.8476	876.2564
890.8116	892.1901	913.9710
914.2836	925.2481	927.8573
958.1539	962.8399	968.6677
976.1333	980.8409	995.7207
1003.6664	1010.2647	1010.6743
1012.5758	1016.2473	1026.0849
1026.5471	1031.3927	1039.2094
1040.6282	1045.1312	1056.1146
1058.9190	1060.2349	1063.1092
1066.7431	1068.2406	1071.6631
1086.1371	1093.5128	1100.7013
1107.0810	1119.0022	1127.1001
1132.7024	1136.8001	1148.3986
1158.6448	1165.3982	1167.1747
1169.6726	1173.4457	1190.2632
1191.8328	1199.5834	1206.6400
1218.1896	1229.8202	1233.4016
1258.1622	1263.5593	1275.6958
1283.5702	1293.4235	1296.3386
1300.7660	1315.9960	1318.2620
1327.8508	1329.5492	1339.5121
1339.8929	1351.8479	1352.7543
1353.8048	1356.3569	1362.6921
1370.7701	1375.3130	1391.3907
1402.2425	1409.2017	1412.7031
1424.9806	1426.1975	1454.2020
1455.6709	1456.6613	1464.0706
1475.2677	1475.6177	1477.4682
1480.9638	1481.5948	1482.4133
1485.4503	1489.8905	1491.0447

1498.6073	1501.1707	1506.2127
1510.5763	1512.9474	1540.2572
1541.8875	1542.3108	1556.1332
1636.7305	1666.0682	1667.8585
1668.7668	1678.4056	1686.6092
1686.7843	1687.3126	1689.9293
1693.7878	1867.0564	3062.2021
3065.6906	3068.0652	3070.4894
3078.2639	3079.7832	3082.2956
3082.4682	3092.1842	3113.5147
3127.9636	3131.1200	3132.3185
3133.6452	3136.1763	3140.7603
3143.5581	3159.2156	3160.7294
3162.0969	3166.7406	3167.7882
3190.5621	3200.6477	3207.2091
3211.1752	3221.1409	3224.8402
3226.3070	3231.1284	3231.2779
3237.2859	3238.3435	3243.2674
3252.5652	3252.8666	3261.0619

TS4

Zero-point correction= 0.679987

Thermal correction to Energy= 0.721454

Thermal correction to Enthalpy= 0.722398

Thermal correction to Gibbs Free Energy= 0.605620

Sum of electronic and zero-point Energies= -3144.092366

Sum of electronic and thermal Energies= -3144.050899

Sum of electronic and thermal Enthalpies= -3144.049954

Sum of electronic and thermal Free Energies= -3144.166732

Cartesian coordinates

O	-2.114198	1.989600	-1.555882
C	-0.362858	0.080703	-2.531555
C	1.626166	-0.828154	-1.134589

S	1.956175	-1.981658	-2.340704
C	3.228490	-2.682473	-1.419861
C	3.371583	-2.027154	-0.239268
N	2.465829	-0.979612	-0.106052
C	4.022061	-3.900049	-1.780853
C	3.753248	-5.092339	-0.816478
C	3.093152	-4.743245	0.524019
C	3.874004	-3.809183	1.457751
C	4.329278	-2.475821	0.817120
C	2.574165	-0.044455	0.999919
C	3.583654	0.927103	0.892506
C	3.671516	1.869433	1.909231
C	2.808935	1.841006	3.012496
C	1.874594	0.813883	3.104693
C	1.743187	-0.164036	2.110230
C	2.903531	2.906694	4.070801
C	0.769590	-1.296004	2.295614
C	4.574327	0.921420	-0.240782
H	0.059390	-0.678493	-3.193285
H	-0.260225	1.046096	-3.035090
H	3.821901	-4.194992	-2.813270
H	5.078717	-3.614789	-1.735780
H	3.100913	-5.807953	-1.325530
H	4.704023	-5.605011	-0.637172
H	2.104917	-4.308957	0.328588
H	2.907369	-5.679355	1.060741
H	3.240338	-3.588359	2.323198
H	4.765110	-4.319536	1.837464
H	4.463503	-1.706728	1.580867
H	5.299290	-2.615581	0.328207
H	4.429979	2.646211	1.840302
H	1.225509	0.758483	3.975710
H	2.259340	2.678416	4.922761
H	3.931051	3.012384	4.431156

H	2.600181	3.877717	3.664890
H	1.053429	-1.884598	3.173859
H	-0.237446	-0.906567	2.472696
H	0.723872	-1.959146	1.429589
H	5.043298	1.902857	-0.339307
H	4.115334	0.663252	-1.198503
H	5.367701	0.189214	-0.045697
C	0.481743	0.199916	-1.191848
C	1.042799	1.606606	-1.021748
C	1.983121	2.084542	-1.933099
C	0.615218	2.430169	0.019523
C	2.530156	3.357708	-1.790490
H	2.308236	1.460232	-2.762805
C	1.151039	3.703335	0.175619
H	-0.126417	2.066523	0.719904
C	2.113022	4.146946	-0.726447
H	3.270975	3.724082	-2.492731
H	0.830419	4.339957	0.993504
C	-2.601151	0.877024	-1.867860
C	-4.096384	0.698394	-1.711550
C	-4.853076	1.824523	-1.370174
C	-4.744590	-0.538722	-1.805248
C	-6.217610	1.722158	-1.117906
H	-4.334933	2.774401	-1.285180
C	-6.109010	-0.647002	-1.544781
H	-4.182043	-1.434548	-2.049488
C	-6.849803	0.481558	-1.195943
H	-6.788398	2.606449	-0.849116
H	-6.593094	-1.617721	-1.605113
H	-7.911737	0.393817	-0.985987
O	-0.376759	-0.045645	-0.104961
C	-1.189619	-1.157792	-0.286445
C	-2.424831	-1.067332	0.549022
C	-2.870108	0.136938	1.102342

C	-3.169599	-2.232654	0.733385
C	-4.063944	0.179089	1.814731
H	-2.311265	1.049455	0.920694
C	-4.367172	-2.204361	1.440038
H	-2.806232	-3.159643	0.302124
C	-4.800935	-0.991726	1.965305
H	-4.428766	1.112164	2.230648
H	-4.955812	-3.105297	1.576612
C	-1.801292	-0.218864	-2.247308
O	-0.711719	-2.231761	-0.651790
H	-2.237073	-1.108570	-2.682772
Cl	-6.319506	-0.932571	2.839082
Cl	2.810734	5.740437	-0.515710

Vibrational frequencies

-202.7691	21.1626	27.7545
29.4520	31.7740	38.3314
44.4297	47.3290	49.4900
58.4918	63.7539	71.7800
83.7729	86.4972	98.2052
99.1893	109.4633	118.9576
127.0595	132.4312	141.5366
144.9064	149.4386	170.1521
173.3392	181.5294	188.6037
203.3965	209.1293	211.7062
217.3471	233.6188	247.5792
252.3419	257.5967	270.3045
281.2185	284.8433	289.9149
306.4356	320.7927	325.2169
334.5076	343.9276	349.0439
361.2600	380.8800	393.2215
396.5464	412.6208	415.4854
418.6882	423.1828	427.1055
440.3258	447.2524	469.6920

474.1552	498.6264	500.0395
506.6867	525.2104	532.5754
542.9626	547.9166	556.3376
563.4376	578.3638	584.9000
594.6433	599.0351	610.1456
628.1274	638.6403	640.3383
656.9013	670.2303	688.3093
698.5545	711.8288	716.0796
719.9377	726.5759	740.2403
748.0204	752.0804	758.3593
758.8560	764.1003	782.4156
804.9709	816.7454	825.8252
844.0453	847.0785	852.0789
852.6193	857.0903	870.7407
885.2020	890.5007	909.2247
918.3480	923.7919	936.3820
958.4979	970.9808	973.0036
977.8809	979.1307	981.8263
991.8466	996.1310	998.4977
1005.0341	1014.4073	1017.4337
1020.6418	1023.2112	1031.3399
1037.4787	1042.4063	1050.3487
1057.6001	1059.6778	1061.9939
1065.2284	1066.1032	1066.6225
1075.0117	1083.9511	1090.4474
1105.9683	1115.7041	1123.0966
1128.7964	1129.1284	1137.5979
1143.4801	1147.8458	1159.9916
1167.3087	1182.6057	1186.7513
1191.8184	1198.0033	1203.7299
1208.9409	1225.8955	1238.8858
1257.2857	1266.9973	1271.7419
1277.5622	1290.7342	1294.2404
1297.8172	1314.0181	1315.4993

1323.7933	1332.3748	1333.4810
1338.2345	1344.9115	1346.7254
1350.9182	1352.8803	1360.8458
1365.8514	1373.6226	1384.6235
1404.1146	1416.8425	1418.8565
1431.0961	1433.7338	1451.5987
1456.5460	1457.2277	1464.6686
1465.9311	1472.9583	1475.3973
1476.3120	1480.0668	1484.5157
1487.0776	1489.6058	1491.6929
1495.0850	1498.6733	1500.4189
1502.3853	1511.2255	1538.0611
1540.7688	1548.6531	1548.8791
1635.2051	1660.4890	1667.1916
1673.3444	1682.4152	1684.6255
1685.3715	1685.5790	1690.2580
1693.5869	1717.2838	3066.6429
3067.5452	3069.9300	3075.5918
3077.3875	3078.8827	3090.2367
3094.7743	3097.0820	3112.4190
3125.8327	3128.4129	3136.7638
3139.0454	3145.9428	3148.5799
3152.6731	3162.0666	3166.0326
3173.2998	3180.5864	3199.1469
3200.0667	3200.4137	3201.4444
3212.7735	3221.8135	3221.8692
3227.0153	3228.7200	3229.1136
3233.5006	3241.5267	3242.7263
3247.5364	3248.2258	3266.6405

M4

Zero-point correction= 0.681225

Thermal correction to Energy= 0.722924

Thermal correction to Enthalpy= 0.723869

Thermal correction to Gibbs Free Energy= 0.604335

Sum of electronic and zero-point Energies= -3144.109054

Sum of electronic and thermal Energies= -3144.067354

Sum of electronic and thermal Enthalpies= -3144.066410

Sum of electronic and thermal Free Energies= -3144.185944

Cartesian coordinates

O	-2.169903	2.221145	-1.357631
C	-0.275167	0.573366	-2.482103
C	1.728011	-0.365839	-1.168635
S	2.416680	-0.979336	-2.595852
C	3.666493	-1.805617	-1.729278
C	3.528388	-1.595471	-0.395337
N	2.431428	-0.766591	-0.110414
C	4.719027	-2.602383	-2.445517
C	4.752633	-4.082330	-2.031974
C	4.675098	-4.324997	-0.513963
C	5.348666	-3.232320	0.328004
C	4.377833	-2.112869	0.730503
C	2.171618	-0.343172	1.256559
C	2.844614	0.778226	1.737150
C	2.573847	1.176618	3.051893
C	1.687585	0.473632	3.860773
C	1.077625	-0.678393	3.346994
C	1.314262	-1.120933	2.050365
C	1.395503	0.917371	5.269121
C	0.724666	-2.405222	1.542467
C	3.839800	1.557958	0.919580
H	0.178241	-0.084221	-3.224108
H	-0.318370	1.584783	-2.886203
H	4.559604	-2.530680	-3.525108
H	5.687820	-2.133188	-2.249229
H	3.934009	-4.615037	-2.526151
H	5.685359	-4.499979	-2.425284

H	3.624971	-4.403676	-0.205146
H	5.127997	-5.297085	-0.298050
H	5.735256	-3.659283	1.257352
H	6.213691	-2.819002	-0.201206
H	3.703900	-2.499077	1.504020
H	4.919299	-1.273767	1.184764
H	3.073613	2.061197	3.440767
H	0.406301	-1.254106	3.980325
H	1.663832	0.135799	5.986926
H	1.951651	1.822076	5.524385
H	0.328298	1.122325	5.399597
H	1.495792	-3.187460	1.525562
H	-0.069386	-2.744855	2.212898
H	0.321924	-2.306886	0.526241
H	3.570657	2.618829	0.910800
H	3.905315	1.217073	-0.115668
H	4.835434	1.475611	1.367663
C	0.505639	0.566112	-1.118616
C	0.963680	1.970618	-0.729567
C	1.799869	2.700487	-1.576065
C	0.523862	2.546183	0.460197
C	2.195049	3.993478	-1.245692
H	2.147896	2.269325	-2.512471
C	0.914819	3.835163	0.810715
H	-0.125058	1.974517	1.114370
C	1.744981	4.543775	-0.050708
H	2.841141	4.562542	-1.905290
H	0.574704	4.282736	1.738698
C	-2.596740	1.135203	-1.721165
C	-4.081516	0.890570	-1.730107
C	-4.916907	1.939396	-1.330862
C	-4.649334	-0.338747	-2.082054
C	-6.295136	1.767325	-1.284479
H	-4.463153	2.885215	-1.052865

C	-6.029864	-0.513476	-2.029054
H	-4.022504	-1.172275	-2.381460
C	-6.854152	0.537450	-1.631754
H	-6.934277	2.587984	-0.973683
H	-6.461439	-1.473083	-2.296452
H	-7.930093	0.397458	-1.590897
O	-0.374920	0.064031	-0.165398
C	-1.230081	-0.937293	-0.904150
C	-2.353236	-1.255252	0.084939
C	-2.859451	-0.327831	0.999750
C	-2.914428	-2.529212	0.031630
C	-3.925867	-0.658217	1.831786
H	-2.422536	0.664799	1.056231
C	-3.986770	-2.878468	0.848683
H	-2.490206	-3.240835	-0.669508
C	-4.481062	-1.930076	1.736856
H	-4.321839	0.060171	2.541916
H	-4.429819	-3.867733	0.799381
C	-1.655817	0.031015	-2.116250
O	-0.559009	-1.949980	-1.345917
H	-2.077476	-0.597368	-2.900849
Cl	-5.834531	-2.349582	2.773260
Cl	2.241295	6.168178	0.382153

Vibrational frequencies

9.1374	17.3027	20.3153
25.5886	30.1374	33.3238
41.9016	45.1122	55.0132
64.8709	72.9601	82.0848
87.7687	94.4093	98.2528
109.4201	121.9024	129.1581
132.5872	138.3055	145.6108
153.6414	162.5902	168.9205
177.3978	187.9447	195.7707

198.7895 203.8781 213.2985

231.4485 249.0315 249.6538

258.4780 271.5193 276.8337

289.9295 298.1655 316.3917

321.2390 333.5087 339.9569

351.6787 356.6999 359.6550

364.9697 383.1151 407.9738

414.8859 416.4903 418.2994

427.1738 429.0481 437.4841

445.5466 465.4529 470.0715

493.3802 501.8169 509.9492

520.6677 527.8664 534.0071

547.3541 553.2945 573.7442

576.8319 578.0574 590.0753

596.1444 599.2385 620.9535

626.1747 638.1378 638.7478

663.2758 675.7093 693.6310

705.6807 713.4813 727.4626

731.2123 740.3172 747.8219

750.2645 756.3176 765.7311

778.2497 796.8246 802.2702

815.6312 845.6696 855.7224

862.5915 864.0443 871.8574

881.0053 883.1375 886.2782

894.6582 914.0700 919.1416

930.6985 951.8865 963.4673

974.4043 976.9994 982.4412

982.7640 986.6070 989.1514

999.8701 1006.1795 1012.9097

1014.8743 1016.9972 1021.2635

1023.4921 1033.8613 1034.9334

1042.3573 1043.8265 1048.3203

1051.8561 1053.0387 1064.7159

1066.3430 1070.8620 1072.1250

1074.9619	1088.0591	1096.2047
1114.5992	1118.2732	1118.9828
1122.9518	1124.6218	1127.5901
1134.1736	1147.1215	1168.3605
1170.4655	1178.8920	1184.2432
1190.9782	1195.7567	1198.8548
1205.2345	1224.8545	1226.1550
1239.8694	1252.8012	1255.4964
1273.5396	1276.0850	1288.5840
1298.2035	1309.7259	1312.1401
1318.5903	1323.2028	1329.3926
1338.0510	1340.9221	1343.2856
1345.0426	1356.2791	1363.4359
1373.0136	1373.7859	1394.6686
1396.3969	1401.8988	1411.7515
1415.2610	1420.2415	1421.3458
1437.9728	1448.2403	1451.2545
1462.0609	1463.4240	1465.4003
1469.0705	1474.9366	1477.6815
1480.1281	1486.5920	1489.3893
1497.4963	1498.4616	1501.2925
1509.3476	1511.2479	1525.7654
1538.6509	1539.9136	1543.1290
1547.4399	1666.9871	1668.3977
1673.2543	1683.0127	1684.0741
1684.4338	1686.4535	1693.0076
1693.2076	1799.6671	3028.4036
3065.7258	3068.2992	3072.9590
3079.1584	3082.2458	3086.6418
3094.5039	3099.5015	3115.1504
3119.7005	3125.0260	3129.9573
3136.5253	3136.8307	3142.5239
3145.1501	3147.9588	3150.2317
3167.2461	3171.1569	3183.9034

3188.2369	3197.6218	3201.7645
3204.9818	3212.7858	3220.1461
3222.4414	3223.9454	3229.4218
3230.1268	3237.6073	3239.2836
3245.8213	3246.5693	3250.9477

TS5

Zero-point correction= 0.678124

Thermal correction to Energy= 0.720678

Thermal correction to Enthalpy= 0.721623

Thermal correction to Gibbs Free Energy= 0.600288

Sum of electronic and zero-point Energies= -3144.086781

Sum of electronic and thermal Energies= -3144.044227

Sum of electronic and thermal Enthalpies= -3144.043283

Sum of electronic and thermal Free Energies= -3144.164617

Cartesian coordinates

O	-2.341009	2.937766	-0.990612
C	-0.446600	1.302216	-2.136192
C	1.594229	-0.350704	-1.186449
S	1.973028	-1.070682	-2.689189
C	2.955439	-2.328540	-1.989705
C	2.971906	-2.181237	-0.642345
N	2.212354	-1.062356	-0.241371
C	3.647920	-3.373656	-2.818244
C	3.207372	-4.810075	-2.491951
C	3.126068	-5.128767	-0.988127
C	4.159039	-4.382609	-0.131955
C	3.629620	-3.043096	0.398201
C	2.167402	-0.671516	1.152463
C	3.203799	0.129917	1.641589
C	3.165202	0.483837	2.989391
C	2.132832	0.055415	3.829027
C	1.125925	-0.751348	3.297381

C	1.125960	-1.137118	1.955116
C	2.117820	0.462939	5.278983
C	0.067594	-2.045365	1.396762
C	4.312836	0.596464	0.738051
H	0.051598	0.740683	-2.927912
H	-0.461848	2.352376	-2.442235
H	3.472726	-3.174651	-3.879336
H	4.726922	-3.272078	-2.664219
H	2.233917	-5.004143	-2.954255
H	3.925088	-5.483338	-2.973283
H	2.124449	-4.883113	-0.613423
H	3.241444	-6.209069	-0.857920
H	4.428047	-4.984700	0.740513
H	5.085884	-4.232084	-0.695972
H	2.880737	-3.247978	1.173862
H	4.431700	-2.479528	0.891009
H	3.955669	1.115115	3.390201
H	0.318583	-1.093692	3.940586
H	1.248830	0.050701	5.796843
H	3.019267	0.114414	5.792817
H	2.090194	1.552556	5.378928
H	0.456560	-3.065792	1.285245
H	-0.795958	-2.087650	2.065771
H	-0.265394	-1.702616	0.415039
H	4.957753	1.308995	1.257194
H	3.913217	1.077988	-0.160954
H	4.933228	-0.245069	0.407567
C	0.281850	1.202338	-0.776127
C	1.378468	2.232445	-0.550916
C	2.166526	2.739214	-1.588527
C	1.588242	2.688344	0.747910
C	3.165857	3.671901	-1.331732
H	2.016724	2.394357	-2.608743
C	2.586732	3.618168	1.027311

H	0.964180	2.284521	1.539279
C	3.366254	4.093425	-0.019786
H	3.784185	4.061248	-2.133371
H	2.760575	3.962212	2.041837
C	-2.801935	1.898247	-1.422415
C	-4.290006	1.689616	-1.448623
C	-5.085793	2.596735	-0.740990
C	-4.897393	0.626999	-2.126961
C	-6.466333	2.443250	-0.704405
H	-4.601925	3.414515	-0.216802
C	-6.280969	0.476975	-2.094020
H	-4.304520	-0.091735	-2.684907
C	-7.065862	1.381204	-1.381604
H	-7.075788	3.146813	-0.145961
H	-6.746214	-0.348765	-2.622688
H	-8.144073	1.257314	-1.352427
O	-0.399651	0.847980	0.209927
C	-1.923884	-0.559939	-1.319354
C	-2.813521	-0.890845	-0.153252
C	-3.077614	-0.006181	0.896514
C	-3.368259	-2.171904	-0.128155
C	-3.898999	-0.390952	1.949549
H	-2.602263	0.967861	0.914708
C	-4.199269	-2.569201	0.914411
H	-3.149336	-2.861064	-0.937352
C	-4.454354	-1.667242	1.940377
H	-4.099515	0.288052	2.771207
H	-4.639135	-3.560255	0.930061
C	-1.893630	0.819027	-1.999566
O	-1.262050	-1.446985	-1.826929
H	-2.274090	0.618103	-3.010623
Cl	-5.499495	-2.149532	3.259224
Cl	4.641995	5.248740	0.319448

Vibrational frequencies

-149.0038	14.8063	18.2237
22.6910	23.5136	30.6909
37.0944	46.3256	49.8312
59.7099	60.9439	65.8275
72.4545	76.1718	88.1036
90.6900	97.9633	111.3183
120.3348	123.8574	130.6540
134.2266	138.2769	140.1483
152.2041	160.0102	168.0272
174.1808	184.1565	188.5497
197.6220	213.7767	241.4953
248.0566	255.5502	257.5955
266.3015	276.5843	283.1048
296.4486	315.0654	318.0863
328.7549	338.2603	346.2944
351.1909	351.7608	371.7269
380.4315	399.8485	414.8855
418.5892	422.8568	425.9198
430.6527	450.7982	457.1041
464.0667	464.8521	486.8310
505.8347	512.1622	529.2138
531.6729	534.0366	551.1479
553.3802	566.9697	574.6782
579.8012	585.5157	587.2281
591.8919	618.3853	625.4104
638.4756	638.8675	660.1740
669.5949	683.9617	702.8163
710.5371	719.5478	733.4174
738.6568	748.9770	751.3369
767.1633	772.7237	798.0440
799.8917	808.9804	845.3164
848.2928	855.6790	861.0111
862.8704	871.8155	878.3127

882.1743 896.8225 908.9624

923.0255 936.6795 959.5713

963.0499 966.2065 974.8423

977.8481 983.9939 986.3964

991.1532 996.8652 1005.7725

1010.5803 1015.4688 1016.4711

1019.1928 1023.5937 1026.7503

1036.7378 1037.5413 1042.9790

1044.5674 1054.3810 1058.9777

1060.3850 1064.8391 1066.4842

1072.1953 1077.2713 1095.6259

1112.5508 1117.5955 1118.0447

1125.5017 1128.1074 1132.2344

1133.4970 1140.2632 1171.6127

1188.4779 1188.6197 1192.9417

1201.2662 1208.1288 1216.0072

1219.3581 1241.6063 1251.3610

1258.5943 1262.3207 1262.9527

1275.8013 1281.6979 1299.1151

1299.2994 1314.7592 1315.3867

1316.4864 1337.0378 1344.8712

1347.4612 1348.8636 1355.2485

1359.1336 1365.8393 1370.3724

1372.1725 1378.8888 1393.1405

1400.4504 1408.9568 1411.5505

1414.1820 1427.1386 1443.8583

1445.1572 1447.2238 1455.6225

1460.2292 1464.3616 1467.9227

1475.2107 1476.0820 1478.8969

1479.6100 1488.0554 1491.0362

1499.2209 1500.8275 1515.7773

1516.4574 1537.0257 1539.5500

1544.8101 1551.1337 1620.6085

1662.7526 1674.8913 1676.4465

1680.2410	1681.6070	1686.6688
1690.3390	1692.6583	1694.8025
1795.9773	1833.7647	3057.7099
3062.5735	3062.8410	3063.8063
3066.6981	3070.9772	3074.6337
3082.3508	3091.1453	3103.9710
3115.4815	3115.6563	3124.7931
3130.6818	3133.5038	3134.0763
3137.3741	3137.8722	3159.2505
3159.3344	3167.4233	3183.8835
3184.4607	3192.7979	3199.8642
3210.0894	3214.1222	3214.7881
3222.3646	3223.4435	3225.3904
3226.4691	3229.4716	3233.6486
3237.2786	3240.2623	3247.2172

P

Zero-point correction= 0.333262

Thermal correction to Energy= 0.356258

Thermal correction to Enthalpy= 0.357202

Thermal correction to Gibbs Free Energy= 0.278310

Sum of electronic and zero-point Energies= -2031.368670

Sum of electronic and thermal Energies= -2031.345675

Sum of electronic and thermal Enthalpies= -2031.344731

Sum of electronic and thermal Free Energies= -2031.423622

Cartesian coordinates

C	-1.343224	-2.139841	-0.152057
O	-0.376294	-2.799825	0.177137
C	-1.156583	-0.689954	-0.598261
C	0.314490	-0.429748	-0.936523
C	-1.738877	0.253728	0.458448
O	-2.312456	-0.169906	1.440848
C	1.203521	-0.352039	0.285577

C	2.680667	-0.533726	0.114541
O	0.740783	-0.101540	1.382820
C	3.474364	-0.577441	1.265597
C	4.849966	-0.735333	1.174667
C	5.426488	-0.837524	-0.088753
C	4.664074	-0.786139	-1.250073
C	3.285314	-0.636800	-1.141243
C	-1.667961	2.569613	1.341921
C	-1.597873	3.948103	1.194515
C	-1.505408	4.477599	-0.090086
C	-1.478227	3.666322	-1.218588
C	-1.532780	2.285811	-1.053172
C	-1.627370	1.730072	0.225042
H	0.664212	-1.219794	-1.604709
H	0.429683	0.515371	-1.480494
H	2.997697	-0.488565	2.236141
H	5.467130	-0.776186	2.065506
H	5.137600	-0.863900	-2.222358
H	2.696253	-0.594442	-2.051291
H	-1.749553	2.129030	2.330155
H	-1.616068	4.603064	2.058554
H	-1.415431	4.102763	-2.209078
H	-1.522042	1.653468	-1.935650
C	-2.710417	-2.746676	-0.178757
C	-3.846826	-2.028924	-0.566363
C	-2.836781	-4.091038	0.187717
C	-5.091529	-2.650610	-0.586336
H	-3.775180	-0.983277	-0.848950
C	-4.080181	-4.710663	0.167570
H	-1.947136	-4.637076	0.484700
C	-5.209781	-3.990182	-0.220430
H	-5.969827	-2.087976	-0.886027
H	-4.170766	-5.753987	0.453090
H	-6.182190	-4.472974	-0.237681

H	-1.738289	-0.534484	-1.516634
Cl	-1.427308	6.213169	-0.291190
Cl	7.158323	-1.036023	-0.217718

Vibrational frequencies

-4.6421	26.1508	31.4496
35.6775	44.7624	62.8519
65.6918	74.6590	83.8260
108.8719	114.2404	137.2494
152.5787	161.3658	196.2934
218.7369	251.0069	257.7304
273.0169	297.3278	321.7894
326.1231	352.9511	380.2400
416.0604	418.2533	422.9948
430.2457	438.7267	456.8516
473.7741	490.9242	530.1507
534.9145	544.0094	573.0529
613.3797	626.6584	637.9044
638.3906	658.4923	678.6313
708.0170	722.8925	733.2102
743.3294	761.7379	781.2322
793.3256	829.1789	853.8997
861.3691	868.3508	869.4274
883.3258	929.5508	954.6730
973.7403	978.4366	1000.3848
1003.3256	1008.8860	1014.7156
1015.8146	1018.5534	1020.8318
1028.1971	1035.7790	1042.5930
1064.4480	1071.0053	1106.0917
1125.3878	1127.1695	1129.1787
1138.9178	1141.0514	1170.8784
1194.3226	1196.1793	1207.8705
1219.7851	1246.3732	1253.6021
1273.0215	1321.3523	1326.8878

1330.7661	1342.2862	1346.5330
1347.9909	1366.6080	1378.6625
1413.6071	1443.7582	1453.5577
1454.9852	1499.9687	1546.0753
1546.7878	1551.4372	1664.3422
1664.5229	1673.8448	1683.5159
1684.9136	1696.4897	1821.2227
1826.7592	1839.9418	3086.2656
3091.8421	3151.9053	3206.5680
3219.9757	3225.4399	3233.7482
3234.1411	3237.7608	3238.1378
3240.6233	3240.8050	3245.2619
3245.9759	3249.9849	3251.9838

R1'

Zero-point correction= 0.148607

Thermal correction to Energy= 0.158501

Thermal correction to Enthalpy= 0.159445

Thermal correction to Gibbs Free Energy= 0.112205

Sum of electronic and zero-point Energies= -497.876601

Sum of electronic and thermal Energies= -497.866707

Sum of electronic and thermal Enthalpies= -497.865762

Sum of electronic and thermal Free Energies= -497.913003

Cartesian coordinates

C	2.749401	-0.916478	-0.168909
C	1.397994	-1.233708	-0.195944
C	0.436630	-0.236790	0.012534
C	0.841043	1.078589	0.268055
C	2.197174	1.389132	0.307233
C	3.149300	0.396810	0.082927
H	3.492417	-1.688796	-0.339794
H	1.067598	-2.250558	-0.383482
H	0.104896	1.854256	0.442872

H	2.509968	2.407944	0.512015
H	4.205958	0.645468	0.106713
C	-0.993694	-0.643662	0.003953
O	-1.345409	-1.805518	0.073232
C	-2.095765	0.424635	-0.159502
C	-3.411476	0.102373	0.480841
H	-3.797148	-0.834886	0.070634
H	-3.270160	-0.051576	1.555446
H	-4.118715	0.912255	0.304124
O	-1.881898	1.410579	-0.830187

Vibrational frequencies

37.9248	57.7236	126.3248
134.3515	178.6020	262.4060
299.6302	358.0355	411.5337
428.5781	461.9457	583.3203
604.9962	625.6592	701.0441
718.0578	721.1943	808.8082
882.8926	919.4683	973.4820
1009.7748	1015.9547	1023.1569
1037.9489	1043.1263	1065.6153
1116.8309	1173.9228	1187.9800
1209.5658	1332.2199	1346.6257
1361.8969	1396.5126	1448.7422
1454.9705	1498.3405	1544.4466
1670.4604	1689.2079	1822.0253
1865.8620	3083.4567	3163.4593
3200.3357	3218.8763	3222.5783
3232.0860	3242.7695	3256.1981

TS1[a]

Zero-point correction= 0.494334

Thermal correction to Energy= 0.522465

Thermal correction to Enthalpy= 0.523409

Thermal correction to Gibbs Free Energy= 0.436434

Sum of electronic and zero-point Energies= -1610.600786

Sum of electronic and thermal Energies= -1610.572654

Sum of electronic and thermal Enthalpies= -1610.571710

Sum of electronic and thermal Free Energies= -1610.658685

Cartesian coordinates

C	-4.950691	0.359702	-1.126485
C	-4.058750	-0.249983	-2.006409
C	-2.987403	-0.996968	-1.521590
C	-2.796803	-1.136807	-0.139481
C	-3.707652	-0.529108	0.737268
C	-1.670861	-1.906567	0.493985
C	-0.580767	-2.615929	-0.363723
O	-1.645785	-2.050391	1.703526
C	1.017147	-1.415347	0.318873
N	1.170260	-0.090586	0.299483
C	2.484905	0.428977	0.253963
C	3.404446	-0.565887	0.225721
S	2.583955	-2.105675	0.263591
C	2.756198	1.907340	0.280314
C	3.531206	2.425413	-0.944867
C	4.714412	1.544373	-1.376630
C	5.462251	0.898674	-0.202257
C	4.905493	-0.486413	0.163894
C	-1.569328	1.997797	1.661542
C	-0.479048	1.129603	1.619559
C	0.020063	0.783012	0.361801
C	-0.528476	1.255432	-0.831914
C	-1.615841	2.124755	-0.740622
C	-2.143576	2.508376	0.493963
C	-3.312482	3.454617	0.564992
C	0.014136	0.792019	-2.155286
C	0.130570	0.554421	2.867449

O	-0.554457	-2.511845	-1.600568
H	-5.783430	0.942240	-1.510063
H	-4.197037	-0.145329	-3.078348
H	-2.295787	-1.473686	-2.202419
H	-3.558871	-0.647185	1.805824
H	1.813792	2.452316	0.371464
H	3.324248	2.124735	1.190236
H	2.844165	2.548744	-1.788762
H	3.895080	3.426630	-0.689356
H	4.359575	0.750473	-2.045714
H	5.400108	2.157278	-1.969501
H	6.517505	0.761753	-0.455952
H	5.440891	1.562133	0.669209
H	5.244109	-1.204067	-0.593216
H	5.326379	-0.826199	1.117610
H	-1.983987	2.276107	2.627791
H	-2.068011	2.498912	-1.656608
H	-2.971428	4.495693	0.543046
H	-3.879326	3.311709	1.488637
H	-3.987726	3.311448	-0.283263
H	-0.538162	1.249130	-2.979315
H	-0.069577	-0.299030	-2.231503
H	1.073859	1.050837	-2.265367
H	-0.001176	-0.533366	2.883976
H	-0.341356	0.976176	3.757084
H	1.206152	0.757763	2.916458
C	-4.776068	0.213394	0.250004
H	-5.472214	0.679639	0.940867
C	-0.120951	-3.914599	0.287203
H	0.760632	-4.291062	-0.236959
H	0.079551	-3.802758	1.351886
H	-0.923898	-4.650032	0.157177

Vibrational frequencies

-130.2928 15.2767 33.9387

43.5240 51.8906 65.0635

77.9594 88.2084 98.4283

100.3500 121.4087 123.0133

139.3046 145.1732 169.0488

175.5614 183.2533 194.6132

205.4962 214.0818 221.6860

243.5764 250.6530 257.6646

260.1189 281.8281 288.5281

294.4409 310.3269 336.6283

354.4397 368.6788 378.9359

411.4976 420.5164 421.3332

428.4571 453.7555 465.1549

500.1058 505.3213 529.4239

536.9648 550.6746 584.4131

588.2967 590.7989 592.1250

599.6761 627.2520 632.4638

667.8138 700.0349 713.2534

716.3080 725.8075 743.0827

762.5785 808.0230 809.8539

845.4996 860.6366 879.1360

887.2649 908.6762 917.9943

919.0005 937.4198 964.1230

973.9596 976.9871 980.9007

994.5868 1002.9312 1006.0749

1019.7977 1020.7585 1026.5873

1033.5060 1035.0593 1039.3459

1060.1564 1063.1362 1064.3597

1066.6018 1067.0467 1073.7873

1092.1136 1110.3615 1113.0671

1128.0836 1165.5664 1168.9595

1186.0738 1197.2367 1197.9235

1212.8124 1246.5089 1261.6121

1274.7107 1275.8331 1298.8712

1302.7758	1328.0364	1334.6193
1342.3084	1355.0329	1355.7812
1360.1302	1368.1285	1377.3673
1391.2187	1398.4531	1408.9263
1411.3917	1411.6143	1426.1804
1449.1332	1455.3270	1471.4089
1474.3730	1476.1217	1477.0650
1478.3855	1480.1732	1482.8070
1483.8629	1488.0548	1488.9175
1490.8488	1498.0231	1509.2477
1516.0842	1535.7855	1545.7975
1661.0553	1674.8093	1682.9613
1687.2333	1691.9571	1697.2095
1807.2238	3053.0902	3058.7237
3061.2488	3064.2868	3068.0657
3068.5846	3070.1824	3078.3787
3093.5416	3106.6328	3111.4055
3122.3437	3122.7399	3125.9581
3127.7109	3135.9694	3146.0208
3148.3862	3154.1073	3162.9041
3163.8529	3190.1361	3196.2421
3197.6277	3202.3753	3217.5240
3222.8321	3234.5091	3272.9610

M1[a]

Zero-point correction= 0.495951

Thermal correction to Energy= 0.524337

Thermal correction to Enthalpy= 0.525282

Thermal correction to Gibbs Free Energy= 0.437014

Sum of electronic and zero-point Energies= -1610.610077

Sum of electronic and thermal Energies= -1610.581691

Sum of electronic and thermal Enthalpies= -1610.580747

Sum of electronic and thermal Free Energies= -1610.669014

Cartesian coordinates

C	5.187687	0.045489	-0.788884
C	4.315182	0.617729	-1.712023
C	3.106123	1.171772	-1.293358
C	2.766132	1.154949	0.066387
C	3.654109	0.584908	0.990425
C	1.477367	1.696340	0.610664
C	0.323877	2.199647	-0.325167
O	1.329243	1.806575	1.818750
C	-0.968559	1.433813	0.109757
N	-1.117160	0.111383	0.191653
C	-2.445330	-0.349320	0.282173
C	-3.336759	0.670948	0.256977
S	-2.497362	2.191369	0.141822
C	-2.767048	-1.810427	0.417717
C	-3.616400	-2.370493	-0.737039
C	-4.784083	-1.467181	-1.163748
C	-5.457456	-0.743765	0.010398
C	-4.840338	0.635767	0.297058
C	1.613209	-2.077923	1.411484
C	0.521207	-1.213433	1.429416
C	0.007590	-0.803608	0.192866
C	0.477453	-1.287522	-1.030932
C	1.576725	-2.148950	-0.992878
C	2.164363	-2.538652	0.211140
C	3.379283	-3.425887	0.225349
C	-0.182462	-0.901141	-2.322995
C	-0.106376	-0.761040	2.718117
O	0.416776	2.011444	-1.634086
H	6.125670	-0.388575	-1.122655
H	4.575556	0.631308	-2.766115
H	2.400502	1.612297	-1.987579
H	3.377364	0.577343	2.039896
H	-1.842574	-2.385301	0.504798

H	-3.301913	-1.942167	1.362947
H	-2.975900	-2.572761	-1.601493
H	-4.005487	-3.337805	-0.401814
H	-4.429933	-0.718825	-1.883634
H	-5.516412	-2.080532	-1.696882
H	-6.516123	-0.576708	-0.206660
H	-5.424869	-1.370231	0.908055
H	-5.205425	1.339641	-0.459968
H	-5.187190	1.015623	1.264797
H	2.043835	-2.399459	2.356937
H	1.975992	-2.527416	-1.930771
H	3.320902	-4.166084	1.027965
H	4.282529	-2.828632	0.395428
H	3.499912	-3.949786	-0.725600
H	0.308377	-1.394638	-3.164667
H	-0.121092	0.188692	-2.431370
H	-1.239504	-1.193475	-2.322229
H	-0.228531	0.325133	2.738154
H	0.512498	-1.056652	3.567720
H	-1.096484	-1.215439	2.845103
C	4.857470	0.033734	0.567899
H	5.537181	-0.407950	1.290460
C	0.162927	3.694420	0.060163
H	-0.640564	4.132517	-0.540044
H	-0.023424	3.857542	1.124654
H	1.089505	4.205567	-0.219260

Vibrational frequencies

16.5701	26.4721	37.4078
45.1239	46.3977	61.6442
68.3120	82.7137	114.1313
124.7994	131.3623	135.7574
156.3716	160.9054	165.4226
179.4391	189.7252	210.4011

222.7709 232.1420 244.6054

253.8248 265.7233 275.7158

279.7545 283.8566 292.6649

308.4597 333.0707 345.8252

369.4108 382.7658 400.1062

411.2983 415.5483 431.4176

450.9063 461.2599 486.5085

504.0403 513.7745 527.3863

547.1420 553.4383 575.9203

588.3158 594.5248 600.8484

626.5741 642.9670 653.7449

693.9295 706.8823 719.9912

732.6761 745.8094 748.2656

774.0066 811.0670 833.3926

848.2441 879.5990 885.1692

892.2613 913.8107 923.0814

942.5520 956.8546 966.7379

979.7977 982.7864 985.3555

986.0256 1006.2907 1019.1260

1022.2853 1036.9178 1040.7001

1045.3883 1046.6403 1058.3236

1063.6251 1063.8140 1066.9666

1072.5544 1076.2616 1095.5356

1104.6101 1114.0914 1115.2880

1138.6548 1162.2265 1170.2384

1187.4969 1189.9911 1202.4527

1216.6538 1249.5430 1262.7102

1272.1928 1279.1664 1283.6737

1299.2870 1308.5051 1333.5055

1337.2729 1345.7609 1352.3148

1355.6207 1362.9592 1369.7241

1371.3984 1394.5779 1399.4039

1401.8876 1411.4475 1415.2305

1422.5794 1452.1026 1465.2910

1470.2968	1475.6195	1475.9312
1477.2659	1478.0049	1483.2821
1486.9121	1490.2532	1492.3809
1496.7027	1498.9808	1502.8133
1511.7802	1517.8484	1533.3700
1537.3241	1660.7674	1676.2020
1681.7764	1683.9827	1690.3279
1789.8615	3040.9049	3070.0184
3070.0832	3071.4957	3073.5149
3074.1799	3083.0172	3090.4159
3105.6766	3113.7215	3119.2426
3122.9096	3133.3338	3138.5747
3143.6389	3145.4275	3150.8752
3159.7966	3166.3960	3171.1227
3173.1344	3178.9057	3208.0781
3212.0707	3216.2514	3225.3406
3235.1103	3243.1193	3249.3787

TS2[a]

Zero-point correction= 0.494880

Thermal correction to Energy= 0.522961

Thermal correction to Enthalpy= 0.523905

Thermal correction to Gibbs Free Energy= 0.436086

Sum of electronic and zero-point Energies= -1610.595403

Sum of electronic and thermal Energies= -1610.567322

Sum of electronic and thermal Enthalpies= -1610.566378

Sum of electronic and thermal Free Energies= -1610.654197

Cartesian coordinates

C	-6.614754	-0.307933	-0.163144
C	-5.805177	0.725175	-0.633298
C	-4.424955	0.677514	-0.450826
C	-3.835946	-0.409394	0.203609
C	-4.656854	-1.433132	0.687389

C	-2.355101	-0.571905	0.448727
C	-1.402168	-0.193816	-0.656043
O	-1.966521	-1.116987	1.500106
C	-0.053257	-0.814481	-0.374932
N	1.032737	-0.193390	0.065996
C	2.117253	-1.033157	0.376158
C	1.835688	-2.336842	0.128962
S	0.207515	-2.493387	-0.457402
C	3.408332	-0.492867	0.919214
C	4.613423	-0.730752	-0.006582
C	4.684108	-2.147140	-0.600803
C	4.220572	-3.241801	0.370256
C	2.716142	-3.549208	0.263217
C	1.130682	3.313811	1.263017
C	0.910949	1.940128	1.267147
C	1.178351	1.250234	0.082284
C	1.670054	1.857548	-1.070616
C	1.874775	3.240156	-1.024180
C	1.608617	3.978884	0.127280
C	1.826006	5.468739	0.160683
C	1.975478	1.056172	-2.308366
C	0.405907	1.203344	2.472658
O	-1.623891	1.007138	-0.021402
H	-7.690255	-0.268054	-0.307777
H	-6.252116	1.578193	-1.135696
H	-3.786870	1.486488	-0.788444
H	-4.196134	-2.262023	1.215424
H	3.305113	0.574375	1.125258
H	3.584401	-0.978706	1.883441
H	4.607044	0.006722	-0.816582
H	5.512953	-0.537330	0.587622
H	4.073123	-2.199760	-1.510990
H	5.714620	-2.337570	-0.915008
H	4.748405	-4.176785	0.162442

H	4.479632	-2.966806	1.398143
H	2.553129	-4.169463	-0.625927
H	2.387073	-4.146146	1.121378
H	0.925026	3.881692	2.167818
H	2.258353	3.742810	-1.908608
H	0.871318	5.998855	0.243137
H	2.329211	5.816471	-0.744372
H	2.431782	5.757312	1.024788
H	2.461774	1.682558	-3.058546
H	1.062613	0.642850	-2.750734
H	2.636062	0.210180	-2.086121
H	-0.490985	0.630556	2.209906
H	0.172339	1.901238	3.279752
H	1.159109	0.496993	2.843535
C	-6.036131	-1.387698	0.501340
H	-6.660035	-2.193112	0.877831
C	-1.745788	-0.267414	-2.137916
H	-1.519294	-1.245354	-2.574466
H	-2.806806	-0.061448	-2.287486
H	-1.173930	0.496998	-2.674306

Vibrational frequencies

-233.5780	26.1960	30.9355
33.1426	42.0564	56.6123
59.0708	73.6536	78.5700
109.8213	115.3259	117.0518
125.4437	147.1258	153.4419
166.6916	170.7748	187.5674
205.4969	217.4687	228.4714
238.6226	250.5573	257.7853
264.0954	281.8308	285.0334
300.8482	332.0286	361.0904
369.5930	374.9788	386.6605
422.9100	429.6389	431.5556

444.8310 469.7119 496.3947

506.3189 511.2860 527.7429

544.5381 557.6082 575.7444

588.7382 594.7916 606.7098

613.0031 630.5018 650.9078

665.3784 701.9251 725.0639

728.7165 745.4871 756.1849

781.3621 796.2919 844.9022

859.5472 884.0442 887.3818

891.6362 915.5981 926.1242

954.1061 958.2764 965.0102

969.7089 982.5357 984.8986

987.5320 1004.0770 1015.5374

1020.6957 1035.4700 1036.1809

1044.3265 1053.7001 1057.3598

1061.6191 1067.6376 1070.4434

1073.5168 1083.8074 1102.6919

1108.5454 1114.8819 1136.3992

1162.2183 1169.5053 1185.9201

1186.8901 1197.1255 1213.9443

1220.3101 1243.7803 1250.9526

1273.5140 1276.0834 1288.6664

1304.8762 1327.7292 1334.2488

1339.0933 1346.7636 1356.1664

1357.8254 1367.7429 1369.9049

1393.8887 1394.7216 1402.5081

1404.4652 1414.2061 1417.6188

1429.8223 1456.6523 1464.9775

1466.5147 1469.6553 1475.9216

1477.8994 1478.5274 1480.9421

1487.4113 1490.3849 1493.6230

1499.3388 1500.0286 1510.5489

1518.0997 1528.8656 1539.7787

1550.5217 1632.6144 1675.5553

1681.6695	1690.3761	1693.1600
1695.7393	3051.9717	3064.6034
3065.2194	3067.8899	3070.7165
3073.3224	3073.6504	3087.2084
3098.9707	3113.7958	3116.1470
3123.7548	3125.8325	3132.3216
3133.9768	3141.8123	3143.5474
3153.5691	3159.7852	3162.9774
3166.6252	3172.7099	3195.2908
3196.8800	3199.2943	3207.8732
3220.4020	3231.8041	3236.4991

M2[a]

Zero-point correction= 0.496615

Thermal correction to Energy= 0.525201

Thermal correction to Enthalpy= 0.526145

Thermal correction to Gibbs Free Energy= 0.437490

Sum of electronic and zero-point Energies= -1610.651833

Sum of electronic and thermal Energies= -1610.623247

Sum of electronic and thermal Enthalpies= -1610.622303

Sum of electronic and thermal Free Energies= -1610.710959

Cartesian coordinates

C	5.221545	-0.159189	0.345516
C	5.420704	-0.423184	-1.009796
C	4.508168	0.040318	-1.957577
C	3.385895	0.756084	-1.552209
C	3.185347	1.015905	-0.194085
C	4.105197	0.563081	0.753933
C	1.966517	1.712565	0.300067
O	1.026537	1.822179	-0.665306
O	1.815275	2.119297	1.428178
C	-0.207491	2.375186	-0.292124
C	-1.241973	1.537035	-0.103541

N	-1.248611	0.135915	-0.161591
C	-2.531170	-0.432798	0.031166
C	-3.514271	0.459142	0.227318
S	-2.886671	2.120868	0.232447
C	-2.641923	-1.931801	-0.024570
C	-4.072553	-2.478152	-0.130299
C	-4.902579	-1.764489	-1.205952
C	-5.676182	-0.537549	-0.689179
C	-4.981119	0.215921	0.455775
C	-0.078260	-0.645111	0.148323
C	0.639309	-1.244259	-0.892374
C	1.730825	-2.050657	-0.565536
C	2.122560	-2.249564	0.759167
C	1.399737	-1.614850	1.772282
C	0.294204	-0.810900	1.488869
C	0.262128	-0.982147	-2.323840
C	-0.466702	-0.111450	2.582024
C	3.301897	-3.126170	1.091337
H	5.931657	-0.523365	1.081290
H	6.290110	-0.990911	-1.327429
H	4.668501	-0.162315	-3.011750
H	2.664868	1.108625	-2.281976
H	3.924848	0.767461	1.804586
H	-2.075061	-2.267055	-0.903141
H	-2.132796	-2.366958	0.845355
H	-3.989700	-3.543067	-0.367354
H	-4.577571	-2.421042	0.840183
H	-4.228085	-1.460986	-2.016321
H	-5.617661	-2.462861	-1.651797
H	-5.856916	0.151192	-1.521390
H	-6.660022	-0.851112	-0.321943
H	-5.488628	1.173437	0.609130
H	-5.106052	-0.338478	1.392099
H	2.301280	-2.515497	-1.366964

H	1.703810	-1.745293	2.808924
H	-0.727051	-1.388442	-2.562200
H	0.221457	0.095382	-2.513156
H	0.989537	-1.430232	-3.004901
H	-0.119287	-0.437435	3.564782
H	-0.321664	0.972257	2.506978
H	-1.542747	-0.307024	2.512281
H	3.997616	-3.185745	0.250316
H	3.842140	-2.746831	1.963226
H	2.977520	-4.146193	1.326497
C	-0.248653	3.861105	-0.166816
H	-1.257392	4.248254	-0.341124
H	0.081490	4.200557	0.821816
H	0.411394	4.312132	-0.914286

Vibrational frequencies

13.0332	35.8854	41.5499
48.6373	56.6087	62.8745
89.9173	94.2773	95.2322
105.4093	120.3364	129.2420
144.3967	149.5989	156.2935
176.6695	178.1683	189.7233
194.9110	206.0144	219.2363
233.8798	247.0260	259.3447
278.5588	285.3142	305.8740
319.9061	330.5120	347.4233
368.1476	388.0555	397.7901
413.5217	427.1294	432.8093
443.4901	467.2823	501.6347
505.0467	520.1642	531.9375
554.6201	562.2900	568.0600
577.3099	588.5794	591.8570
606.3963	624.4643	646.9256
695.8207	702.9563	715.5723

731.1971	752.3767	793.2947
818.4850	826.6234	842.7820
875.0320	880.6338	883.9206
889.5024	912.0075	926.3493
937.5054	959.7784	968.1914
975.7670	980.9949	986.5597
1011.3009	1016.8405	1017.9829
1032.2415	1036.5763	1041.8018
1052.7180	1055.1951	1058.7404
1060.3456	1061.8855	1061.9282
1066.5996	1073.3179	1091.9118
1113.6256	1115.6216	1137.9624
1150.0041	1175.0826	1187.3753
1193.8064	1202.6957	1206.0492
1230.0273	1249.2841	1263.1288
1272.9804	1283.3421	1300.8538
1311.2270	1318.6511	1331.6450
1333.3133	1345.8255	1356.3682
1363.4057	1370.9030	1375.0582
1392.8068	1405.6266	1406.6871
1409.3600	1416.9420	1424.4289
1427.9622	1455.5978	1466.3922
1468.1473	1472.1952	1477.2059
1479.1622	1482.0328	1483.6024
1485.2191	1485.3937	1487.4165
1497.4251	1499.6535	1510.1478
1513.1921	1541.5655	1546.4173
1673.4842	1676.9468	1690.1864
1691.3240	1738.5954	1777.0423
1851.9787	3054.8142	3055.2126
3059.5651	3060.6181	3062.8512
3063.6389	3066.6644	3071.8710
3082.2851	3094.7837	3107.8681
3116.9091	3124.1959	3125.0167

3126.3169	3129.4046	3130.6514
3132.3386	3146.1134	3156.5081
3162.1954	3163.7203	3182.2402
3194.3628	3217.5079	3226.4255
3233.3002	3242.1724	3248.7589

TS3[a]

Zero-point correction= 0.643235

Thermal correction to Energy= 0.680571

Thermal correction to Enthalpy= 0.681515

Thermal correction to Gibbs Free Energy= 0.571678

Sum of electronic and zero-point Energies= -2033.293671

Sum of electronic and thermal Energies= -2033.256335

Sum of electronic and thermal Enthalpies= -2033.255391

Sum of electronic and thermal Free Energies= -2033.365227

Cartesian coordinates

O	3.838127	0.968853	-0.201703
C	1.546842	-0.246730	0.899755
C	0.004605	1.029474	-0.931771
S	1.016018	2.339102	-1.476249
C	-0.190332	3.519681	-1.030890
C	-1.262781	2.923900	-0.477841
N	-1.148771	1.527204	-0.401325
C	-0.026157	5.007667	-1.108315
C	0.071354	5.677301	0.289788
C	-0.517213	4.871763	1.455001
C	-2.001407	4.495669	1.360525
C	-2.405417	3.711057	0.085920
C	-2.215113	0.738065	0.167205
C	-3.216437	0.275456	-0.699754
C	-4.268322	-0.448178	-0.153912
C	-4.332721	-0.724980	1.218159
C	-3.329408	-0.231039	2.044596

C	-2.258957	0.522628	1.543360
C	-5.463238	-1.555095	1.764315
C	-1.232500	1.075895	2.497112
C	-3.119505	0.543209	-2.175654
H	0.738363	-0.728345	1.443149
H	1.568703	0.839497	0.954519
H	0.847289	5.269321	-1.710950
H	-0.897586	5.401801	-1.643759
H	1.125493	5.863203	0.519111
H	-0.413995	6.658033	0.234206
H	0.073611	3.955726	1.579859
H	-0.372592	5.449944	2.374276
H	-2.251866	3.895364	2.241453
H	-2.617547	5.399874	1.411672
H	-3.264848	3.068000	0.288162
H	-2.716470	4.417842	-0.690998
H	-5.049037	-0.822984	-0.812642
H	-3.373522	-0.422418	3.114709
H	-5.428067	-1.608187	2.854694
H	-6.432944	-1.143075	1.468892
H	-5.412744	-2.576534	1.370982
H	-0.499544	1.713796	1.998721
H	-1.725478	1.663435	3.277615
H	-0.692943	0.266424	2.998691
H	-3.964483	0.098803	-2.705931
H	-2.192320	0.124643	-2.585063
H	-3.107876	1.618899	-2.385640
C	0.471061	-0.302270	-0.933217
C	3.910343	-0.163975	0.309812
C	5.267666	-0.822637	0.387516
C	6.289651	-0.321687	-0.425267
C	5.549097	-1.891530	1.245500
C	7.560894	-0.885329	-0.399088
H	6.060646	0.516807	-1.075266

C	6.823254	-2.453490	1.278555
H	4.778154	-2.276226	1.905989
C	7.830662	-1.955380	0.453965
H	8.342775	-0.491978	-1.042081
H	7.031598	-3.278670	1.953093
H	8.822805	-2.396149	0.479921
O	-0.605287	-1.225440	-0.869607
C	-0.419532	-2.464834	-0.382344
O	0.618334	-2.876879	0.082157
C	-1.661756	-3.285268	-0.470509
C	-2.678132	-3.006902	-1.386245
C	-1.775219	-4.374905	0.396760
C	-3.809602	-3.818159	-1.427395
H	-2.578563	-2.167294	-2.066215
C	-2.913430	-5.172003	0.364279
H	-0.970394	-4.579547	1.095408
C	-3.930677	-4.894277	-0.549487
H	-4.597409	-3.609036	-2.144417
H	-3.007901	-6.009487	1.047901
H	-4.817906	-5.519349	-0.578794
C	2.775548	-0.884653	0.801250
H	2.847330	-1.949419	0.984955
C	1.538776	-0.700417	-1.909976
H	1.130602	-0.802638	-2.922333
H	2.347528	0.034540	-1.907790
H	1.975457	-1.651104	-1.593867

Vibrational frequencies

-428.8048	18.1373	19.1759
23.9949	28.8717	32.3730
39.7709	50.1571	54.3654
54.8652	64.8040	77.5204
83.6349	95.7189	100.7151
106.6956	111.1541	126.1761

127.1333	151.6442	154.9148
164.7407	175.3542	181.5879
185.6792	198.9078	211.4395
215.0477	222.4909	247.3363
253.7910	265.9335	281.3147
288.1664	290.5848	307.3374
315.0492	325.7518	331.7410
349.6027	364.0833	372.6501
387.0388	402.9288	405.8485
417.7193	420.6609	427.2787
435.3896	442.2761	452.8466
471.9643	505.1609	512.2563
527.4603	531.3995	544.0197
551.8306	569.2756	576.5888
592.9265	597.6331	627.3619
629.0902	629.6222	644.9356
660.2193	685.8758	700.5721
706.3152	710.4305	721.3334
724.4268	728.8293	750.1314
755.5635	760.9587	793.5923
808.5505	816.8497	826.6098
831.6955	857.6787	873.4863
879.8193	887.7101	894.7692
912.6853	921.5306	928.9748
954.6210	965.4476	966.4350
968.0034	972.5375	979.7374
983.3360	1004.4234	1008.1605
1012.5813	1014.9621	1019.3942
1021.6161	1030.5188	1032.4658
1041.6322	1044.6324	1051.2294
1055.9468	1060.3026	1061.3189
1063.3321	1064.4515	1065.9684
1079.3738	1083.1843	1089.6150
1104.8535	1112.4092	1117.1195

1125.7974	1139.8165	1152.9380
1166.5446	1170.1708	1181.7728
1185.1044	1192.1704	1198.0407
1203.7077	1217.3600	1237.3909
1240.4120	1260.2990	1268.7160
1278.0313	1280.6721	1285.3389
1295.5736	1321.9418	1324.6213
1332.2315	1335.7301	1347.7233
1349.5541	1361.1308	1362.2447
1366.1641	1366.7916	1385.4122
1390.4666	1403.1732	1409.2520
1412.7153	1413.5103	1422.9240
1424.4157	1428.9040	1459.5723
1462.5720	1468.8178	1471.7573
1473.0917	1475.3490	1475.9627
1481.6022	1487.4014	1489.5319
1491.6514	1493.5962	1497.3345
1501.5101	1502.8438	1503.9767
1513.6118	1542.3432	1547.0924
1551.3258	1589.2183	1660.9928
1679.9326	1685.8075	1691.1899
1696.1763	1697.8833	1700.3673
1709.3619	1843.5491	3056.4223
3061.4006	3063.1486	3063.9039
3072.3356	3076.2000	3077.8932
3079.6229	3085.7103	3107.9935
3120.5535	3121.4247	3126.1291
3130.8392	3146.1128	3146.2904
3150.1849	3150.9593	3153.6008
3162.6492	3163.1522	3168.0003
3168.6657	3187.3297	3188.8658
3197.8944	3207.2213	3212.0358
3214.7629	3216.3505	3223.1509
3228.4631	3229.6581	3229.9862

3237.4715 3238.3961 3256.4887

M3[a]

Zero-point correction= 0.646482

Thermal correction to Energy= 0.683129

Thermal correction to Enthalpy= 0.684074

Thermal correction to Gibbs Free Energy= 0.576398

Sum of electronic and zero-point Energies= -2033.311711

Sum of electronic and thermal Energies= -2033.275064

Sum of electronic and thermal Enthalpies= -2033.274120

Sum of electronic and thermal Free Energies= -2033.381796

Cartesian coordinates

O	-3.113081	-3.118951	-0.158721
C	-1.116113	-1.203960	0.591351
C	0.956373	-1.184124	-0.826933
S	1.345001	-2.667963	-1.577019
C	3.008964	-2.517979	-1.160199
C	3.223316	-1.361827	-0.482779
N	2.047870	-0.635840	-0.291480
C	4.086636	-3.522642	-1.422544
C	4.591619	-4.182298	-0.115672
C	4.488596	-3.314133	1.145271
C	5.142408	-1.929150	1.087563
C	4.573956	-0.954472	0.017851
C	2.061547	0.600643	0.466299
C	2.264457	1.794442	-0.238080
C	2.279347	2.970606	0.501733
C	2.123603	2.964864	1.893820
C	1.977260	1.746050	2.548912
C	1.953823	0.532265	1.853075
C	2.123756	4.265058	2.651960
C	1.867081	-0.772124	2.600661
C	2.447761	1.790422	-1.730002

H	-0.545958	-0.768312	1.413931
H	-0.942492	-2.288142	0.573235
H	3.746995	-4.284820	-2.127463
H	4.908396	-2.985480	-1.909581
H	4.018379	-5.097620	0.062026
H	5.631673	-4.485192	-0.275860
H	3.430877	-3.194287	1.409982
H	4.944091	-3.868084	1.972746
H	5.029861	-1.468126	2.073513
H	6.217725	-2.035776	0.911883
H	4.545238	0.065875	0.405256
H	5.235108	-0.940874	-0.855073
H	2.408073	3.916990	-0.019415
H	1.875739	1.726951	3.631415
H	1.911443	4.107512	3.711546
H	3.093476	4.766017	2.566790
H	1.371393	4.949341	2.246253
H	1.551197	-1.603582	1.966528
H	2.845207	-1.026353	3.024653
H	1.160619	-0.689192	3.430580
H	2.577697	2.808459	-2.102196
H	1.582574	1.345410	-2.232533
H	3.330585	1.204772	-2.012761
C	-0.485716	-0.704461	-0.749722
C	-3.450475	-1.996419	0.336867
C	-4.943005	-1.752393	0.502037
C	-5.819039	-2.577561	-0.211399
C	-5.495147	-0.766546	1.330846
C	-7.199137	-2.411250	-0.127458
H	-5.378307	-3.353142	-0.829813
C	-6.874712	-0.597591	1.421449
H	-4.843919	-0.136144	1.929004
C	-7.734522	-1.416149	0.688984
H	-7.859422	-3.058698	-0.698386

H	-7.281297	0.169246	2.075046
H	-8.810084	-1.283799	0.761027
O	-0.486751	0.719306	-0.982355
C	-0.775969	1.686985	-0.085996
O	-0.939720	1.538492	1.099247
C	-0.846227	3.019741	-0.762365
C	-0.800732	3.161325	-2.150630
C	-0.938346	4.148860	0.056540
C	-0.839738	4.434023	-2.715313
H	-0.740834	2.281966	-2.782665
C	-0.971999	5.416970	-0.510710
H	-0.973352	4.014002	1.133196
C	-0.920453	5.559651	-1.898089
H	-0.806821	4.546233	-3.794253
H	-1.035734	6.293998	0.125620
H	-0.945890	6.550360	-2.341545
C	-2.585510	-0.981994	0.710091
H	-2.940126	-0.021405	1.061138
C	-1.270894	-1.269233	-1.932562
H	-1.436988	-2.342431	-1.808699
H	-2.253738	-0.796860	-1.915437
H	-0.776682	-1.044886	-2.881534

Vibrational frequencies

13.9233	16.7461	26.1642
28.8725	36.2196	40.2711
48.9022	55.6002	59.0757
73.6881	84.3597	100.2123
107.7343	119.9997	129.3924
140.2433	149.2032	151.1809
154.8276	165.0603	172.4854
182.3605	183.8442	190.0510
222.3195	225.3056	233.8166
239.0643	256.1204	266.1946

284.1168 284.7743 295.6916

304.3793 314.6799 325.5291

335.3576 343.1753 355.6378

376.5358 382.6822 387.6192

410.0417 418.3354 420.3547

424.4078 434.3299 449.0400

454.7269 466.6652 491.8228

501.5865 512.2134 529.8297

533.1247 545.1994 563.9376

581.1490 583.4047 595.2071

609.9062 626.4107 627.8372

632.0645 656.4757 672.1143

676.4007 699.8992 700.8451

705.9901 718.7401 720.2863

734.7167 747.5502 752.8570

764.4192 780.1188 800.5198

808.2311 813.1894 815.3353

840.7774 871.8497 883.9753

885.5657 886.4663 900.7977

919.3373 922.4492 933.4245

953.8159 958.6685 963.6938

969.9742 972.6196 976.5944

982.0133 1006.6241 1014.7085

1017.8423 1018.8213 1021.3018

1022.3199 1035.0887 1041.0654

1046.5185 1047.7383 1054.8368

1056.2204 1060.9564 1064.7781

1067.9407 1069.0926 1069.9040

1081.8057 1096.5435 1102.1322

1107.4131 1118.2768 1128.5273

1156.1798 1159.6617 1165.5018

1166.3841 1171.3451 1179.3415

1184.6139 1193.1046 1196.1255

1201.4303 1217.3829 1227.1374

1246.8569	1267.2123	1280.8755
1287.5599	1294.4039	1302.4962
1308.4071	1327.5560	1328.1841
1331.3801	1332.5052	1337.2791
1346.9273	1353.0984	1355.8968
1364.0083	1366.0657	1374.3372
1386.9904	1401.0382	1410.7888
1413.0241	1417.6111	1427.3199
1429.8934	1440.1308	1461.1820
1465.3617	1468.8151	1471.2275
1479.2142	1480.9521	1483.1299
1485.0107	1488.3043	1488.5730
1489.8258	1491.2186	1495.7223
1500.1765	1501.7774	1504.8680
1512.7018	1515.6855	1540.4224
1542.0960	1542.4835	1636.2503
1670.0281	1677.4077	1680.0125
1686.8743	1689.1889	1693.9105
1693.9924	1857.3663	3055.7173
3066.9678	3067.6701	3069.4573
3070.0046	3076.4545	3078.8892
3084.4931	3087.5339	3095.8550
3116.7887	3126.8104	3133.9368
3136.6777	3137.9691	3141.0482
3148.7531	3155.8303	3158.3854
3166.2267	3169.8508	3170.1712
3175.5886	3183.5379	3194.6723
3196.0523	3200.6221	3202.6149
3207.3766	3216.3542	3219.9222
3221.8504	3225.0314	3227.6154
3232.3037	3241.4198	3253.5254

TS4[a]

Zero-point correction= 0.646051

Thermal correction to Energy= 0.681756

Thermal correction to Enthalpy= 0.682700

Thermal correction to Gibbs Free Energy= 0.579081

Sum of electronic and zero-point Energies= -2033.312692

Sum of electronic and thermal Energies= -2033.276987

Sum of electronic and thermal Enthalpies= -2033.276042

Sum of electronic and thermal Free Energies= -2033.379662

Cartesian coordinates

O	-2.859590	0.546143	-2.408435
C	-0.825460	-1.380615	-2.092963
C	1.483947	-0.796035	-1.094911
S	2.002098	-2.394690	-1.374932
C	3.495278	-2.129342	-0.558802
C	3.564818	-0.851180	-0.113716
N	2.426274	-0.111959	-0.440157
C	4.536904	-3.162282	-0.256953
C	4.657968	-3.453656	1.267232
C	4.059445	-2.398832	2.207711
C	4.662470	-0.989533	2.142144
C	4.697014	-0.357404	0.729455
C	2.401793	1.318877	-0.182440
C	3.076958	2.130510	-1.109904
C	3.086355	3.500247	-0.877176
C	2.470776	4.057625	0.250718
C	1.858779	3.206556	1.164447
C	1.819739	1.818883	0.978584
C	2.488597	5.548017	0.459262
C	1.190178	0.948771	2.029367
C	3.783724	1.538897	-2.299739
H	-0.357622	-2.364316	-2.020900
H	-0.987500	-1.170594	-3.155470
H	4.330246	-4.085513	-0.802927
H	5.488423	-2.778203	-0.639820

H	4.156423	-4.402663	1.479008
H	5.717627	-3.599009	1.502083
H	2.979889	-2.333112	2.022887
H	4.165535	-2.764732	3.234272
H	4.078740	-0.342951	2.805747
H	5.686150	-1.002378	2.530448
H	4.695364	0.732590	0.795333
H	5.622653	-0.646094	0.219981
H	3.588941	4.150244	-1.589646
H	1.398170	3.620746	2.058359
H	1.996283	5.824346	1.394167
H	3.515370	5.925586	0.485545
H	1.976210	6.059767	-0.361462
H	1.699420	1.096395	2.986860
H	0.142212	1.231663	2.170157
H	1.209637	-0.111238	1.772313
H	4.095596	2.328742	-2.985515
H	3.147540	0.838249	-2.849742
H	4.680254	0.990686	-1.986562
C	0.129180	-0.244050	-1.551217
C	-3.098962	-0.446264	-1.682609
C	-4.485993	-0.545448	-1.081973
C	-5.446561	0.373658	-1.516728
C	-4.837114	-1.451896	-0.074623
C	-6.724119	0.392046	-0.965728
H	-5.157683	1.079685	-2.288550
C	-6.109935	-1.426248	0.490723
H	-4.108236	-2.163268	0.300678
C	-7.058683	-0.505323	0.047272
H	-7.456990	1.111919	-1.318924
H	-6.359393	-2.123391	1.285681
H	-8.049964	-0.486331	0.490452
O	-0.498071	0.353019	-0.433774
C	-1.060530	-0.616424	0.398709

C	-2.135034	-0.040959	1.268158
C	-2.797238	1.151983	0.960949
C	-2.496777	-0.760428	2.408759
C	-3.825903	1.603652	1.783030
H	-2.529487	1.688463	0.056017
C	-3.527957	-0.307774	3.227301
H	-1.965431	-1.680347	2.631496
C	-4.196533	0.874643	2.914437
H	-4.348594	2.523185	1.536182
H	-3.809569	-0.876132	4.108779
H	-5.003424	1.228831	3.548994
C	-2.120701	-1.403049	-1.332932
O	-0.382384	-1.591075	0.747413
H	-2.426256	-2.345169	-0.894523
C	0.303205	0.837573	-2.613532
H	0.824880	1.712229	-2.223308
H	0.853925	0.435578	-3.468821
H	-0.704228	1.119419	-2.924759

Vibrational frequencies

-251.4780	16.1875	27.9558
37.1745	40.6671	42.9626
53.3343	55.6066	66.8941
80.8486	81.5642	92.2024
103.0170	106.3502	123.6270
129.4142	133.7107	139.6137
164.4806	169.9741	174.1208
179.4185	195.6594	200.3436
210.1908	223.1891	236.7694
247.5351	259.9750	271.3413
283.9141	288.4346	291.9568
300.9715	309.8723	318.3941
330.7576	344.5977	352.0296
373.7945	377.5770	390.6743

412.0230 414.1148 418.9492

423.3448 437.7655 457.5349

473.8101 480.6726 496.7445

505.0030 514.2050 528.9565

534.1147 550.2035 565.3613

577.6733 587.7675 595.6292

608.3622 616.1496 626.7772

627.3548 665.0297 672.1780

686.9151 698.9726 706.8574

711.1333 722.7745 736.5097

747.2970 750.8398 754.0759

759.7504 776.0861 797.4066

806.5985 816.0860 830.2677

854.3463 867.3294 880.4006

881.5896 885.5807 897.2088

916.0666 919.4114 935.0376

948.2778 954.6796 957.6694

973.9302 977.9125 980.5813

983.5644 1003.7447 1004.7976

1015.3136 1016.5650 1020.3581

1024.2925 1026.1657 1045.2983

1047.4179 1049.8097 1055.2930

1059.1802 1060.6681 1062.7575

1063.1232 1068.7457 1071.3838

1085.3725 1087.7539 1102.7916

1111.6726 1116.0942 1118.4530

1147.3992 1150.8490 1165.1685

1165.2801 1174.0541 1183.6837

1189.0899 1192.5569 1194.1772

1196.4510 1214.8553 1222.1297

1254.6951 1267.2378 1272.4583

1280.5211 1287.0833 1295.9260

1297.9465 1312.2618 1326.2051

1326.6590 1336.2367 1342.6963

1346.7442	1347.6971	1359.9195
1363.6913	1367.2374	1378.1216
1386.5830	1393.4258	1400.0362
1411.3670	1417.2693	1426.9232
1430.1055	1458.7040	1462.6830
1467.1533	1473.3250	1477.0925
1478.3323	1480.6247	1482.2100
1484.3046	1488.5722	1489.6259
1492.0241	1495.4931	1497.6667
1501.7083	1503.1437	1504.0729
1510.7417	1515.1631	1541.7580
1544.6608	1547.3508	1636.0296
1662.6349	1674.0516	1683.9773
1689.4690	1690.8126	1693.4722
1695.6826	1703.6359	3061.2800
3065.7890	3070.8376	3072.7130
3077.2892	3078.3077	3079.6297
3083.7074	3086.9342	3096.6159
3111.0466	3124.6031	3127.9276
3135.0171	3136.4869	3144.7308
3148.5070	3149.8982	3154.2676
3163.5082	3168.2503	3173.8292
3185.2919	3193.2169	3193.4119
3195.0612	3195.1394	3201.3706
3207.2625	3213.8690	3215.4788
3220.4587	3220.5228	3226.4428
3231.3945	3234.7188	3238.8245

M4[a]

Zero-point correction= 0.647897

Thermal correction to Energy= 0.683520

Thermal correction to Enthalpy= 0.684464

Thermal correction to Gibbs Free Energy= 0.581413

Sum of electronic and zero-point Energies= -2033.326915

Sum of electronic and thermal Energies= -2033.291293

Sum of electronic and thermal Enthalpies= -2033.290348

Sum of electronic and thermal Free Energies= -2033.393400

Cartesian coordinates

O	-2.963451	-0.255049	-2.487246
C	-0.810761	-1.835043	-1.710155
C	1.465152	-0.961729	-0.914221
S	2.109047	-2.537199	-0.941632
C	3.583325	-2.033205	-0.185827
C	3.551770	-0.699407	0.057426
N	2.349489	-0.117447	-0.382546
C	4.686952	-3.012180	0.098732
C	5.059356	-3.101879	1.586838
C	5.210879	-1.742274	2.293472
C	5.728882	-0.616641	1.387332
C	4.596520	0.163729	0.705643
C	2.185132	1.327173	-0.329357
C	2.696728	2.077843	-1.389768
C	2.530239	3.465458	-1.336673
C	1.906345	4.085985	-0.257296
C	1.465325	3.293890	0.807602
C	1.604286	1.908435	0.805904
C	1.706027	5.577496	-0.223079
C	1.201087	1.087813	1.997148
C	3.441051	1.456119	-2.543431
H	-0.319556	-2.766432	-1.427029
H	-1.118265	-1.911699	-2.754561
H	4.396100	-4.002738	-0.262555
H	5.560580	-2.717636	-0.490325
H	4.308206	-3.700152	2.112451
H	6.002489	-3.655384	1.644810
H	4.244129	-1.432675	2.710140
H	5.881603	-1.872029	3.147908

H	6.294700	0.108084	1.979143
H	6.426791	-1.012119	0.641882
H	4.094806	0.778102	1.462422
H	5.002104	0.860614	-0.037853
H	2.902062	4.067431	-2.162389
H	1.001169	3.768989	1.668994
H	2.091052	6.002822	0.708585
H	2.209848	6.066679	-1.059655
H	0.640762	5.825482	-0.274799
H	2.089090	0.833563	2.591707
H	0.534525	1.667000	2.641952
H	0.702554	0.153099	1.708110
H	3.255672	2.017634	-3.462312
H	3.165574	0.413879	-2.719626
H	4.519992	1.483557	-2.351731
C	0.105842	-0.580145	-1.516452
C	-3.132043	-0.890640	-1.455873
C	-4.507520	-0.940977	-0.844823
C	-5.541637	-0.269579	-1.506882
C	-4.781414	-1.593802	0.362134
C	-6.825328	-0.247921	-0.975023
H	-5.315669	0.238251	-2.438928
C	-6.065569	-1.564544	0.900011
H	-3.994357	-2.110383	0.901046
C	-7.088756	-0.893647	0.233179
H	-7.620665	0.275703	-1.496437
H	-6.265692	-2.066004	1.841859
H	-8.089334	-0.872159	0.654412
O	-0.556849	0.247136	-0.606119
C	-1.234926	-0.695133	0.341553
C	-2.155852	0.196863	1.175070
C	-2.749826	1.357863	0.671710
C	-2.442056	-0.200472	2.480610
C	-3.634896	2.093772	1.457164

H	-2.518739	1.674752	-0.340849
C	-3.333082	0.528435	3.266402
H	-1.949656	-1.093123	2.855097
C	-3.935467	1.676696	2.753741
H	-4.091210	2.994995	1.057285
H	-3.556684	0.204766	4.279222
H	-4.629595	2.248065	3.363020
C	-1.991854	-1.587747	-0.770695
O	-0.402649	-1.436758	1.005806
H	-2.327858	-2.498529	-0.275006
C	0.292125	0.164662	-2.837649
H	0.762957	1.136551	-2.684707
H	0.891349	-0.424662	-3.538404
H	-0.704645	0.318784	-3.255268

Vibrational frequencies

23.9323	25.9573	33.6574
40.9562	44.3447	50.3673
57.2645	69.7970	75.2095
91.4468	97.9807	109.8536
113.2499	114.4041	130.8182
139.7280	151.3449	157.8739
162.3365	171.8329	185.8905
196.0730	204.1229	211.0642
231.3623	249.6364	256.4399
263.3652	271.4637	284.9663
286.0041	297.7350	299.0316
314.5827	324.4163	333.6820
343.5484	354.5974	367.2129
385.7211	398.0327	412.7747
416.9387	418.7234	420.4664
440.3982	447.8605	466.3444
475.7562	491.3858	504.6935
526.6654	531.1208	540.4100

540.7003	573.1219	576.9314
578.3092	589.1789	595.6270
600.8378	627.5006	627.6765
641.0427	667.3847	678.4048
689.8355	709.5474	713.6394
720.7567	725.1328	739.6858
749.7381	762.5686	770.7056
779.1841	800.2639	808.3300
825.2955	849.7740	879.2552
882.5344	888.2682	888.5934
895.2623	917.2035	918.4369
932.1046	945.6354	950.2276
957.3971	964.7378	970.4248
974.9513	983.7927	987.7690
1000.6311	1004.6300	1014.5587
1016.0526	1019.5052	1019.8719
1022.7946	1024.7026	1037.0616
1040.1388	1049.9841	1060.2616
1060.9885	1063.7543	1066.6292
1068.5045	1069.8873	1078.5913
1088.4910	1092.2888	1097.4538
1106.8431	1119.3351	1121.3245
1130.1129	1145.8514	1165.2073
1171.7058	1174.7933	1176.6625
1190.2201	1192.2952	1200.4986
1207.2628	1220.2473	1224.8688
1237.9542	1250.3458	1257.4795
1268.9219	1277.3044	1286.5190
1296.5427	1309.6279	1318.8619
1328.9439	1333.3642	1339.8398
1343.1419	1355.8405	1356.0145
1363.6648	1365.2351	1373.9474
1393.3816	1399.2408	1401.4207
1402.5975	1406.0013	1415.5112

1420.2426	1422.9026	1435.9368
1461.5768	1465.2345	1470.4665
1471.1227	1477.9111	1478.9606
1481.2566	1486.5860	1486.7282
1490.5984	1496.3320	1498.3364
1500.3353	1501.6471	1509.7224
1510.8728	1512.3236	1527.0973
1536.8466	1545.8108	1548.1650
1672.2992	1675.3505	1682.9502
1688.7128	1691.4572	1694.5790
1694.9983	1788.1182	3025.4398
3065.4059	3068.7147	3073.3707
3073.5846	3075.0798	3085.4053
3086.2716	3095.2936	3099.2198
3111.9442	3114.4961	3117.9812
3124.8224	3132.6686	3140.9585
3141.1455	3143.2016	3149.5772
3150.2075	3167.8299	3169.8505
3172.8283	3176.8279	3193.4841
3195.2199	3196.2988	3201.1888
3203.6292	3204.8346	3214.0733
3219.7021	3219.8685	3224.1010
3225.3558	3241.1657	3249.2802

TS5[a]

Zero-point correction= 0.644445

Thermal correction to Energy= 0.681284

Thermal correction to Enthalpy= 0.682228

Thermal correction to Gibbs Free Energy= 0.575515

Sum of electronic and zero-point Energies= -2033.300992

Sum of electronic and thermal Energies= -2033.264154

Sum of electronic and thermal Enthalpies= -2033.263210

Sum of electronic and thermal Free Energies= -2033.369923

Cartesian coordinates

O	-3.205065	0.654355	-2.463684
C	-0.996744	-0.974049	-2.281323
C	1.573909	-0.633442	-1.295858
S	2.052297	-2.258897	-1.518924
C	3.460979	-2.127116	-0.501022
C	3.535873	-0.865064	-0.011880
N	2.471489	-0.068658	-0.483776
C	4.409000	-3.271500	-0.275712
C	4.564902	-3.670048	1.200058
C	4.769492	-2.490428	2.169161
C	5.504588	-1.289207	1.557838
C	4.546187	-0.270096	0.928382
C	2.411587	1.340145	-0.154224
C	3.109451	2.232914	-0.973719
C	3.055173	3.587336	-0.646479
C	2.342044	4.042416	0.466068
C	1.678130	3.111114	1.265198
C	1.700009	1.745418	0.975085
C	2.292153	5.514060	0.783038
C	0.997696	0.739683	1.841829
C	3.902179	1.741714	-2.155917
H	-0.405409	-1.890272	-2.320139
H	-1.390614	-0.800664	-3.287519
H	4.074265	-4.141344	-0.848367
H	5.383353	-2.993891	-0.690628
H	3.687822	-4.245892	1.513247
H	5.423001	-4.348567	1.258370
H	3.796572	-2.145070	2.540611
H	5.314177	-2.854754	3.045457
H	6.063186	-0.760013	2.335130
H	6.245176	-1.625468	0.824110
H	3.995590	0.229702	1.735595
H	5.107070	0.517598	0.409519

H	3.584296	4.302424	-1.272566
H	1.122720	3.452130	2.135906
H	1.771925	5.698914	1.725606
H	3.299885	5.933802	0.859660
H	1.770983	6.064903	-0.006651
H	1.719652	0.145312	2.416325
H	0.335170	1.240760	2.552459
H	0.406184	0.056789	1.227624
H	4.270035	2.583595	-2.746043
H	3.298381	1.100407	-2.805803
H	4.766250	1.150027	-1.831931
C	-0.164454	0.265262	-1.862826
C	-3.328161	-0.234167	-1.641562
C	-4.660157	-0.460028	-0.981291
C	-5.649085	0.512224	-1.165400
C	-4.934632	-1.576135	-0.184056
C	-6.891557	0.377312	-0.557896
H	-5.420688	1.374731	-1.783163
C	-6.180716	-1.712510	0.421828
H	-4.182733	-2.343110	-0.024098
C	-7.158417	-0.736481	0.238286
H	-7.650994	1.139704	-0.699939
H	-6.388145	-2.581244	1.038463
H	-8.127459	-0.843811	0.716061
O	-0.571830	0.907124	-0.864463
C	-1.643394	-1.171313	0.126787
C	-2.274192	-0.379313	1.237821
C	-2.733412	0.932882	1.087249
C	-2.374222	-1.007621	2.481794
C	-3.303134	1.596187	2.169444
H	-2.596790	1.437767	0.137480
C	-2.954058	-0.345389	3.560849
H	-1.998005	-2.020230	2.591269
C	-3.422178	0.957454	3.404374

H	-3.650788	2.618013	2.051631
H	-3.040386	-0.844760	4.520987
H	-3.874831	1.477171	4.243451
C	-2.170558	-1.170019	-1.319229
O	-0.745795	-1.952378	0.389505
H	-2.559694	-2.188372	-1.456411
C	0.386479	1.040985	-3.052089
H	1.070595	1.822690	-2.714399
H	0.888990	0.392418	-3.776090
H	-0.468950	1.519669	-3.544504

Vibrational frequencies

-179.6583	21.7881	24.0903
30.5778	37.6183	46.1600
50.9373	56.4036	64.7281
72.1804	81.2794	90.4303
92.7560	99.7123	108.8943
116.8001	122.1269	128.6776
132.8223	140.8566	157.7419
158.1909	162.6349	175.6474
194.0954	204.6142	207.0753
220.8884	240.8070	244.5967
246.2466	255.5183	281.2552
290.2914	308.0590	311.0743
321.0770	336.5520	347.3861
360.4416	363.5155	370.0463
382.4456	401.5572	416.1059
419.1833	423.4642	441.9582
449.9380	460.5888	463.3067
478.9597	504.2111	519.3007
527.2041	543.6234	550.1270
557.9824	572.7009	577.1663
585.8706	593.3821	617.7577
623.4403	626.7886	634.1833

662.1029 668.9185 690.4244

704.5771 713.3267 715.6172

724.3904 747.4538 757.4687

767.9507 786.2115 796.9272

799.9075 812.8089 847.2124

871.5099 881.8198 883.9009

884.7591 891.9026 914.4768

924.1271 935.3559 938.9972

960.3781 966.2200 973.6726

978.2225 982.2161 985.6503

994.5203 1003.0435 1012.8300

1016.2847 1020.1816 1021.4293

1023.9879 1030.7903 1036.3212

1037.5193 1040.3744 1043.1293

1053.6125 1061.6969 1066.4124

1067.2870 1069.1540 1069.6391

1071.3400 1080.2631 1094.9692

1108.7744 1119.6655 1121.6125

1128.3742 1140.4947 1172.3192

1178.5197 1179.5392 1188.2656

1198.8864 1200.4989 1204.5431

1218.6846 1222.5565 1245.2209

1248.8361 1260.6832 1261.7964

1273.2411 1286.2388 1300.1562

1302.4329 1315.0943 1336.5591

1341.0137 1343.1053 1355.0800

1357.6467 1358.8200 1360.4344

1364.4521 1374.4944 1377.3363

1389.8333 1395.5912 1400.3107

1406.4645 1411.2691 1415.3952

1426.3262 1442.9658 1456.4552

1463.9800 1465.8965 1469.9660

1471.5993 1475.8007 1476.8167

1478.4281 1480.7477 1486.0814

1486.8369	1496.0240	1497.3357
1502.5932	1502.8964	1506.6617
1516.3199	1544.0458	1544.3659
1548.2903	1615.2695	1673.7423
1675.7930	1683.8212	1690.0097
1690.4657	1691.6147	1695.3139
1790.4401	1830.0264	3054.9569
3056.4014	3066.8055	3069.0603
3069.1478	3071.5699	3071.6582
3076.6434	3081.9076	3089.9292
3104.6440	3107.8692	3114.4402
3124.2381	3132.2223	3133.6589
3134.8839	3136.7087	3137.7453
3141.8678	3161.5575	3163.0944
3166.9474	3168.4693	3184.0748
3188.8995	3199.4188	3207.0601
3214.5493	3219.4688	3222.8193
3229.3443	3231.8129	3235.5825
3241.8304	3246.6627	3248.5245

P[a]

Zero-point correction= 0.298551

Thermal correction to Energy= 0.317016

Thermal correction to Enthalpy= 0.317961

Thermal correction to Gibbs Free Energy= 0.250192

Sum of electronic and zero-point Energies= -920.592560

Sum of electronic and thermal Energies= -920.574095

Sum of electronic and thermal Enthalpies= -920.573150

Sum of electronic and thermal Free Energies= -920.640919

Cartesian coordinates

C	1.463780	0.907868	-0.235766
O	1.688090	2.071375	0.042551
C	0.068093	0.496499	-0.699249

C	-0.728577	1.739892	-1.109327
C	-0.605846	-0.330921	0.401039
O	-0.028544	-0.574221	1.441917
C	-1.061921	2.636143	0.068096
O	-1.376679	2.157499	1.139686
H	-0.172618	2.296649	-1.867403
H	-1.683536	1.447159	-1.561010
C	2.548206	-0.119314	-0.160762
C	2.334129	-1.463217	-0.484600
C	3.819600	0.296246	0.249654
C	3.380000	-2.377045	-0.397378
H	1.355136	-1.810730	-0.799934
C	4.862931	-0.617192	0.336790
H	3.972813	1.341240	0.498659
C	4.643572	-1.956223	0.013242
H	3.206998	-3.418871	-0.647359
H	5.846113	-0.288144	0.657984
H	5.456968	-2.672075	0.082712
H	0.165474	-0.150654	-1.580231
C	-1.976868	-0.876991	0.143596
C	-2.754854	-1.229761	1.251345
C	-2.477634	-1.079836	-1.145822
C	-4.024550	-1.765225	1.073510
H	-2.349536	-1.071000	2.245537
C	-3.745186	-1.630326	-1.322287
H	-1.881002	-0.828039	-2.017838
C	-4.520458	-1.967497	-0.215151
H	-4.628277	-2.027289	1.936659
H	-4.126431	-1.794637	-2.325073
H	-5.510638	-2.390257	-0.355219
C	-1.035430	4.118470	-0.181631
H	-1.637559	4.361771	-1.063084
H	-1.405624	4.660307	0.689178
H	-0.005146	4.417937	-0.398611

Vibrational frequencies

25.0194	41.3982	52.4134
58.7803	65.7002	73.2917
116.1456	131.5811	155.5539
161.2399	166.5422	173.7335
208.5107	242.4889	301.8618
337.7340	352.7707	407.6977
414.5820	423.4726	438.2002
454.1827	477.5872	492.9853
515.8257	582.5957	617.9912
625.3812	626.7651	656.4078
702.2238	710.7652	715.2929
733.1681	770.0712	774.9539
810.5257	820.7758	884.7114
886.7816	893.1907	929.1870
974.0559	978.0394	983.9876
998.1110	1015.2936	1018.5846
1020.4058	1021.4281	1029.5672
1040.0740	1042.4671	1067.0398
1069.0925	1077.7432	1094.5803
1119.9649	1125.4827	1175.8698
1177.8628	1190.5146	1203.2844
1208.6746	1220.7024	1244.9310
1255.8728	1316.6987	1342.5826
1344.7819	1361.5886	1365.7133
1375.3964	1378.4788	1419.2637
1456.5553	1457.3702	1466.6766
1498.5450	1500.9440	1546.5711
1549.7700	1674.2064	1675.1654
1689.9765	1693.9226	1820.8168
1830.5297	1854.4268	3076.3775
3089.6640	3095.4342	3152.6830
3155.2099	3189.8894	3210.8974

3217.8418	3218.5199	3223.8247
3229.0135	3231.3522	3233.9203
3235.3523	3238.0448	3247.0298

TS1[b]

Zero-point correction= 0.493891

Thermal correction to Energy= 0.522336

Thermal correction to Enthalpy= 0.523280

Thermal correction to Gibbs Free Energy= 0.435062

Sum of electronic and zero-point Energies= -1610.600986

Sum of electronic and thermal Energies= -1610.572541

Sum of electronic and thermal Enthalpies= -1610.571597

Sum of electronic and thermal Free Energies= -1610.659815

Cartesian coordinates

C	-4.004847	-0.045604	-2.054866
C	-2.890899	-0.705970	-2.574052
C	-1.983139	-1.330873	-1.722578
C	-2.178633	-1.298540	-0.338561
C	-3.300088	-0.643835	0.174276
C	-1.248185	-1.950495	0.677265
C	-0.774401	-3.390105	0.349289
O	-1.419448	-1.696240	1.888697
C	0.540970	-1.168694	0.104081
N	0.870988	0.108802	0.295839
C	2.238956	0.447823	0.242487
C	3.007965	-0.638663	-0.017468
S	1.982960	-2.040516	-0.181051
C	2.713166	1.849030	0.508177
C	3.500692	2.486515	-0.650657
C	4.510122	1.547745	-1.328589
C	5.221968	0.603352	-0.350136
C	4.498748	-0.743276	-0.187633
C	-1.663577	2.363110	1.799440

C	-0.617936	1.440242	1.712161
C	-0.164562	1.110291	0.435881
C	-0.657334	1.705304	-0.731002
C	-1.699882	2.619136	-0.592369
C	-2.223971	2.946291	0.662313
C	-3.376400	3.909535	0.769248
C	-0.055769	1.397685	-2.075848
C	0.023744	0.843754	2.933824
O	-0.791060	-3.853371	-0.772252
H	-4.707958	0.443896	-2.722301
H	-2.723012	-0.726843	-3.647070
H	-1.111564	-1.831750	-2.129619
H	-3.432787	-0.623204	1.251090
H	1.858196	2.481021	0.760590
H	3.344165	1.816149	1.401927
H	2.804815	2.876172	-1.400704
H	4.028318	3.352129	-0.235508
H	4.000605	0.946893	-2.092450
H	5.243706	2.159504	-1.862326
H	6.232016	0.381308	-0.706406
H	5.340783	1.090722	0.623859
H	4.687119	-1.346400	-1.084175
H	4.923086	-1.302922	0.654036
H	-2.044365	2.632602	2.781698
H	-2.114953	3.083750	-1.484334
H	-3.599587	4.149562	1.811220
H	-4.278493	3.481134	0.319371
H	-3.161754	4.841612	0.237981
H	-0.705012	1.756424	-2.877577
H	0.105078	0.324964	-2.215279
H	0.917994	1.890803	-2.182470
H	-0.099593	-0.242900	2.928284
H	-0.431860	1.246543	3.841122
H	1.095548	1.072774	2.959640

C	-4.210236	-0.019971	-0.676907
H	-5.076549	0.489044	-0.263691
C	-0.306348	-4.177461	1.545576
H	0.205378	-5.081819	1.214673
H	0.338260	-3.568636	2.182464
H	-1.178522	-4.446964	2.150219

Vibrational frequencies

-147.1593	20.1858	34.0916
39.1700	50.0711	54.7613
63.4712	82.9091	85.3380
95.2643	107.5370	113.7914
125.2081	129.5704	132.2375
167.8430	174.1211	181.4908
196.1120	211.3858	229.4769
237.2627	244.5366	254.7796
258.0075	279.7211	289.5954
299.2154	318.9549	333.0293
354.0815	366.6105	376.8612
408.9461	419.3936	427.8103
447.6308	456.0984	493.4287
503.2598	512.9488	525.2469
533.6723	551.2257	581.5362
588.6768	593.6786	595.2261
601.7808	625.1263	629.5895
647.1648	672.3531	716.1017
718.7057	729.1701	742.8938
760.8910	787.4692	812.0782
844.6431	868.0967	879.8515
886.1227	911.1268	916.3632
919.6364	937.0059	958.9657
962.9366	972.8731	980.0455
991.8767	1001.7632	1010.1849
1012.5844	1022.6189	1026.0100

1032.6024	1034.7747	1041.5660
1055.1711	1062.6803	1065.1796
1066.7385	1067.7129	1072.9977
1091.5691	1107.4924	1112.6253
1128.4037	1167.0112	1179.9906
1183.4800	1197.2868	1199.4676
1213.1516	1248.5234	1260.8831
1274.6744	1275.5243	1296.6353
1299.5634	1330.6952	1330.9197
1338.2936	1354.8666	1359.6283
1362.0577	1368.9312	1390.5722
1393.0637	1393.7263	1404.0673
1409.5475	1414.0766	1425.1175
1448.7032	1451.5449	1456.9010
1458.5585	1468.0343	1473.3459
1476.7408	1481.2644	1482.2412
1485.5755	1488.4749	1489.2469
1492.4638	1496.9621	1508.8970
1516.3641	1540.7892	1544.6340
1618.3415	1678.3953	1684.8152
1686.1558	1691.0950	1694.1756
1852.8601	3059.0460	3060.7161
3064.6776	3066.8930	3067.6765
3078.1230	3082.3016	3087.4667
3098.7908	3105.2299	3112.8606
3127.1250	3129.1541	3134.8064
3135.8068	3138.3839	3150.6142
3162.7082	3164.4095	3168.3702
3169.6050	3189.0421	3192.7135
3196.6580	3199.4642	3203.3454
3218.2566	3228.8336	3230.8214

M1[b]

Zero-point correction= 0.495954

Thermal correction to Energy= 0.524100

Thermal correction to Enthalpy= 0.525044

Thermal correction to Gibbs Free Energy= 0.439250

Sum of electronic and zero-point Energies= -1610.612578

Sum of electronic and thermal Energies= -1610.584432

Sum of electronic and thermal Enthalpies= -1610.583488

Sum of electronic and thermal Free Energies= -1610.669282

Cartesian coordinates

C	4.152760	0.041038	-1.566982
C	3.136880	0.668955	-2.288122
C	2.064681	1.254665	-1.616932
C	1.992099	1.194629	-0.224005
C	3.021238	0.591731	0.494943
C	0.836911	1.843608	0.588235
C	0.853440	3.322026	0.111242
O	0.935993	1.744062	1.905884
C	-0.542635	1.211203	0.201635
N	-0.844162	-0.086266	0.297783
C	-2.215717	-0.399842	0.288827
C	-2.983493	0.710625	0.165968
S	-1.978064	2.120815	0.036809
C	-2.705013	-1.812687	0.438861
C	-3.531011	-2.323589	-0.755331
C	-4.547714	-1.312578	-1.306958
C	-5.224658	-0.472047	-0.216406
C	-4.479757	0.840955	0.076163
C	1.603876	-2.561937	1.581933
C	0.605231	-1.585632	1.584058
C	0.162444	-1.127341	0.342866
C	0.604651	-1.657006	-0.874405
C	1.607069	-2.623240	-0.822598
C	2.129483	-3.072638	0.394246
C	3.255707	-4.070843	0.411108

C	0.002404	-1.228483	-2.185010
C	0.017280	-1.047960	2.857319
O	0.166409	3.741866	-0.802206
H	4.987894	-0.416653	-2.088929
H	3.182262	0.705952	-3.372818
H	1.276797	1.755720	-2.175864
H	2.929686	0.582484	1.577211
H	-1.858782	-2.480841	0.612235
H	-3.316572	-1.848074	1.345810
H	-2.860162	-2.641508	-1.559749
H	-4.057112	-3.221524	-0.413907
H	-4.051137	-0.638061	-2.015894
H	-5.300389	-1.860099	-1.882134
H	-6.238381	-0.199769	-0.523450
H	-5.330929	-1.061064	0.701205
H	-4.698879	1.549136	-0.731974
H	-4.860422	1.297081	0.997194
H	1.980502	-2.926622	2.534561
H	1.989282	-3.033756	-1.754575
H	3.387465	-4.506376	1.404165
H	4.196440	-3.585070	0.128044
H	3.080583	-4.879681	-0.303795
H	0.650224	-1.515576	-3.016170
H	-0.158269	-0.148342	-2.230892
H	-0.971092	-1.710208	-2.335043
H	0.140519	0.041331	2.868106
H	0.514790	-1.488426	3.724424
H	-1.051583	-1.286133	2.921753
C	4.097544	0.011015	-0.172932
H	4.893181	-0.469535	0.390229
C	1.792507	4.199432	0.891369
H	1.912537	5.160984	0.391279
H	1.374969	4.339927	1.891646
H	2.758289	3.703747	1.019928

Vibrational frequencies

28.2891	47.0393	52.2100
55.8172	61.7549	80.7059
100.1644	104.7022	111.1762
115.8575	135.0405	141.1203
150.5035	174.8524	179.0569
181.7593	184.3379	192.2440
215.0331	218.0763	236.7193
254.6045	257.6048	268.3231
273.8217	284.1204	285.9122
311.1511	326.6616	342.1980
369.0408	385.7580	386.2786
416.5738	424.9135	431.7827
460.4736	462.3867	498.6205
505.6601	510.9967	527.9463
550.3535	569.8590	580.6510
590.4515	591.4025	600.4511
622.0798	625.7638	654.4649
679.2053	694.8709	731.2712
738.2614	746.1557	766.0144
777.4535	814.3698	845.5995
861.5626	885.7238	897.2204
898.9655	916.0723	930.4848
930.8141	955.5558	965.8466
966.4533	981.5476	985.3385
1004.0371	1013.6536	1016.4920
1020.6469	1032.8931	1040.4635
1042.0017	1043.9284	1057.4356
1060.0605	1061.3972	1066.0286
1070.9863	1073.6973	1091.2733
1094.6248	1113.3926	1119.7944
1139.7591	1164.2705	1167.7780
1185.7090	1192.8941	1202.8698

1210.7081	1232.9360	1249.7934
1265.5556	1275.0348	1277.5771
1298.2026	1306.0433	1327.7397
1335.5841	1341.1015	1356.2645
1357.0450	1364.6314	1369.4841
1381.6236	1395.6014	1397.9221
1402.3554	1413.8899	1416.6330
1427.3399	1448.4792	1456.5058
1462.6268	1467.0583	1470.7155
1476.7548	1480.3442	1482.0811
1484.3418	1491.2234	1492.3647
1494.6339	1502.8930	1505.3729
1510.0292	1519.8255	1530.5551
1542.0649	1674.3484	1681.7702
1682.7384	1688.3470	1694.2718
1827.5693	3039.5599	3063.6363
3065.5922	3067.5007	3073.0757
3080.5340	3081.8557	3089.0889
3100.2875	3108.8130	3116.0452
3117.6276	3127.9637	3129.7710
3135.7670	3145.9514	3154.3939
3156.3361	3168.1146	3169.3520
3170.1208	3196.2316	3197.2707
3205.3127	3209.7540	3211.8960
3216.1995	3221.4851	3227.4995

TS2[b]

Zero-point correction= 0.494690

Thermal correction to Energy= 0.522640

Thermal correction to Enthalpy= 0.523584

Thermal correction to Gibbs Free Energy= 0.436521

Sum of electronic and zero-point Energies= -1610.592209

Sum of electronic and thermal Energies= -1610.564260

Sum of electronic and thermal Enthalpies= -1610.563316

Sum of electronic and thermal Free Energies= -1610.650379

Cartesian coordinates

C	-1.461296	-1.764671	-1.484641
C	-1.601378	-0.820646	-0.292286
O	-0.538343	-1.684008	-2.309257
C	-0.664832	0.344863	-0.337857
N	0.668812	0.323577	-0.289354
C	1.288294	1.582835	-0.412330
C	0.391034	2.583503	-0.581700
S	-1.221251	1.949321	-0.557127
C	2.770902	1.779573	-0.277403
C	3.145400	2.572187	0.987137
C	2.314553	3.847386	1.211938
C	1.943961	4.567208	-0.090920
C	0.622120	4.065683	-0.706519
C	3.093550	-2.468702	-0.632949
C	2.268456	-1.401924	-0.993665
C	1.479818	-0.842640	0.013970
C	1.530216	-1.261263	1.344861
C	2.377880	-2.323699	1.654809
C	3.157406	-2.945377	0.677524
C	4.063476	-4.098134	1.021193
C	0.676836	-0.606240	2.393677
C	2.300585	-0.844878	-2.390068
O	-1.077957	-2.008118	0.187024
H	3.288902	0.820292	-0.264489
H	3.118000	2.312574	-1.167521
H	3.061072	1.918446	1.862294
H	4.203983	2.837214	0.892042
H	1.393609	3.603144	1.755788
H	2.883348	4.518826	1.861950
H	1.820950	5.638136	0.092898
H	2.759897	4.473615	-0.814968

H	-0.207781	4.568803	-0.197848
H	0.557614	4.354868	-1.761601
H	3.712404	-2.931272	-1.399208
H	2.428219	-2.671945	2.683677
H	3.787356	-4.993746	0.455781
H	4.013215	-4.338417	2.085581
H	5.103924	-3.866346	0.772288
H	0.964519	-0.943794	3.391399
H	-0.373424	-0.868152	2.223921
H	0.760096	0.486333	2.360965
H	1.334610	-0.421481	-2.662022
H	2.539050	-1.637478	-3.103591
H	3.078731	-0.077202	-2.478809
C	-2.969346	-0.433186	0.226803
C	-3.877424	0.277232	-0.564277
C	-3.347699	-0.835116	1.509076
C	-5.130727	0.619994	-0.061046
H	-3.613038	0.545964	-1.585023
C	-4.599076	-0.490478	2.013141
H	-2.657076	-1.437861	2.091769
C	-5.490929	0.243583	1.231593
H	-5.830163	1.169741	-0.683581
H	-4.883413	-0.800899	3.014272
H	-6.468337	0.508748	1.623002
C	-2.647405	-2.674839	-1.736383
H	-3.237020	-2.273718	-2.568009
H	-2.265999	-3.653361	-2.040853
H	-3.290773	-2.791705	-0.864796

Vibrational frequencies

-270.0585	17.7043	28.7344
40.8931	51.8714	59.7772
75.8014	78.5985	91.8088
107.5899	122.4670	127.7056

134.0168	149.0209	155.6097
161.3511	177.5015	185.1462
204.4807	205.5883	221.4142
232.7106	249.8977	264.5466
272.2865	280.6883	293.1746
316.8955	334.4233	341.2774
377.4388	380.0338	408.8924
422.6873	424.3138	435.8844
452.8315	477.8521	496.4877
502.5820	518.4149	524.1787
542.8880	549.3635	559.2700
578.3838	590.4929	596.8277
610.7944	626.5257	635.4840
670.2019	704.8674	723.8099
725.7391	744.8990	756.7537
775.4956	820.2038	851.1542
878.6729	881.9363	885.5017
894.4948	915.9243	924.4893
945.5123	958.8142	964.9261
969.8969	982.3855	986.3178
1006.0405	1008.0927	1009.3393
1018.7958	1023.8990	1035.3357
1035.7896	1048.6906	1050.4680
1060.1933	1062.2057	1067.1263
1069.1207	1071.4040	1090.9096
1099.6352	1112.1980	1115.0905
1141.3850	1168.7088	1181.5844
1187.4870	1190.4673	1205.7066
1216.7652	1221.7448	1254.3013
1276.8452	1277.8313	1284.6718
1305.4113	1311.5759	1331.7037
1337.8017	1345.0337	1355.4743
1359.2192	1363.5969	1369.0655
1388.1887	1393.4916	1395.8327

1397.4551	1409.0254	1417.3351
1426.8095	1458.3249	1463.4104
1470.0285	1470.2768	1475.0471
1477.8135	1478.7156	1480.3944
1482.0912	1489.7521	1492.6252
1494.3194	1496.0044	1505.4734
1515.9531	1516.8447	1541.9867
1547.1367	1654.0765	1673.2111
1684.8396	1689.8992	1694.9218
1696.3551	3060.1694	3064.3707
3065.8954	3066.4722	3070.5450
3075.0527	3077.5237	3085.3816
3105.8348	3113.9965	3117.7927
3125.9567	3131.1430	3135.1919
3139.8829	3141.9946	3144.5189
3164.2278	3165.4310	3169.2039
3183.9054	3184.8675	3190.5615
3198.1377	3199.0265	3204.4142
3212.3124	3219.5620	3225.5941

M2[b]

Zero-point correction= 0.496420

Thermal correction to Energy= 0.525190

Thermal correction to Enthalpy= 0.526134

Thermal correction to Gibbs Free Energy= 0.437024

Sum of electronic and zero-point Energies= -1610.651856

Sum of electronic and thermal Energies= -1610.623087

Sum of electronic and thermal Enthalpies= -1610.622142

Sum of electronic and thermal Free Energies= -1610.711253

Cartesian coordinates

C	-1.997950	2.009512	-0.043025
O	-1.592481	0.977901	-0.832915
O	-2.299858	1.875364	1.115005

C	-1.609386	-0.305071	-0.266767
C	-0.402526	-0.881346	-0.014381
C	-2.933245	-0.920041	-0.169095
C	-3.228102	-1.969386	0.717572
C	-4.500494	-2.532309	0.760861
C	-5.517087	-2.053758	-0.061660
C	-5.246330	-0.992444	-0.925395
C	-3.976551	-0.431822	-0.978670
N	0.841284	-0.261061	-0.076218
C	1.942370	-1.127119	0.111494
C	1.599069	-2.409097	0.315830
S	-0.159709	-2.602000	0.329640
C	3.323626	-0.532704	0.082753
C	4.467088	-1.554200	0.039091
C	4.258634	-2.629543	-1.035356
C	3.501028	-3.875166	-0.539428
C	2.479899	-3.600747	0.575618
C	1.018076	1.160915	0.048030
C	1.290850	1.917512	-1.097730
C	1.512895	3.284868	-0.944034
C	1.450229	3.900408	0.309945
C	1.154562	3.116766	1.426170
C	0.942314	1.740110	1.318779
C	1.276753	1.270086	-2.454124
C	0.601765	0.900987	2.519561
C	1.707463	5.377383	0.452122
H	-2.476958	-2.325363	1.414723
H	-4.699152	-3.339867	1.459316
H	-6.509050	-2.492353	-0.022007
H	-6.029282	-0.599441	-1.567334
H	-3.780690	0.388469	-1.661908
H	3.395884	0.104031	-0.807988
H	3.442075	0.138844	0.943082
H	5.384144	-0.994470	-0.167390

H	4.607997	-2.017288	1.021411
H	3.716540	-2.176493	-1.874875
H	5.225034	-2.949610	-1.436977
H	2.994638	-4.349693	-1.386548
H	4.215171	-4.609190	-0.149576
H	1.856505	-4.490493	0.709309
H	3.000055	-3.456485	1.528579
H	1.725033	3.887327	-1.824781
H	1.088552	3.583701	2.406442
H	1.989029	0.440541	-2.517764
H	0.283062	0.856267	-2.658070
H	1.519490	1.994800	-3.234305
H	0.745536	1.467570	3.442127
H	-0.446137	0.583555	2.470305
H	1.219961	-0.002509	2.566377
H	1.397395	5.920316	-0.444566
H	1.172710	5.790798	1.311029
H	2.774707	5.573900	0.603097
C	-2.064516	3.287733	-0.825871
H	-3.066437	3.367744	-1.260989
H	-1.908812	4.133464	-0.156084
H	-1.334522	3.296070	-1.635809

Vibrational frequencies

22.0960	37.8854	49.8227
52.6859	59.5028	61.1471
68.5762	78.4295	91.6302
98.4139	107.9437	113.0209
122.1360	130.8030	149.1994
160.7474	179.3252	182.4290
182.8720	212.1423	214.8542
236.2464	252.5408	255.0609
271.0516	280.8362	301.6891
319.4219	339.6368	351.3018

357.2866	371.2438	399.5987
421.8744	426.3925	439.7649
460.6915	501.2595	508.9347
514.7002	534.2844	545.4700
567.2777	569.9180	575.1554
587.4059	591.9011	601.7670
617.2628	623.0975	630.6884
650.5530	698.0682	718.8498
739.2130	751.0296	789.1856
791.5616	795.5703	842.3790
873.3806	881.8592	885.2926
913.3322	917.2805	931.0337
941.2723	948.8692	961.5314
973.2434	985.0231	991.8889
1007.3471	1013.9457	1016.8753
1024.3963	1028.1477	1034.6690
1037.5234	1058.6826	1062.4827
1063.9315	1067.2148	1069.3619
1070.1443	1073.7730	1094.2005
1103.0393	1120.0959	1122.1026
1154.3464	1168.9463	1188.9063
1204.3209	1205.0392	1208.3827
1233.1995	1251.7742	1262.8860
1272.7924	1285.2037	1290.9947
1309.8907	1324.7400	1333.2448
1337.3255	1356.4533	1359.0172
1363.2687	1376.6377	1381.1319
1395.7603	1403.6502	1405.6185
1409.4840	1415.2215	1418.8447
1428.3973	1454.9164	1460.9409
1462.8557	1471.2432	1475.7427
1476.2875	1479.1473	1481.6975
1482.5228	1485.0320	1485.4541
1490.6732	1498.5247	1514.8036

1516.0898	1543.8811	1547.7359
1648.1014	1665.2864	1676.0856
1694.9917	1699.2620	1749.8206
1881.5902	3057.0267	3061.7721
3062.4061	3063.0461	3065.3730
3072.3957	3077.7134	3082.4872
3087.5018	3099.1332	3110.7356
3117.0679	3127.7451	3130.7925
3131.5034	3132.6692	3136.3630
3158.8481	3158.9096	3161.0021
3165.1703	3195.0219	3197.5085
3200.1255	3201.2878	3207.5354
3218.8047	3224.4568	3233.0669

TS3[b]

Zero-point correction= 0.643471

Thermal correction to Energy= 0.680686

Thermal correction to Enthalpy= 0.681630

Thermal correction to Gibbs Free Energy= 0.572637

Sum of electronic and zero-point Energies= -2033.292813

Sum of electronic and thermal Energies= -2033.255598

Sum of electronic and thermal Enthalpies= -2033.254654

Sum of electronic and thermal Free Energies= -2033.363647

Cartesian coordinates

O	-2.696335	1.735668	-1.145872
C	-0.853178	-0.413296	-1.068346
C	0.780951	0.450429	0.892573
S	0.359410	1.980440	1.596020
C	1.869140	2.686472	1.099440
C	2.624333	1.787483	0.439559
N	2.005146	0.532611	0.311725
C	2.260444	4.122108	1.270934
C	2.299018	4.890925	-0.074846

C	2.544919	4.027689	-1.318306
C	3.812854	3.165173	-1.329818
C	3.948405	2.150787	-0.161725
C	2.726326	-0.560326	-0.308076
C	3.479936	-1.397155	0.531439
C	4.217384	-2.414683	-0.059034
C	4.223973	-2.606195	-1.448108
C	3.489158	-1.734041	-2.242739
C	2.738526	-0.683111	-1.695617
C	5.016076	-3.735675	-2.050680
C	2.026076	0.271015	-2.618305
C	3.471512	-1.194342	2.021004
H	-0.172350	-1.201179	-1.386461
H	-0.488700	0.597488	-1.242877
H	1.593804	4.626198	1.975068
H	3.257006	4.129376	1.727277
H	1.343505	5.406377	-0.215398
H	3.068092	5.667298	-0.000689
H	1.673633	3.378804	-1.471742
H	2.580269	4.691001	-2.189277
H	3.832069	2.616538	-2.276974
H	4.699008	3.808719	-1.322933
H	4.486258	1.259409	-0.490663
H	4.544185	2.599707	0.640370
H	4.802329	-3.077555	0.574969
H	3.503012	-1.851683	-3.324079
H	4.975135	-3.711702	-3.141840
H	6.065374	-3.686073	-1.744002
H	4.627305	-4.702815	-1.715264
H	1.623251	1.138453	-2.091483
H	2.716813	0.627127	-3.388110
H	1.196347	-0.226114	-3.131058
H	4.165304	-1.884484	2.504879
H	2.470097	-1.364855	2.430973

H	3.762847	-0.171155	2.283916
C	-0.122824	-0.660989	0.862680
C	-1.257015	-0.653798	1.822556
C	-2.252750	0.327975	1.727560
C	-1.364119	-1.625885	2.827206
C	-3.313800	0.350051	2.631851
H	-2.205711	1.072912	0.939200
C	-2.430670	-1.606441	3.719136
H	-0.603285	-2.395517	2.920424
C	-3.411293	-0.617626	3.626571
H	-4.074252	1.120382	2.541716
H	-2.494540	-2.365132	4.493488
H	-4.243772	-0.606817	4.323312
C	-3.084130	0.558315	-1.286719
C	-4.563020	0.326724	-1.493105
C	-5.442018	1.339758	-1.095898
C	-5.088980	-0.838381	-2.062201
C	-6.817014	1.187795	-1.242180
H	-5.019440	2.244260	-0.669825
C	-6.464927	-0.988471	-2.219420
H	-4.424095	-1.625351	-2.404543
C	-7.332693	0.020753	-1.805188
H	-7.488194	1.977996	-0.918548
H	-6.860597	-1.894521	-2.668601
H	-8.405292	-0.100573	-1.924199
O	0.612156	-1.867295	0.833904
C	0.051931	-3.021371	0.397966
O	-1.102437	-3.134340	0.073738
C	-2.228073	-0.581796	-1.222198
H	-2.651423	-1.577937	-1.209243
C	1.082975	-4.112330	0.377739
H	1.771657	-3.925104	-0.452686
H	1.664082	-4.112384	1.302692
H	0.592010	-5.073907	0.235430

Vibrational frequencies

-461.9117	13.9037	15.8823
23.8048	28.1253	39.0416
47.0380	52.9435	64.2156
73.7634	79.1992	90.0896
92.6173	94.3442	102.7048
105.5112	124.0209	127.9565
133.6401	135.6797	152.6751
164.6862	176.1739	178.7094
181.9708	206.4272	211.6980
219.0919	227.2828	241.7033
243.1307	256.8713	273.5795
277.5489	279.0673	295.7671
308.5664	315.4774	334.4618
340.7218	356.0698	373.3938
379.2210	402.0428	409.3501
416.9692	425.7593	432.3405
440.1621	465.0862	478.6251
500.3939	510.9621	526.9457
529.1103	541.1576	550.1386
558.1996	570.9261	580.9711
592.5567	598.6264	607.4640
626.1545	627.4514	642.0479
651.2537	666.7696	689.8893
704.2659	715.6750	723.4318
731.4369	742.2104	746.6107
751.3267	761.2775	776.2991
792.8339	798.4381	815.7703
824.3904	858.9938	880.8242
884.8091	889.4247	895.9948
914.0619	920.4983	938.0991
963.0784	966.7488	971.7366
973.5790	977.6019	981.1007

1000.5380	1012.2792	1013.6047
1015.2143	1019.0001	1019.9137
1027.5419	1028.5762	1038.9534
1044.1334	1051.9664	1054.6099
1059.5359	1060.1523	1060.8613
1062.4193	1063.7513	1068.9603
1072.9126	1087.2990	1092.7107
1100.6721	1109.8717	1117.2522
1121.1064	1140.0950	1153.9136
1164.8830	1170.2815	1172.5671
1190.1615	1194.1711	1201.7160
1214.4930	1218.0435	1224.2428
1262.3547	1271.2085	1276.1529
1277.1269	1281.6748	1288.3958
1294.3681	1312.4130	1319.7224
1333.2724	1335.3948	1339.1219
1349.4810	1358.4843	1360.3927
1367.4663	1368.8140	1385.3019
1386.1031	1400.7636	1402.5445
1408.9086	1415.0732	1420.4270
1425.4723	1429.7422	1457.5711
1461.7478	1463.1207	1468.3373
1473.3771	1474.0668	1474.6218
1476.3760	1477.8425	1483.0823
1488.8962	1489.9314	1491.7208
1492.6253	1500.7602	1501.5015
1510.7625	1539.3479	1541.0159
1552.3572	1561.5146	1655.7695
1665.7742	1684.5965	1687.3973
1692.0388	1693.7028	1695.9330
1704.4006	1876.5476	3065.0266
3065.1505	3071.1683	3073.2499
3077.7173	3078.7193	3079.1590
3082.1239	3087.9164	3109.4947

3123.2357	3125.6872	3131.4771
3137.3770	3140.5318	3141.1969
3147.5565	3155.3720	3162.8920
3163.4606	3169.5337	3173.2040
3194.7806	3201.2244	3201.8777
3204.8451	3206.8778	3209.5682
3215.0143	3215.8865	3219.0972
3225.4604	3226.5057	3228.2669
3230.6281	3232.0899	3241.8274

M3[b]

Zero-point correction= 0.645251

Thermal correction to Energy= 0.682400

Thermal correction to Enthalpy= 0.683344

Thermal correction to Gibbs Free Energy= 0.575071

Sum of electronic and zero-point Energies= -2033.310204

Sum of electronic and thermal Energies= -2033.273055

Sum of electronic and thermal Enthalpies= -2033.272111

Sum of electronic and thermal Free Energies= -2033.380384

Cartesian coordinates

O	3.277369	-1.462658	-1.908048
C	1.082847	0.045080	-0.766764
C	-1.012554	-0.828511	0.287361
S	-1.319248	-2.500524	0.196474
C	-2.961287	-2.247224	-0.279297
C	-3.234728	-0.916999	-0.343543
N	-2.108819	-0.142186	-0.028599
C	-3.893080	-3.401462	-0.517135
C	-4.501912	-3.418321	-1.928446
C	-5.020680	-2.055012	-2.418155
C	-5.585462	-1.163562	-1.303623
C	-4.522937	-0.233233	-0.702939
C	-2.197912	1.306610	-0.023638

C	-2.547477	1.922261	1.186055
C	-2.633306	3.309898	1.189936
C	-2.409083	4.062406	0.029945
C	-2.115325	3.397017	-1.156034
C	-2.006795	2.003531	-1.214175
C	-2.468856	5.564985	0.083666
C	-1.750295	1.321917	-2.532435
C	-2.808439	1.107156	2.422894
H	0.467163	0.820531	-1.229638
H	1.007142	-0.853413	-1.390521
H	-3.365311	-4.342020	-0.336284
H	-4.686417	-3.347674	0.234542
H	-3.761801	-3.801148	-2.638046
H	-5.324075	-4.141316	-1.907838
H	-4.211423	-1.511122	-2.922037
H	-5.785261	-2.231286	-3.180129
H	-6.373728	-0.519149	-1.701693
H	-6.052704	-1.772064	-0.522327
H	-4.290559	0.544232	-1.440131
H	-4.909974	0.286155	0.182605
H	-2.883721	3.818240	2.118387
H	-1.962358	3.967308	-2.069440
H	-2.549275	5.995682	-0.916817
H	-3.320384	5.904349	0.679768
H	-1.562249	5.965124	0.550773
H	-1.509577	0.262016	-2.423363
H	-2.637820	1.401396	-3.170056
H	-0.924877	1.807219	-3.060038
H	-3.087016	1.755339	3.255860
H	-1.921414	0.532888	2.712027
H	-3.621877	0.390999	2.259180
C	0.395765	-0.302354	0.586614
C	1.118622	-1.407533	1.370542
C	1.959815	-2.323351	0.733183

C	0.855223	-1.548218	2.738183
C	2.524625	-3.366948	1.468467
H	2.211985	-2.218655	-0.323059
C	1.425662	-2.588818	3.463647
H	0.203428	-0.837942	3.237374
C	2.261940	-3.505172	2.828108
H	3.183989	-4.070945	0.969051
H	1.214239	-2.684443	4.524228
H	2.708358	-4.319343	3.391069
C	3.481908	-0.355834	-1.304280
C	4.924648	0.110002	-1.229383
C	5.929000	-0.853555	-1.376842
C	5.311309	1.444055	-1.047441
C	7.275826	-0.507084	-1.312573
H	5.617039	-1.879224	-1.547213
C	6.657729	1.797220	-0.989784
H	4.554041	2.219106	-0.970747
C	7.647220	0.822634	-1.117119
H	8.038986	-1.273177	-1.420409
H	6.935712	2.838872	-0.854606
H	8.696670	1.098901	-1.074207
O	0.263819	0.782017	1.523619
C	0.481285	2.107935	1.306544
O	0.708026	2.625061	0.245638
C	2.525023	0.420135	-0.679256
H	2.792614	1.331309	-0.159516
C	0.427576	2.831026	2.624647
H	1.352589	2.623392	3.172142
H	0.346947	3.902221	2.442992
H	-0.408466	2.481894	3.233477

Vibrational frequencies

17.9250	19.1290	25.1948
35.6756	42.3615	45.0377

50.4836	54.4785	69.3710
73.2497	84.0388	95.3109
105.0114	116.1356	121.7614
128.3924	129.2290	140.6121
148.1986	152.8551	157.1054
164.2707	172.6872	178.7152
199.2788	206.6137	227.6166
231.6883	237.0181	249.6339
260.8577	265.9718	273.7762
280.9043	291.3508	309.3573
325.5213	333.3638	344.7184
353.9622	376.0802	386.3234
411.4587	418.1897	420.5827
424.2702	426.6838	449.8098
472.2274	484.5461	501.7077
504.5616	529.8212	534.9602
543.9663	559.0747	572.2315
578.2936	584.9533	588.9927
596.8663	599.8517	624.4394
627.8409	628.8285	638.7402
660.6503	668.1807	694.3646
707.6113	718.1376	723.1393
729.4059	749.6168	754.2718
761.5147	792.0948	803.1997
807.8743	812.6390	849.6502
865.5370	881.5634	884.2379
889.9867	892.0562	918.9637
931.2315	934.0237	953.5495
955.3650	966.7506	972.1526
981.4227	983.8704	991.0012
1005.6575	1010.2624	1014.2961
1021.7351	1025.5822	1026.4321
1026.4925	1039.0840	1041.0519
1044.7424	1049.8355	1057.3444

1061.1307	1062.9091	1064.5596
1065.2786	1065.4780	1067.2179
1074.5166	1095.8207	1097.0596
1099.2711	1105.1170	1118.9249
1135.0323	1150.0326	1159.2744
1164.3669	1167.6702	1169.1638
1188.3099	1190.1109	1207.3183
1210.8797	1218.8597	1223.2440
1244.1985	1251.5143	1256.7612
1277.1281	1277.5924	1280.5894
1301.2207	1307.9512	1322.4598
1324.0518	1331.3046	1339.9319
1353.0483	1354.0018	1356.6034
1369.0691	1373.0443	1374.6459
1393.7216	1401.4322	1406.0605
1409.9862	1412.6430	1413.8190
1424.5180	1455.4701	1458.0902
1460.9421	1464.4833	1466.8976
1469.4532	1477.8895	1480.3817
1481.3328	1486.9080	1487.5718
1488.7786	1491.4557	1494.3729
1501.8732	1503.8678	1510.0524
1511.1686	1513.8163	1537.9002
1541.1492	1549.9703	1636.2626
1674.1852	1677.3719	1680.2712
1687.6670	1688.5604	1690.5033
1692.5752	1885.2570	3067.3517
3067.8968	3068.9558	3070.5992
3071.3687	3080.2460	3083.9537
3084.8888	3086.3149	3095.9616
3111.4959	3122.9566	3130.4807
3133.8834	3135.2227	3140.7954
3141.2555	3143.7490	3144.1171
3148.4397	3167.3727	3169.0103

3170.5453	3170.6958	3191.7792
3194.5194	3194.7048	3202.5454
3203.0603	3209.2513	3209.8445
3215.3784	3219.0081	3221.1799
3227.0485	3229.9152	3240.4323

TS4[b]

Zero-point correction= 0.644840

Thermal correction to Energy= 0.681002

Thermal correction to Enthalpy= 0.681947

Thermal correction to Gibbs Free Energy= 0.576918

Sum of electronic and zero-point Energies= -2033.311631

Sum of electronic and thermal Energies= -2033.275469

Sum of electronic and thermal Enthalpies= -2033.274525

Sum of electronic and thermal Free Energies= -2033.379553

Cartesian coordinates

O	-3.785409	2.558946	-0.525080
C	-1.485657	1.111688	-1.480531
C	0.423778	-0.453060	-0.784078
S	-0.272451	-1.684094	-1.718412
C	0.914811	-2.835204	-1.214142
C	1.806251	-2.248951	-0.370743
N	1.515374	-0.896144	-0.161680
C	0.848177	-4.260939	-1.691265
C	1.631191	-5.260499	-0.820704
C	1.467579	-4.999347	0.682765
C	2.523236	-4.040949	1.261643
C	2.965438	-2.922407	0.301399
C	2.455061	-0.009922	0.506392
C	3.526986	0.453477	-0.276508
C	4.398833	1.363651	0.307987
C	4.238054	1.786599	1.633606
C	3.201865	1.244295	2.386125

C	2.292857	0.324047	1.847429
C	5.172010	2.812728	2.215416
C	1.238175	-0.285200	2.727974
C	3.769707	-0.056068	-1.672322
H	-1.283582	0.764089	-2.502831
H	-1.662072	2.190330	-1.530085
H	-0.206425	-4.557988	-1.695148
H	1.188805	-4.308470	-2.731697
H	1.257498	-6.256742	-1.072418
H	2.691850	-5.253695	-1.092612
H	0.463354	-4.595857	0.862297
H	1.520089	-5.942558	1.234229
H	2.140655	-3.595087	2.185886
H	3.424244	-4.602710	1.528994
H	3.557309	-2.183567	0.846155
H	3.615848	-3.333122	-0.476462
H	5.224913	1.752858	-0.283057
H	3.087261	1.534620	3.428063
H	5.041757	2.901908	3.296086
H	6.215445	2.557654	2.009130
H	4.984831	3.795381	1.768508
H	1.719454	-0.880759	3.511059
H	0.659821	0.499794	3.224615
H	0.541719	-0.916046	2.175627
H	4.435106	0.620701	-2.212578
H	2.847765	-0.161826	-2.250293
H	4.251669	-1.040953	-1.635077
C	-0.200944	0.938408	-0.613361
C	0.800529	2.034056	-0.948540
C	1.350807	2.086518	-2.231237
C	1.121932	3.023826	-0.019657
C	2.245271	3.098679	-2.569829
H	1.090810	1.326571	-2.965328
C	2.012425	4.038742	-0.363388

H	0.683503	2.988836	0.971079
C	2.583540	4.074737	-1.634310
H	2.676190	3.124152	-3.566126
H	2.262831	4.801373	0.368330
H	3.282089	4.863212	-1.896823
C	-3.782245	1.307586	-0.512561
C	-5.048272	0.607110	-0.063034
C	-6.258106	1.299259	-0.165812
C	-5.054002	-0.688064	0.470011
C	-7.455054	0.704818	0.223827
H	-6.235274	2.312217	-0.555509
C	-6.248959	-1.279314	0.874407
H	-4.114324	-1.220921	0.598116
C	-7.453578	-0.588497	0.744745
H	-8.389764	1.249892	0.127223
H	-6.239925	-2.280085	1.296583
H	-8.384520	-1.053183	1.056014
O	-0.610341	1.082868	0.723143
C	-1.649518	0.215897	1.142897
C	-2.674944	0.489104	-0.830151
O	-1.465585	-1.001621	1.167396
H	-2.860500	-0.566390	-0.992594
C	-2.482208	0.947620	2.165408
H	-2.815372	1.915941	1.789356
H	-3.339412	0.335783	2.449012
H	-1.861539	1.105096	3.055802

Vibrational frequencies

-249.9508	19.8457	25.7375
34.3904	40.6586	45.9941
51.2087	56.7575	57.2306
65.6518	72.0949	86.6942
100.4935	100.9339	115.6244
131.4558	133.0003	136.0036

152.2304	156.4169	165.5643
181.7623	196.4785	203.3097
210.0405	215.0704	223.2531
231.8223	246.5417	252.8900
257.7208	269.6523	283.3196
286.0251	298.5391	303.6410
321.0929	339.8046	342.4243
364.6081	374.8495	387.7067
398.1395	417.6926	418.5900
427.7169	431.8733	435.1926
462.9989	482.1408	499.5421
508.0390	518.2613	528.4604
545.1434	550.5136	564.4230
572.5136	581.7553	586.2423
597.4082	610.9710	623.7761
628.1936	631.5741	651.2957
674.6067	689.1085	710.3412
715.7583	725.9030	727.8972
741.7004	751.5502	772.6860
782.0741	791.2035	812.7710
818.4747	833.8831	849.8829
878.8985	881.7278	884.1466
887.0069	889.3149	914.0599
916.2925	926.3073	954.5023
958.6361	964.2116	967.9403
974.8001	979.4471	984.4454
1004.3231	1008.1430	1008.9023
1014.0647	1017.2151	1020.0524
1022.6641	1028.0308	1034.7777
1039.3256	1045.3108	1047.9333
1054.1640	1059.4605	1062.6751
1065.6302	1066.5754	1067.1723
1068.9604	1087.6550	1098.7853
1106.7713	1112.6968	1116.3867

1137.0379	1152.9680	1155.1348
1167.4348	1169.3350	1174.9364
1177.4255	1192.1967	1194.4177
1201.1151	1202.6791	1215.7499
1248.7332	1250.7089	1262.3731
1269.5875	1275.1181	1279.3358
1289.7495	1304.9682	1323.2077
1330.0110	1332.3801	1341.5252
1352.9328	1358.8966	1362.3516
1362.9164	1370.7939	1377.7715
1397.1059	1397.7551	1398.5896
1412.5265	1413.4736	1418.9448
1426.6890	1459.1249	1460.6923
1465.1744	1468.5206	1468.8771
1474.0637	1477.0933	1480.7947
1483.8206	1486.5942	1486.8161
1489.7268	1495.4367	1496.6025
1500.0394	1503.7705	1508.5542
1510.6324	1514.0294	1538.8788
1544.4952	1545.3841	1648.4984
1670.9488	1675.6386	1682.1305
1686.7315	1690.7306	1691.1525
1693.5728	1706.1559	3054.0527
3064.4429	3067.4485	3068.5488
3069.8280	3071.5974	3078.2147
3079.6689	3088.2598	3096.6771
3116.9876	3120.2642	3128.9737
3130.1930	3137.9284	3138.8746
3139.4615	3141.5731	3152.9953
3157.3528	3169.0777	3170.0449
3186.3208	3188.3736	3189.8777
3190.5492	3192.1362	3198.5176
3199.7713	3202.2636	3204.6776
3208.7452	3216.8699	3218.4937

3219.7528 3224.2662 3237.1416

M4[b]

Zero-point correction= 0.647117

Thermal correction to Energy= 0.682858

Thermal correction to Enthalpy= 0.683802

Thermal correction to Gibbs Free Energy= 0.580321

Sum of electronic and zero-point Energies= -2033.322985

Sum of electronic and thermal Energies= -2033.287244

Sum of electronic and thermal Enthalpies= -2033.286300

Sum of electronic and thermal Free Energies= -2033.389782

Cartesian coordinates

O	-3.549097	0.826259	-1.112003
C	-1.473389	-0.931278	-1.625740
C	0.934676	-0.701870	-0.758120
S	1.413301	-2.059907	-1.665723
C	3.012087	-2.041625	-1.001395
C	3.140217	-1.016043	-0.122386
N	1.952849	-0.271064	-0.014232
C	4.046471	-3.044933	-1.427327
C	4.622150	-3.869645	-0.265193
C	5.004291	-3.048592	0.979615
C	5.488521	-1.626140	0.667927
C	4.346695	-0.600995	0.670745
C	1.909720	0.908498	0.833922
C	2.342877	2.123519	0.307861
C	2.278668	3.244554	1.144401
C	1.829085	3.152819	2.457270
C	1.470201	1.894867	2.959018
C	1.517463	0.749418	2.171724
C	1.740939	4.370955	3.337697
C	1.227847	-0.609928	2.738355
C	2.883326	2.273112	-1.088734

H	-1.029894	-1.856376	-1.996359
H	-1.896219	-0.391977	-2.473639
H	3.614237	-3.721509	-2.170018
H	4.849286	-2.505512	-1.939085
H	3.903252	-4.644455	0.019744
H	5.506627	-4.386290	-0.652557
H	4.143229	-2.981607	1.656496
H	5.777783	-3.594808	1.527303
H	6.204538	-1.298753	1.426627
H	6.023552	-1.603087	-0.287250
H	4.028512	-0.438134	1.707249
H	4.698251	0.370560	0.301004
H	2.596483	4.207010	0.749554
H	1.156373	1.804082	3.996539
H	2.265318	4.209746	4.284383
H	2.173452	5.246491	2.848248
H	0.697599	4.597896	3.580191
H	2.160520	-1.184613	2.823225
H	0.811479	-0.517579	3.744948
H	0.537192	-1.184707	2.103351
H	2.278856	2.988775	-1.654255
H	2.899118	1.332107	-1.642458
H	3.905685	2.662324	-1.048926
C	-0.439708	-0.015425	-0.877024
C	-0.261726	1.312727	-1.612382
C	0.181957	1.325672	-2.937276
C	-0.589950	2.514745	-0.988609
C	0.296455	2.527013	-3.631906
H	0.429613	0.391696	-3.438441
C	-0.468633	3.718259	-1.681174
H	-0.941753	2.492406	0.036729
C	-0.027631	3.728952	-3.003616
H	0.637003	2.523338	-4.662812
H	-0.725144	4.650277	-1.185829

H	0.060463	4.667629	-3.542239
C	-3.673897	-0.284393	-0.618329
C	-5.000650	-0.681676	-0.024774
C	-6.047141	0.246094	-0.078516
C	-5.225208	-1.927473	0.571703
C	-7.294089	-0.062313	0.451466
H	-5.861349	1.209301	-0.542815
C	-6.474323	-2.236109	1.105250
H	-4.429695	-2.662939	0.630988
C	-7.509671	-1.306042	1.046003
H	-8.098920	0.664943	0.403400
H	-6.637324	-3.204455	1.568011
H	-8.483082	-1.548885	1.461605
O	-0.951441	0.188648	0.396618
C	-1.634645	-1.122408	0.760971
C	-2.526201	-1.250120	-0.566578
O	-0.793761	-2.103555	0.840671
H	-2.869730	-2.282534	-0.625673
C	-2.394821	-0.772655	2.042143
H	-3.063833	0.086428	1.928992
H	-2.979117	-1.637350	2.368500
H	-1.662503	-0.543544	2.822224

Vibrational frequencies

16.2064	25.8043	35.6212
43.7274	44.8604	48.6653
55.2365	76.4048	84.0260
89.8059	93.4666	100.8282
114.7676	121.0041	131.3083
139.4967	149.3460	155.7923
175.0252	184.8439	191.8929
199.5931	205.5636	216.8045
226.3674	233.3813	237.9195
252.1630	254.8963	273.3980

276.3046	287.2292	305.1913
315.4446	324.2458	326.2300
341.5156	350.3800	362.7824
378.7275	405.0021	411.7567
415.1821	418.7375	420.3440
432.9951	445.9405	467.0407
489.6311	496.6852	506.0230
519.9325	531.6474	540.0236
552.1080	571.8702	577.0236
579.9218	590.5810	595.5500
615.2702	624.1012	625.3074
631.0390	659.8895	670.8883
687.2844	697.1037	708.3928
710.6586	721.1321	725.6325
735.6830	749.1239	772.8159
775.1741	795.7061	800.9978
814.3947	846.5997	876.3826
881.8539	883.0692	885.8848
886.8206	895.3406	913.2186
930.9250	950.5042	952.5250
968.3805	969.8098	973.3830
981.9687	982.5510	988.0421
1008.7458	1013.1547	1017.8496
1020.9966	1022.6106	1023.7788
1033.1172	1037.0950	1041.1729
1044.7057	1051.5402	1051.9160
1056.2691	1064.8832	1068.7073
1069.1906	1071.8158	1076.1866
1080.5877	1093.5265	1096.7701
1108.5133	1119.4541	1121.2029
1126.6781	1148.0881	1160.6358
1165.8287	1170.3430	1172.2981
1186.0183	1189.6936	1197.3372
1202.0799	1207.1987	1223.4209

1242.0144	1249.7225	1256.0304
1273.6735	1276.8305	1285.6525
1294.2027	1306.6882	1322.7481
1329.3272	1335.4644	1337.1653
1342.7395	1355.6782	1358.3725
1359.8005	1370.9991	1372.4563
1373.3767	1391.7939	1399.8364
1402.9554	1414.2771	1416.2135
1422.4843	1428.2143	1440.5144
1463.3788	1465.5540	1468.3916
1469.1999	1471.2354	1475.4521
1478.8763	1479.6104	1483.7170
1489.8184	1490.7814	1495.0705
1497.5333	1501.7021	1502.4794
1509.8175	1513.1384	1535.3952
1545.1660	1546.6478	1547.7913
1669.7974	1676.7604	1682.8002
1685.8140	1692.2723	1692.8537
1693.5664	1806.4511	3000.4995
3061.9249	3062.9716	3069.9815
3071.7091	3072.8797	3074.1635
3081.5708	3082.3090	3099.2453
3112.2927	3116.4052	3121.5741
3126.8095	3131.6081	3142.1028
3143.7054	3144.3993	3145.0883
3145.5059	3155.5691	3157.5866
3160.4044	3167.9622	3177.0877
3183.3893	3191.1731	3197.1109
3201.2235	3206.3960	3214.4685
3219.3823	3224.9835	3228.4862
3238.2198	3241.0034	3244.6102

TS5[b]

Zero-point correction= 0.643269

Thermal correction to Energy= 0.680310

Thermal correction to Enthalpy= 0.681254

Thermal correction to Gibbs Free Energy= 0.573210

Sum of electronic and zero-point Energies= -2033.306962

Sum of electronic and thermal Energies= -2033.269921

Sum of electronic and thermal Enthalpies= -2033.268977

Sum of electronic and thermal Free Energies= -2033.377021

Cartesian coordinates

O	-3.704246	1.180967	-0.914827
C	-1.618936	-0.452306	-1.645687
C	1.039397	-0.548724	-0.879893
S	1.408822	-1.928271	-1.820075
C	2.966273	-2.179033	-1.079492
C	3.169271	-1.225583	-0.137998
N	2.077018	-0.334225	-0.069028
C	3.881861	-3.299825	-1.485802
C	4.219169	-4.268256	-0.340365
C	4.579324	-3.585133	0.990988
C	5.299697	-2.238704	0.831809
C	4.327677	-1.051990	0.803235
C	2.108775	0.787904	0.845075
C	2.734661	1.963819	0.433762
C	2.774652	3.025115	1.342245
C	2.216529	2.917571	2.616035
C	1.614933	1.710497	2.988829
C	1.552330	0.625667	2.117355
C	2.242934	4.078703	3.574984
C	0.928829	-0.683512	2.507901
C	3.324595	2.087297	-0.944294
H	-1.072499	-1.286044	-2.088179
H	-2.053032	0.124003	-2.467180
H	3.430480	-3.859340	-2.310085
H	4.802008	-2.862306	-1.885713

H	3.376165	-4.948252	-0.179460
H	5.060051	-4.884211	-0.677728
H	3.667639	-3.420732	1.579510
H	5.196491	-4.273589	1.576066
H	5.976852	-2.074208	1.674751
H	5.926350	-2.242993	-0.066524
H	3.913404	-0.918041	1.810748
H	4.859795	-0.122286	0.566009
H	3.249766	3.955846	1.040730
H	1.185869	1.611403	3.983618
H	2.581226	3.763691	4.566487
H	2.905972	4.871100	3.220043
H	1.241579	4.505623	3.694855
H	1.669205	-1.492943	2.477886
H	0.523825	-0.629740	3.521150
H	0.124459	-0.936326	1.810219
H	3.719835	3.092777	-1.103560
H	2.569542	1.885399	-1.712107
H	4.141508	1.371702	-1.093677
C	-0.717632	0.483268	-0.793385
C	-0.201330	1.711620	-1.535094
C	0.099741	1.695970	-2.901548
C	-0.048561	2.897224	-0.819710
C	0.554560	2.848009	-3.537007
H	-0.007296	0.774639	-3.469921
C	0.411995	4.051582	-1.451687
H	-0.287283	2.886007	0.239889
C	0.714795	4.029938	-2.811678
H	0.787654	2.825012	-4.597526
H	0.535148	4.968914	-0.882239
H	1.072894	4.928089	-3.306125
C	-3.858272	0.020029	-0.587520
C	-5.179003	-0.426026	-0.023933
C	-6.083936	0.561797	0.380037

C	-5.536319	-1.773520	0.095513
C	-7.323053	0.211298	0.901740
H	-5.796489	1.603512	0.280385
C	-6.781577	-2.123818	0.611387
H	-4.854559	-2.559809	-0.214536
C	-7.673944	-1.133944	1.016976
H	-8.016229	0.983804	1.219789
H	-7.054015	-3.171077	0.695323
H	-8.642750	-1.410567	1.421783
O	-1.015727	0.611869	0.417343
C	-2.182352	-1.624875	0.502375
C	-2.757464	-1.010696	-0.789339
O	-1.309637	-2.464273	0.391965
H	-3.206764	-1.854019	-1.330040
C	-2.749685	-1.261249	1.852116
H	-3.039730	-0.210494	1.895430
H	-3.631417	-1.878330	2.055944
H	-1.998644	-1.473517	2.614952

Vibrational frequencies

-155.9612	15.2885	15.9576
29.3092	37.6703	43.4203
50.1915	51.4497	59.0639
69.5808	76.2769	83.6366
89.7677	100.9473	105.6311
125.1797	127.4565	137.7107
139.3331	150.0695	158.3127
163.8281	165.1781	184.9858
189.5801	196.8740	198.7033
213.5334	215.8767	242.9082
245.4886	255.3347	259.0615
280.5059	300.1510	307.7926
326.4724	333.7582	340.0855
348.9742	364.4479	370.3689

380.0941	408.8808	414.8434
416.3757	418.1373	451.7557
460.0872	460.5966	475.6300
503.2324	505.4608	513.1198
524.0243	527.2537	552.3777
559.6750	573.2252	577.6859
586.1318	591.9137	603.9840
618.7521	625.4573	626.8783
640.1826	666.9571	682.0388
705.1021	707.0597	711.1775
716.2800	747.5134	752.0338
767.5195	775.4939	797.4139
802.2887	811.8524	845.3535
862.4210	868.5911	876.1398
879.3257	881.6703	914.9747
922.0728	937.0789	947.2748
959.1974	965.6462	968.7796
969.9807	984.0398	985.7457
991.8793	996.4833	1003.4076
1013.5137	1014.4255	1018.9629
1020.2750	1022.9202	1025.8120
1035.4742	1037.5412	1043.5050
1051.0042	1052.4062	1059.7948
1064.2102	1065.6492	1067.0777
1068.8957	1075.6779	1095.5420
1096.2563	1108.3023	1117.8148
1119.6617	1141.0863	1165.9418
1166.0478	1187.8636	1189.5075
1195.0312	1201.9689	1204.2904
1218.8277	1219.7796	1246.9409
1249.4487	1256.9886	1263.3590
1275.0972	1283.5480	1285.1855
1301.0519	1314.0882	1331.5024
1335.3347	1337.6327	1353.7756

1359.3621	1360.2465	1361.6064
1361.7823	1371.8554	1378.3261
1387.5074	1392.4530	1399.9413
1402.7894	1411.8542	1414.2372
1426.3640	1444.7298	1449.6213
1455.6711	1457.7309	1467.1486
1471.7897	1478.2461	1479.8267
1480.6359	1482.1617	1486.2272
1486.4489	1492.1498	1494.8859
1495.8136	1497.6983	1510.1004
1516.5327	1542.3989	1545.9883
1546.6326	1605.0872	1673.8207
1678.6368	1684.4800	1691.2291
1691.7958	1692.2618	1696.7291
1816.4486	1839.7552	3056.0992
3060.4321	3061.9193	3065.5476
3069.1999	3072.6253	3080.9461
3081.7864	3082.3151	3090.8311
3105.3598	3109.0629	3112.4285
3122.8942	3128.5751	3129.2214
3133.7285	3136.5490	3139.8199
3158.6428	3163.2388	3164.2822
3164.4599	3169.9022	3190.4569
3190.9122	3196.0290	3198.2674
3202.4356	3205.4611	3209.7792
3213.0886	3218.1490	3224.2232
3225.5858	3229.6469	3229.9022

P^{b}

Zero-point correction= 0.298573

Thermal correction to Energy= 0.316928

Thermal correction to Enthalpy= 0.317872

Thermal correction to Gibbs Free Energy= 0.250248

Sum of electronic and zero-point Energies= -920.593406

Sum of electronic and thermal Energies= -920.575052

Sum of electronic and thermal Enthalpies= -920.574108

Sum of electronic and thermal Free Energies= -920.641732

Cartesian coordinates

C	1.218030	-0.449891	0.138958
O	0.452550	-1.316414	-0.241277
C	0.662732	0.855627	0.702901
C	-0.813203	0.686621	1.062858
C	0.947260	2.037775	-0.233842
O	1.728271	1.942565	-1.156143
C	-1.692222	0.539178	-0.162783
C	-3.040381	-0.096356	-0.018137
O	-1.324938	0.967390	-1.242567
C	-3.776056	-0.347748	-1.181643
C	-5.036311	-0.926553	-1.103690
C	-5.577310	-1.248838	0.141483
C	-4.854621	-0.992535	1.304606
C	-3.586795	-0.421615	1.227369
H	-0.923937	-0.183175	1.713588
H	-1.173329	1.553629	1.631181
H	-3.341261	-0.084724	-2.140429
H	-5.598928	-1.127240	-2.010015
H	-6.563211	-1.699253	0.205386
H	-5.277229	-1.237937	2.273783
H	-3.036854	-0.223038	2.141722
C	2.697013	-0.678450	0.109304
C	3.615432	0.255318	0.600309
C	3.160914	-1.890925	-0.413050
C	4.978589	-0.023182	0.568789
H	3.277934	1.204609	1.002984
C	4.522375	-2.166733	-0.447532
H	2.438091	-2.607296	-0.789455
C	5.433226	-1.232195	0.045281

H	5.686411	0.704558	0.952444
H	4.875779	-3.108604	-0.855220
H	6.497337	-1.446824	0.021675
H	1.202683	1.091134	1.630614
C	0.273025	3.340705	0.115453
H	0.712955	4.144246	-0.476214
H	-0.796396	3.274599	-0.104848
H	0.382699	3.555763	1.182901

Vibrational frequencies

23.4244	29.4191	50.0559
54.6268	78.8075	106.8791
127.6709	139.4302	142.8563
154.9229	161.8189	171.4522
212.8017	297.4158	312.8927
343.1868	355.5000	412.8123
415.1446	418.7001	425.0689
443.6114	481.2677	494.7481
558.9779	564.4919	588.0487
626.3391	626.8728	648.1643
693.2078	708.6089	711.0475
715.0611	763.3367	775.1107
815.2192	834.3994	873.8600
879.0952	884.1369	952.3168
971.5167	977.8196	987.1639
1002.2923	1011.9721	1016.7093
1020.0503	1022.0426	1030.8330
1037.6124	1042.6184	1057.7747
1067.9176	1071.9031	1104.2264
1118.2177	1130.9093	1172.3066
1177.5054	1186.9470	1192.4385
1202.2632	1212.4455	1248.2374
1273.2611	1311.1492	1338.0036
1345.0203	1362.9252	1365.2015

1376.9072	1396.6078	1407.2977
1445.5971	1457.3159	1470.0405
1497.9571	1501.0530	1546.3614
1551.3160	1673.4683	1674.4888
1692.3200	1693.9102	1819.2374
1826.9988	1856.1878	3074.3013
3077.0814	3093.3502	3151.9780
3157.6272	3187.7965	3208.1696
3216.5653	3216.9406	3224.1555
3228.5214	3233.5796	3233.9218
3236.0175	3247.4731	3251.9656

TS3$^{a\prime}$

Zero-point correction= 0.687722

Thermal correction to Energy= 0.729236

Thermal correction to Enthalpy= 0.730180

Thermal correction to Gibbs Free Energy= 0.610988

Sum of electronic and zero-point Energies= -2684.492407

Sum of electronic and thermal Energies= -2684.450893

Sum of electronic and thermal Enthalpies= -2684.449949

Sum of electronic and thermal Free Energies= -2684.569141

Cartesian coordinates

O	-2.969264	1.945255	-1.233655
C	-0.717227	0.237721	-1.368050
C	0.523052	1.029787	0.855300
S	-0.307558	2.279666	1.723415
C	1.010233	3.390486	1.494638
C	2.006823	2.812447	0.796868
N	1.723500	1.488316	0.424731
C	1.021980	4.829970	1.908384
C	0.971835	5.794766	0.694765
C	1.510405	5.226273	-0.624520
C	2.949474	4.695259	-0.617929

C	3.242749	3.561016	0.401618
C	2.735138	0.692766	-0.239686
C	3.587964	-0.065561	0.577109
C	4.573592	-0.822640	-0.041677
C	4.722247	-0.834531	-1.434999
C	3.887391	-0.027866	-2.200412
C	2.887277	0.767226	-1.622664
C	5.764516	-1.713552	-2.072523
C	2.065796	1.677419	-2.498699
C	3.419831	-0.055969	2.071186
H	0.134738	-0.316995	-1.754561
H	-0.568821	1.314805	-1.315162
H	0.199439	5.044209	2.595013
H	1.947438	4.994334	2.471825
H	-0.067143	6.094265	0.524680
H	1.522252	6.703539	0.960554
H	0.839534	4.425959	-0.961033
H	1.444061	6.012706	-1.383897
H	3.173069	4.330756	-1.625539
H	3.646354	5.516623	-0.420042
H	4.000769	2.880906	0.008221
H	3.655228	3.993939	1.319120
H	5.234836	-1.430104	0.572365
H	4.013753	0.001504	-3.280240
H	5.825650	-1.541942	-3.149303
H	6.751597	-1.534693	-1.635741
H	5.524979	-2.769803	-1.908134
H	1.457647	2.375344	-1.919278
H	2.727177	2.256418	-3.149615
H	1.395066	1.103037	-3.145275
H	4.157945	-0.706544	2.544721
H	2.419407	-0.398911	2.359967
H	3.544058	0.954884	2.476341
C	-0.092081	-0.230318	0.542907

C	-3.079082	0.780819	-1.670518
C	-4.442831	0.337539	-2.149272
C	-5.551134	1.093275	-1.751719
C	-4.646697	-0.775522	-2.973014
C	-6.836279	0.736731	-2.147459
H	-5.377481	1.963026	-1.126332
C	-5.931874	-1.130274	-3.376658
H	-3.800222	-1.360155	-3.318937
C	-7.030318	-0.379052	-2.961469
H	-7.687864	1.327672	-1.823373
H	-6.075599	-1.992871	-4.020308
H	-8.031673	-0.659345	-3.274059
O	0.896002	-1.237793	0.415871
C	0.628098	-2.372186	-0.271279
O	-0.401630	-2.586973	-0.862873
C	1.765128	-3.331767	-0.200095
C	2.681354	-3.316180	0.853561
C	1.877156	-4.283162	-1.217558
C	3.713139	-4.250469	0.883425
H	2.580779	-2.584705	1.648281
C	2.919340	-5.202667	-1.193184
H	1.149081	-4.285497	-2.022327
C	3.836857	-5.187033	-0.141654
H	4.421818	-4.245010	1.705594
H	3.015217	-5.933522	-1.989531
C	-2.009663	-0.161395	-1.712092
H	-2.203094	-1.198170	-1.953811
C	-1.255692	-0.657446	1.362588
C	-2.457870	0.062265	1.328926
C	-1.185091	-1.809077	2.159042
C	-3.554095	-0.342299	2.088326
H	-2.552156	0.942601	0.700801
C	-2.274975	-2.229021	2.910264
H	-0.266605	-2.386055	2.208024

C	-3.451879	-1.487440	2.865057
H	-4.480686	0.220976	2.055915
H	-2.208952	-3.118787	3.526672
H	4.646730	-5.909726	-0.119811
Cl	-4.832956	-2.017851	3.804394

Vibrational frequencies

-458.8358	14.5360	18.1902
21.3223	28.4066	32.1744
35.6067	43.3095	47.4594
52.5241	59.3401	68.0368
72.0375	79.1535	89.2832
93.1259	100.2505	113.7023
118.1220	129.4262	132.6325
135.3070	147.9800	153.2573
168.3150	171.3457	179.0368
187.6345	192.8596	204.4015
211.7893	218.7126	220.1676
245.7172	257.4678	269.3333
275.3222	282.9835	305.0078
311.4763	311.8273	334.4568
337.2431	342.0234	363.3119
373.7328	376.1192	400.1864
407.5953	418.8426	420.2966
423.3900	427.6407	436.5176
440.1835	450.1120	472.2068
487.5907	503.9607	505.9830
523.7365	528.3739	532.9238
541.8126	560.4368	572.0403
579.7781	592.1642	608.5587
613.4491	626.7361	627.6054
640.1078	652.5171	664.5405
679.9906	698.1898	705.4707
709.1731	714.1586	727.3616

729.4429 732.2502 748.3859

751.1587 753.4856 769.4798

786.5187 794.1323 813.2092

821.8116 827.7080 855.5331

860.2555 865.5087 881.2335

882.8844 886.9476 887.7175

913.4963 920.3130 925.4859

963.9028 965.3800 969.4837

973.4659 975.5973 976.5531

994.9634 997.5940 1010.6589

1013.7584 1015.2970 1015.7925

1017.5035 1021.7062 1031.7215

1037.3310 1038.0441 1041.7512

1045.7110 1053.9979 1057.0829

1058.2196 1059.7180 1061.7452

1065.0812 1065.4658 1068.5660

1084.7921 1091.5332 1106.1325

1113.9556 1115.9562 1126.4445

1128.3281 1147.4662 1148.8593

1157.4608 1166.1425 1167.6145

1173.2751 1189.5537 1191.0939

1192.7815 1200.6052 1214.7360

1217.9276 1224.0547 1262.4370

1265.6098 1272.6100 1274.8985

1285.9919 1296.6864 1306.3100

1315.1491 1317.2296 1328.9448

1329.9932 1333.0076 1335.5935

1341.5227 1348.5748 1350.0685

1354.7429 1358.2160 1364.0789

1382.5249 1384.6757 1401.9629

1409.8545 1414.1797 1420.5171

1422.4222 1427.2623 1444.0472

1456.8707 1464.6994 1470.9083

1472.7131 1473.9338 1476.1033

1476.2981	1476.7584	1486.0034
1488.0680	1488.9342	1491.0826
1496.5526	1497.6878	1508.9958
1534.5820	1537.2627	1544.3673
1544.9326	1554.5719	1650.1064
1652.5319	1672.4693	1675.9943
1679.2851	1683.3888	1688.3568
1689.4872	1690.3893	1704.7468
1855.3653	3063.7047	3065.7657
3071.3004	3077.3393	3080.6896
3081.4268	3082.5048	3090.6989
3113.8530	3125.5224	3126.6063
3128.3097	3138.4959	3145.7596
3147.5022	3150.3251	3158.3859
3169.0794	3169.2801	3177.2754
3202.6394	3205.3799	3214.2075
3220.6385	3223.3921	3226.0575
3228.4640	3230.6026	3232.3634
3236.5504	3239.3546	3239.8031
3241.0150	3241.2274	3247.3981
3247.5224	3252.5973	3268.4416

TS3$^{b\prime}$

Zero-point correction= 0.687704

Thermal correction to Energy= 0.729128

Thermal correction to Enthalpy= 0.730072

Thermal correction to Gibbs Free Energy= 0.610406

Sum of electronic and zero-point Energies= -2684.490755

Sum of electronic and thermal Energies= -2684.449332

Sum of electronic and thermal Enthalpies= -2684.448388

Sum of electronic and thermal Free Energies= -2684.568054

Cartesian coordinates

O	-4.078855	0.514268	-0.951720

C	-1.363502	-0.275799	-1.059368
C	-0.366996	1.251747	0.908433
S	-1.498507	2.277308	1.726657
C	-0.643621	3.708090	1.231378
C	0.431975	3.388352	0.485583
N	0.576387	2.005533	0.287990
C	-1.079407	5.118313	1.489688
C	-1.532332	5.848072	0.198075
C	-0.957356	5.293421	-1.110913
C	0.570199	5.243270	-1.236413
C	1.307215	4.433394	-0.136688
C	1.711982	1.499677	-0.459846
C	2.879103	1.197864	0.260660
C	3.982285	0.740362	-0.448923
C	3.946564	0.585017	-1.840744
C	2.786008	0.941641	-2.518390
C	1.652958	1.428675	-1.851166
C	5.151515	0.058019	-2.573424
C	0.470593	1.895311	-2.660615
C	2.922320	1.381320	1.751895
H	-0.384630	-0.540467	-1.452319
H	-1.624037	0.776231	-1.155279
H	-1.875546	5.146581	2.237933
H	-0.223058	5.642252	1.929575
H	-2.623300	5.793719	0.126374
H	-1.276126	6.908260	0.298109
H	-1.359747	4.285275	-1.269362
H	-1.343448	5.902908	-1.935130
H	0.808665	4.811779	-2.213919
H	0.975872	6.260562	-1.235107
H	2.221769	3.990805	-0.536759
H	1.610427	5.108826	0.670404
H	4.892133	0.492879	0.093857
H	2.753377	0.864140	-3.602908

H	5.002234	0.086134	-3.655052
H	6.043799	0.643672	-2.332126
H	5.356928	-0.978863	-2.284975
H	-0.273805	2.413648	-2.052542
H	0.811537	2.580810	-3.441866
H	-0.024815	1.056096	-3.158756
H	3.882127	1.047907	2.152405
H	2.123902	0.816956	2.244751
H	2.787473	2.436392	2.018541
C	-0.520550	-0.173360	0.835744
C	-3.769907	-0.672903	-1.179285
C	-4.892993	-1.658797	-1.405778
C	-6.170900	-1.304034	-0.960656
C	-4.719774	-2.892264	-2.043892
C	-7.248997	-2.167136	-1.127185
H	-6.295166	-0.337887	-0.481930
C	-5.799657	-3.754296	-2.219953
H	-3.743518	-3.177825	-2.423149
C	-7.065515	-3.397231	-1.758349
H	-8.233413	-1.881442	-0.768098
H	-5.653031	-4.705852	-2.722295
H	-7.904746	-4.072959	-1.893614
O	0.762462	-0.768150	0.760650
C	0.951277	-1.978299	0.198032
O	0.087842	-2.667806	-0.284778
C	2.397766	-2.336303	0.242179
C	3.201663	-1.983952	1.327272
C	2.942416	-3.012496	-0.849188
C	4.556386	-2.295545	1.321017
H	2.772379	-1.465208	2.178376
C	4.300991	-3.306010	-0.879457
H	2.307440	-3.287249	-1.685300
C	5.089217	-2.936167	0.206652
H	5.190051	-2.030258	2.160282

H	4.742698	-3.807626	-1.733453
C	-2.429237	-1.161695	-1.205797
H	-2.237031	-2.224752	-1.273199
C	-1.422916	-0.841768	1.806609
C	-2.797211	-0.563526	1.806818
C	-0.927157	-1.785092	2.718370
C	-3.644184	-1.189078	2.720301
H	-3.210184	0.133189	1.083712
C	-1.779124	-2.416196	3.617787
H	0.132918	-2.020780	2.735119
C	-3.142258	-2.119539	3.625527
H	-4.705120	-0.956864	2.707874
H	-1.374777	-3.139140	4.319770
H	-3.805594	-2.613517	4.328755
Cl	6.803068	-3.282754	0.166452

Vibrational frequencies

-455.6785	8.0923	16.0170
18.6549	21.7114	33.8782
34.0676	47.5749	52.1447
55.8869	61.2764	65.4733
74.9943	80.0985	86.1496
95.7662	107.1643	119.4574
121.6597	128.8665	131.9203
134.1801	140.2966	156.2222
165.0660	167.2133	183.6018
203.0428	209.9471	214.7029
224.7273	234.8706	237.1548
251.9009	259.3493	270.1558
277.0235	282.9059	285.7078
302.9167	313.2690	314.4582
336.2348	338.1154	354.4171
374.2141	376.7436	402.0144
403.8573	409.6124	419.2818

420.8293 427.2218 434.9458

437.0546 463.2719 474.0905

486.5109 503.7490 520.4809

530.4969 531.9512 539.6766

544.9933 557.9309 571.4465

581.1366 593.7725 595.8564

612.4668 626.1361 627.1549

636.0333 648.7922 665.0782

670.6917 694.2972 706.7106

710.4473 719.3115 723.7797

732.2849 745.5457 748.8415

753.9923 765.0529 771.8098

780.1854 790.3213 796.9477

813.8093 825.7272 857.7983

861.3101 866.9078 873.6289

881.7226 889.6783 898.5660

913.1869 915.2404 924.6876

963.1131 965.5366 968.0132

973.8865 974.1620 978.3387

989.9156 995.7606 1003.5895

1010.7639 1014.5577 1016.3517

1016.7361 1024.2370 1026.9174

1031.8130 1039.3515 1044.3529

1045.8744 1052.6658 1056.8625

1058.6492 1059.5010 1061.2254

1061.8969 1063.8238 1078.9622

1087.0795 1091.5303 1110.1915

1114.6282 1120.5401 1125.7214

1135.3484 1138.2583 1147.7354

1155.3283 1165.1493 1175.1348

1178.9508 1188.7611 1193.9158

1196.1225 1203.1600 1216.2037

1218.4928 1224.7343 1261.6779

1271.5502 1275.2694 1279.0771

1286.5522	1294.3074	1309.7451
1319.8707	1320.7266	1327.5941
1332.6339	1336.2123	1339.7432
1348.8400	1350.4908	1358.3324
1360.1805	1364.3814	1370.9699
1382.7743	1383.5522	1401.3777
1411.9040	1413.1505	1420.2456
1423.1085	1428.4990	1451.5622
1454.0694	1459.2267	1470.0614
1470.6116	1477.0313	1477.4974
1478.8724	1480.2108	1485.1506
1490.2718	1491.8337	1492.2055
1497.9025	1499.9669	1510.9073
1538.5232	1540.5570	1544.3813
1553.3484	1558.2087	1657.2365
1665.2374	1667.9725	1681.8714
1686.4577	1688.6311	1693.1177
1694.4303	1698.1099	1702.5271
1861.7412	3060.8861	3065.4152
3069.4932	3072.0180	3074.1089
3076.3355	3078.2177	3084.4583
3108.1104	3121.9802	3123.6295
3130.9590	3139.1582	3140.6323
3141.9543	3147.3106	3154.9041
3164.0784	3170.0774	3170.9034
3196.6398	3198.0678	3199.5733
3208.9727	3210.3024	3214.6721
3219.5482	3223.4130	3226.1008
3228.8465	3232.6336	3234.8061
3236.5674	3239.5907	3241.0917
3243.4313	3245.6444	3248.7842