Supplementary Data

Mechanistic insight highlights the key-steps and significance of metal in Ir(III)- catalyzed C-H activated chromones generation

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1. Gaussian 09 Full Reference

Gaussian 09, Revision C.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian, Inc., Wallingford CT, **2010**.

2. Computational methods:

Computational Method used:

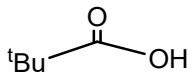
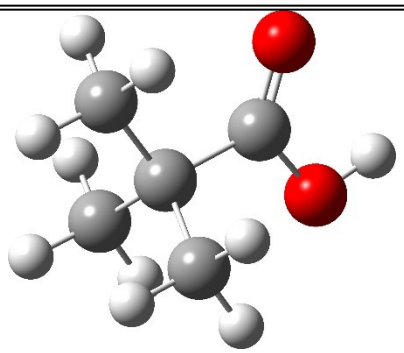
Hybrid DFT functional method M06-2X, M06 and M06L.

Basis set used:

DZ for valence electrons and LANL2 as ECP Iridium atom and 6-31G(d,p), 6-311G++(d,p) basis set for other atoms.

Solvent used for calculation by SMD model:

Methanol

St.Pt.	General Structure	Ball & Stick model
Pivalic Acid		

Cartesian co-ordinate

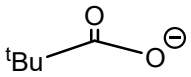
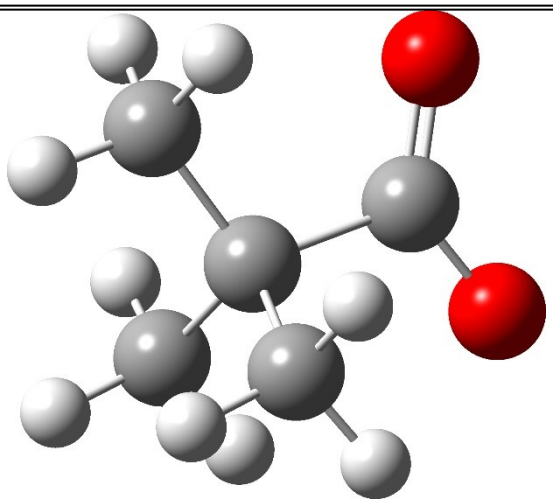
Atoms	X	Y	Z
O	-1.60122	-0.99448	-0.00002
C	-0.93875	0.18211	-0.00002
O	-1.52140	1.23969	-0.00002
C	0.56721	-0.01023	-0.00001
C	0.96763	-0.79514	1.25247
H	0.50531	-1.78731	1.27018
H	2.05713	-0.92109	1.27175
H	0.67603	-0.26176	2.16547
C	0.96771	-0.79524	-1.25238
H	0.67640	-0.26183	-2.16544
H	2.05720	-0.92139	-1.27144
H	0.50523	-1.78734	-1.27016
C	1.23821	1.35696	-0.00004
H	0.95320	1.93884	-0.88298
H	0.95337	1.93880	0.88299
H	2.32802	1.23454	-0.00015
H	-2.54294	-0.76389	-0.00002

Frequencies

20.4974	201.6744	226.9389
248.9615	282.7465	287.1638
347.7622	357.9879	381.0666
513.7520	580.1238	631.5691
740.1999	796.4129	878.5174
948.9897	949.5788	951.7895
1032.7243	1039.3715	1177.3831
1241.6133	1246.0257	1277.1031
1372.4849	1376.9284	1394.9813
1418.4214	1444.4943	1458.7030
1464.9982	1469.0819	1480.8254
1503.6563	1881.6662	3031.7037
3033.8379	3041.1383	3117.9940
3119.1324	3130.6937	3136.8609
3138.5109	3139.5687	3814.5248

Statistical Thermodynamic Analysis

Temperature=298K Pressure=1 atm
Zero-point correction= 0.146555 Electronic Energy = -346.822814957
Internal Energy (E)= -346.667953957 Enthalpy (H)= -346.667009957
Gibbs Free Energy (G)=-346.709206957 Gibbs Free Energy of Solvation=-346.841231237

St.Pt.	General Structure	Ball & Stick model
Pivalate Ion		

Cartesian co-ordinate

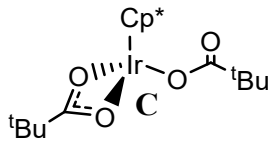
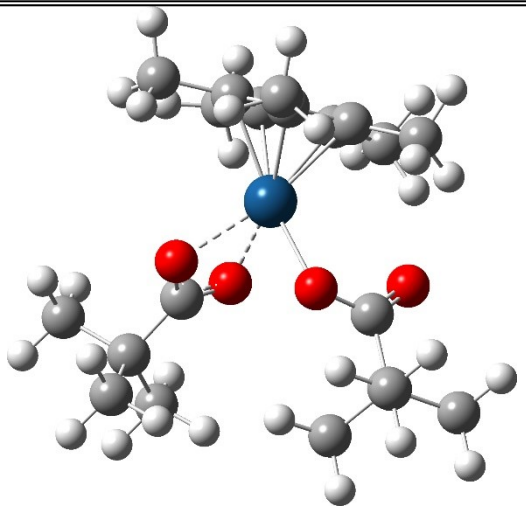
Atoms	X	Y	Z
O	1.58289	-1.10545	0.00004
C	1.05961	0.03245	-0.00002
O	1.59813	1.15933	-0.00014
C	-0.52273	0.01206	-0.00003
C	-0.98361	-0.74499	-1.24093
H	-0.49833	-1.72724	-1.26394
H	-2.07931	-0.87764	-1.25991
H	-0.69516	-0.20539	-2.15484
C	-0.98347	-0.74436	1.24126
H	-0.69531	-0.20415	2.15490
H	-2.07913	-0.87729	1.26012
H	-0.49796	-1.72649	1.26503
C	-1.10092	1.41783	-0.00021
H	-0.75501	1.97531	0.87825
H	-0.75629	1.97490	-0.87951
H	-2.20498	1.39899	0.00028
H	-2.54294	-0.76389	-0.00002

Frequencies

49.2181	228.5306	270.1743
284.2385	308.5546	311.1354
354.3666	372.1142	387.1643
526.4043	582.4226	797.5958
802.1965	872.6220	928.9123
939.3621	943.9884	1030.4954
1035.6613	1239.9927	1240.8582
1266.9822	1350.0168	1352.4313
1372.6158	1425.2934	1448.2067
1457.8882	1466.0236	1475.1283
1476.2987	1501.3685	1803.0588
2973.8366	2973.8859	2983.9040
3057.1887	3060.2599	3085.3348
3120.2592	3120.9704	3124.0990

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.133047 Electronic Energy = -346.245504190
Internal Energy (E)= -346.10463319 Enthalpy (H)= -346.10368819
Gibbs Free Energy (G)=-346.14422819 Gibbs Free Energy of Solvation=-346.384527125

St.Pt.	General Structure	Ball & Stick model
Active Catalyst (**C**)		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-2.14834	-1.57148	-0.04788
C	-2.14723	-0.87221	1.20649
C	-2.52703	0.51322	0.94856
C	-2.73076	0.66105	-0.45815
C	-2.46759	-0.62622	-1.09102
C	1.11231	1.85674	0.00247
O	0.81006	1.18699	1.03698
O	0.44607	1.64631	-1.05845
C	1.50872	-1.86309	0.21161
O	1.01850	-0.99913	-0.62877
O	0.94082	-2.29808	1.20948
C	2.94394	-2.27397	-0.14490
Ir	-0.69742	0.03488	-0.09777
C	2.17105	2.93818	0.03855
C	3.81980	-1.03305	0.05296
H	3.51158	-0.23195	-0.63046
H	3.73947	-0.66062	1.08372
H	4.87364	-1.27291	-0.14199
C	3.01813	-2.72791	-1.60187
H	4.05131	-2.99757	-1.85945
H	2.39038	-3.61237	-1.77288
H	2.68413	-1.93550	-2.27874
C	3.41295	-3.39130	0.77689
H	2.78167	-4.28124	0.67233
H	4.44693	-3.67001	0.53358
H	3.37018	-3.08149	1.82611
C	-2.60711	-0.92339	-2.54197
H	-1.95236	-1.74714	-2.84200
H	-3.63982	-1.20267	-2.78957
H	-2.33764	-0.05448	-3.15118

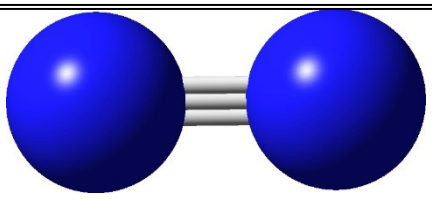
Frequencies

26.6684	33.2471	47.0558
60.4496	70.1386	84.5661
90.1225	106.6644	121.1919
125.9555	135.5812	140.9992
152.1963	159.3481	164.2452
169.9558	176.3076	176.8919
185.6811	195.4474	201.4704
206.7101	212.8003	222.1952
230.1503	234.5767	262.0340
268.9007	280.5801	290.4183
300.6839	308.8103	311.5538
318.4967	323.7102	327.5984
339.5568	364.8207	380.1160
388.1017	389.9593	403.0829
433.8469	441.8672	451.8487
462.2617	464.5086	531.8748
537.9611	541.0484	543.6213
572.6816	579.3283	582.1243
601.4692	620.0447	643.9709
790.8850	793.7404	805.5988
809.2057	815.1769	827.4042
916.2330	932.6454	941.6738
946.1832	947.3183	950.7605
952.2053	953.9881	961.3648
977.0163	1029.0655	1037.5102
1038.3753	1038.8040	1039.4280
1042.9072	1043.7217	1046.5241
1046.9225	1091.7491	1093.9147
1110.1686	1185.2472	1188.4030
1236.3535	1240.0682	1251.6135
1258.8756	1264.6226	1268.2533
1367.5611	1369.1919	1373.1485
1377.2991	1377.5453	1378.7370
1389.5867	1393.1999	1396.1915

C	-1.82418	-3.00933	-0.24263	1398.4516	1400.9744	1415.4104
H	-1.09952	-3.34438	0.50400	1427.1071	1436.3536	1438.8569
H	-2.73387	-3.61871	-0.16728	1442.8885	1445.5266	1447.1134
H	-1.38146	-3.18081	-1.22965	1449.1015	1455.4199	1456.3334
C	-1.84704	-1.46697	2.53573	1458.0581	1460.8399	1461.1274
H	-2.68215	-2.09217	2.87761	1463.4167	1469.5974	1470.5563
H	-0.93854	-2.07532	2.47431	1473.5502	1474.6180	1475.0039
H	-1.67888	-0.68805	3.28589	1483.7774	1485.2704	1486.2688
C	-3.07185	1.91207	-1.18714	1496.8973	1498.6425	1503.5932
H	-4.13929	1.94265	-1.43962	1516.8556	1531.4338	1538.2352
H	-2.83461	2.79782	-0.58940	1545.1445	1605.8949	1765.7582
H	-2.49917	1.98740	-2.11771	3020.2425	3024.7709	3027.2697
C	-2.62467	1.57139	1.99074	3033.0803	3034.5634	3035.0608
H	-2.68625	2.56851	1.54397	3036.6061	3038.5729	3040.9407
H	-3.51371	1.42540	2.61704	3041.0892	3041.6372	3101.6294
H	-1.74282	1.55451	2.64100	3104.5226	3115.0688	3116.8775
C	2.97056	2.92330	-1.26187	3117.5361	3118.1971	3120.6186
H	3.70816	3.73582	-1.25212	3120.9309	3121.6993	3124.0734
H	3.51086	1.97618	-1.38301	3124.9164	3131.6023	3132.6819
H	2.31734	3.05184	-2.13042	3138.3509	3139.2767	3141.1348
C	3.09152	2.75159	1.23844	3142.7174	3145.4007	3145.5625
H	3.83545	3.55792	1.26167	3145.9377	3147.1626	3170.2806
H	2.52974	2.76729	2.17791			
H	3.62302	1.79456	1.18392			
C	1.41120	4.26580	0.16593			
H	2.12330	5.09975	0.20583			
H	0.74359	4.42103	-0.68958			
H	0.81111	4.28620	1.08486			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.495301 Electronic Energy = -1186.96161724
Internal Energy (E)= -1186.43537124 Enthalpy (H)= -1186.43442724
Gibbs Free Energy (G)=-1186.52586024 Gibbs Free Energy of Solvation=-1186.95977

St.Pt.	General Structure	Ball & Stick model
N_2	N≡N	

Cartesian co-ordinate

Atoms	X	Y	Z

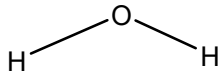
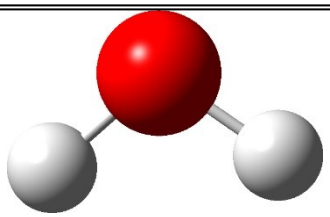
Frequencies

2467.7575

N	0.00000	0.00000	0.55260	
N	0.00000	0.00000	-0.55260	

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.005622 Electronic Energy = -109.458949410
Internal Energy (E)= -109.45096641 Enthalpy (H)= -109.45002241
Gibbs Free Energy (G)=-109.47177641 Gibbs Free Energy of Solvation=-109.514018963

St.Pt.	General Structure	Ball & Stick model
H_2O		

Cartesian co-ordinate

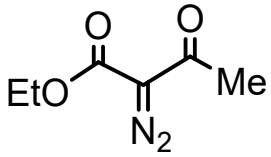
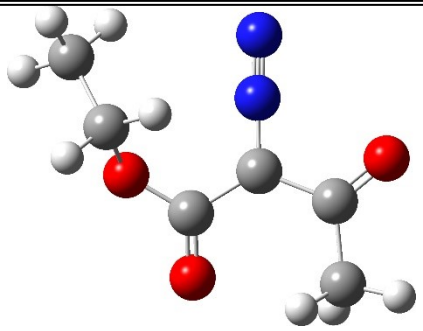
Atoms	X	Y	Z
O	0.00000	0.00000	0.11801
H	0.00000	0.75770	-0.47204
H	0.00000	-0.75770	-0.47204

Frequencies

1646.0646 3890.6078 4023.8385

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.021780 Electronic Energy = -76.3858742185
Internal Energy (E)= -76.3612582185 Enthalpy (H)= -76.3603142185
Gibbs Free Energy (G)=-76.3817342185 Gibbs Free Energy of Solvation=-76.4309807901

St.Pt.	General Structure	Ball & Stick model
R’	 **R'**	

Cartesian co-ordinate

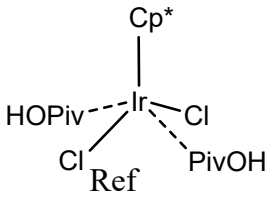
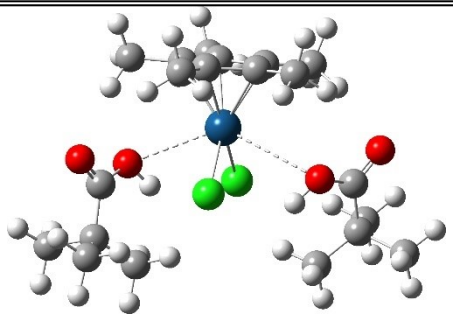
Atoms	X	Y	Z
C	0.58667	0.16374	-0.09328
C	2.04019	0.36268	0.15692
C	-0.13441	-1.10916	-0.28140
C	-2.21338	-0.36705	0.76087
H	-2.57209	-1.12611	1.46728
H	-1.55211	0.30658	1.32239
C	-3.36366	0.37272	0.12968
H	-3.98242	0.84333	0.89983
H	-3.01128	1.15402	-0.55261
H	-3.99018	-0.31866	-0.44162
O	-1.48541	-1.06141	-0.26060
O	0.44322	-2.13989	-0.51492
N	-0.06619	1.28988	-0.29933
N	-0.57577	2.28409	-0.47420
C	2.87725	-0.86588	0.34530
H	3.87203	-0.54937	0.66458
H	2.43326	-1.55035	1.07461
H	2.94092	-1.42776	-0.59190
O	2.49215	1.48983	0.20849

Frequencies

56.6650	64.2566	77.8002
134.2365	154.7361	187.1953
214.6385	235.6462	258.6419
313.7013	344.8023	386.7881
434.0802	477.6360	540.5797
553.8576	614.6542	644.7832
697.0121	759.0141	815.9516
914.6624	985.1918	1027.0155
1037.8068	1112.6951	1131.7952
1166.2099	1225.4431	1299.7181
1303.3216	1331.5353	1383.2476
1391.6654	1418.8628	1438.1226
1461.1607	1461.6095	1489.4020
1525.7509	1813.3877	1862.6104
2268.4567	3047.0800	3055.0691
3060.2864	3098.9973	3145.8204
3147.5108	3152.9698	3179.9821

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.143306 Electronic Energy = -568.256345682
Internal Energy (E)= -568.101513682 Enthalpy (H)= -568.100569682
Gibbs Free Energy (G)=-568.150912682 Gibbs Free Energy of Solvation=-568.370856377

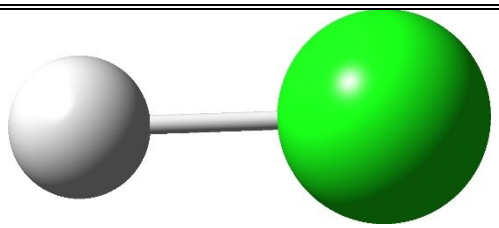
St.Pt.	General Structure	Ball & Stick model
Ref		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.43869	-2.46748	-1.12131
C	0.96918	-2.36340	-0.85390

Frequencies

27.5259	43.2845	45.7495
57.3549	63.4097	68.3445
74.1339	75.6020	79.7309
88.0184	102.0982	105.2664
108.0363	116.4044	132.9700
143.7065	153.2902	155.8018

St.Pt.	General Structure	Ball & Stick model
HCl	H-Cl	

Cartesian co-ordinate

Atoms	X	Y	Z
Cl	0.00000	0.00000	0.07134
H	0.00000	0.00000	-1.21277

Frequencies

2968.6974

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.006763 Electronic Energy = -460.763827404
Internal Energy (E)= -460.754705404 Enthalpy (H)= -460.753761404
Gibbs Free Energy (G)=-460.774938404 Gibbs Free Energy of Solvation=-460.823972498

C	1.15846	-2.37827	0.59797	167.7138	185.7377	190.8915
C	-0.13145	-2.49607	1.21199	192.0744	213.0372	216.9298
C	-1.12072	-2.54086	0.15188	231.7302	233.5941	238.0438
C	3.57958	0.92595	-0.51442	253.1196	258.7785	262.8086
O	2.66155	0.69920	-1.46298	270.6795	272.0867	292.2381
O	4.34879	0.03446	-0.22511	294.8269	298.0097	300.5680
C	3.67740	2.32174	0.09812	306.6758	307.3415	309.9002
Ir	-0.03408	-0.68368	0.03480	315.6642	319.9377	328.8673
Cl	-0.45466	1.03332	-1.57444	345.7908	350.5244	369.2700
H	1.94355	1.35639	-1.48578	369.9029	383.7290	384.2984
Cl	0.27564	0.96085	1.74676	387.8457	403.8652	442.5243
C	-2.58626	-2.69749	0.31869	453.3510	459.2183	516.2333
H	-2.88800	-3.67555	-0.07998	517.4718	532.9319	538.6077
H	-2.87898	-2.64673	1.37068	545.7126	570.7482	576.8730
H	-3.14542	-1.91637	-0.21385	587.5233	590.8061	602.4602
C	-1.11289	-2.48819	-2.44589	632.2833	641.4172	762.1902
H	-0.50112	-2.00375	-3.21241	769.9069	787.4194	788.0230
H	-1.31278	-3.51938	-2.76448	804.9882	813.2983	886.0068
H	-2.06756	-1.95195	-2.39948	888.8470	947.0384	950.7264
C	2.05916	-2.29966	-1.85868	954.4412	954.5914	955.1189
H	2.92923	-1.75649	-1.47762	955.9679	958.5122	973.0794
H	2.36633	-3.31954	-2.12677	1032.1573	1033.8341	1035.4327
H	1.72997	-1.78850	-2.76841	1037.4400	1039.5139	1040.5201
C	2.46602	-2.28452	1.29546	1045.1594	1045.7846	1051.9426
H	2.35056	-1.83648	2.28742	1089.2245	1094.8652	1108.4261
H	2.90040	-3.28523	1.42031	1170.0923	1177.7466	1186.1247
H	3.18078	-1.67113	0.73489	1188.9593	1226.0203	1227.7659
C	-0.43441	-2.53636	2.66684	1238.5116	1240.8957	1266.2933
H	-0.64752	-3.56275	2.99116	1266.9336	1344.5017	1358.9105
H	0.40403	-2.15667	3.25696	1377.8369	1381.3700	1381.6847
H	-1.30552	-1.91402	2.89943	1382.6888	1386.5532	1387.6987
C	3.82535	2.16550	1.61151	1399.2536	1403.9071	1405.9707
H	3.98685	3.14926	2.06974	1413.1496	1418.0891	1427.3703
H	2.92032	1.72716	2.05115	1433.1288	1442.2128	1444.5939
H	4.67806	1.52277	1.85078	1448.7518	1454.0453	1455.4802
C	4.95629	2.93641	-0.48563	1455.8264	1459.6379	1464.6302
H	4.88555	3.04644	-1.57546	1464.7052	1465.9608	1466.8529
H	5.11625	3.93221	-0.05370	1469.9466	1470.9699	1472.1143
H	5.82537	2.31055	-0.25715	1480.1588	1481.4985	1484.3322
C	2.48346	3.21617	-0.22353	1487.1550	1492.4261	1493.9463
H	1.54177	2.79921	0.15926	1501.1858	1501.9667	1507.8354
H	2.62511	4.19310	0.25403	1515.5799	1533.1395	1853.5563
H	2.38369	3.40361	-1.30187	1867.3851	3026.4080	3026.6278
O	-2.75014	0.34338	1.06628	3027.9598	3029.5514	3030.2710
C	-3.49433	0.82433	0.04885	3036.7544	3038.3320	3039.7989
C	-3.71641	2.33277	-0.01803	3040.1850	3044.0590	3047.7564
C	-5.02063	2.57583	0.75630	3107.4408	3109.9034	3110.7189
H	-4.92776	2.25993	1.80334	3115.4395	3118.8362	3122.7947
H	-5.26312	3.64572	0.74355	3123.1682	3124.9798	3126.4409
H	-5.85234	2.02564	0.30162	3129.6172	3129.8460	3134.0848
C	-3.89692	2.73557	-1.47803	3139.1353	3139.7541	3143.4420
H	-4.16404	3.79777	-1.53862	3148.6902	3150.0825	3151.6105
H	-2.96959	2.57764	-2.04038	3151.7477	3156.4478	3159.9250
H	-4.68697	2.14398	-1.94948	3161.3923	3717.2033	3727.0741
C	-2.58720	3.14531	0.61141			
H	-1.61864	2.92636	0.14453			
H	-2.79530	4.21314	0.47372			

H	-2.50163	2.98471	1.69553
O	-4.03908	0.04257	-0.69550
H	-2.15276	1.01038	1.44893

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.522668 Electronic Energy = -2108.56021317
Internal Energy (E)= -2108.00243717 Enthalpy (H)= -2108.00149417
Gibbs Free Energy (G)=-2108.10222217 Gibbs Free Energy of Solvation=-2109.17771283

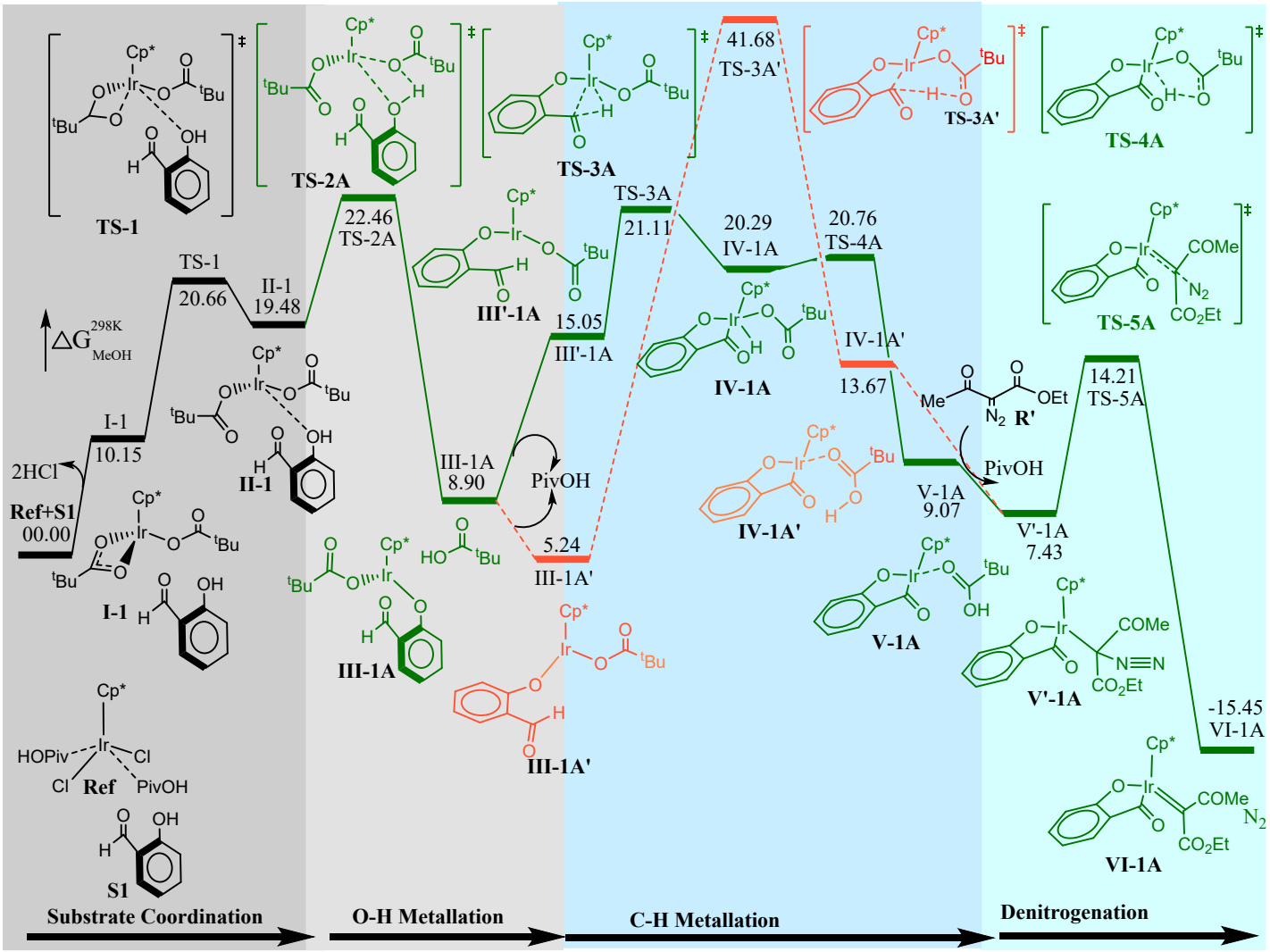


Fig-1: PES with Gibbs free energy (kcal/mol) and the structures of the stationary points for S1 using M06L functional & 6-311++G(d,p) basis set for non-metals and triple-zeta SDD for metal (green, orange and black colour represent path-A, path-A' and common path respectively)

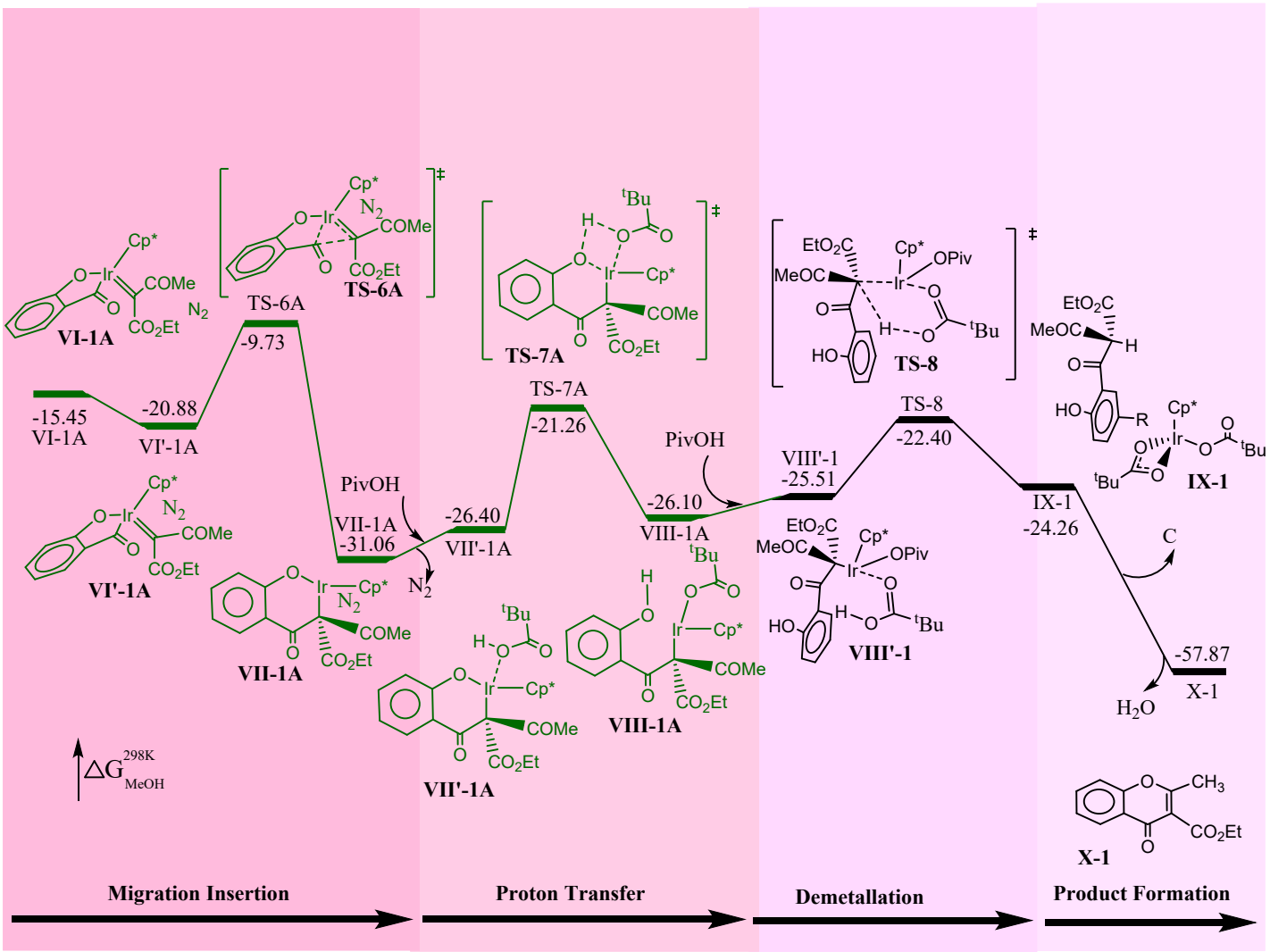


Fig-2: PES with Gibbs free energy (kcal/mol) and the structures of the stationary points for S1 using M06L functional & 6-311++G(d,p) basis set for non-metals and triple-zeta SDD for metal (green and black colour represent path-A, and common path respectively)

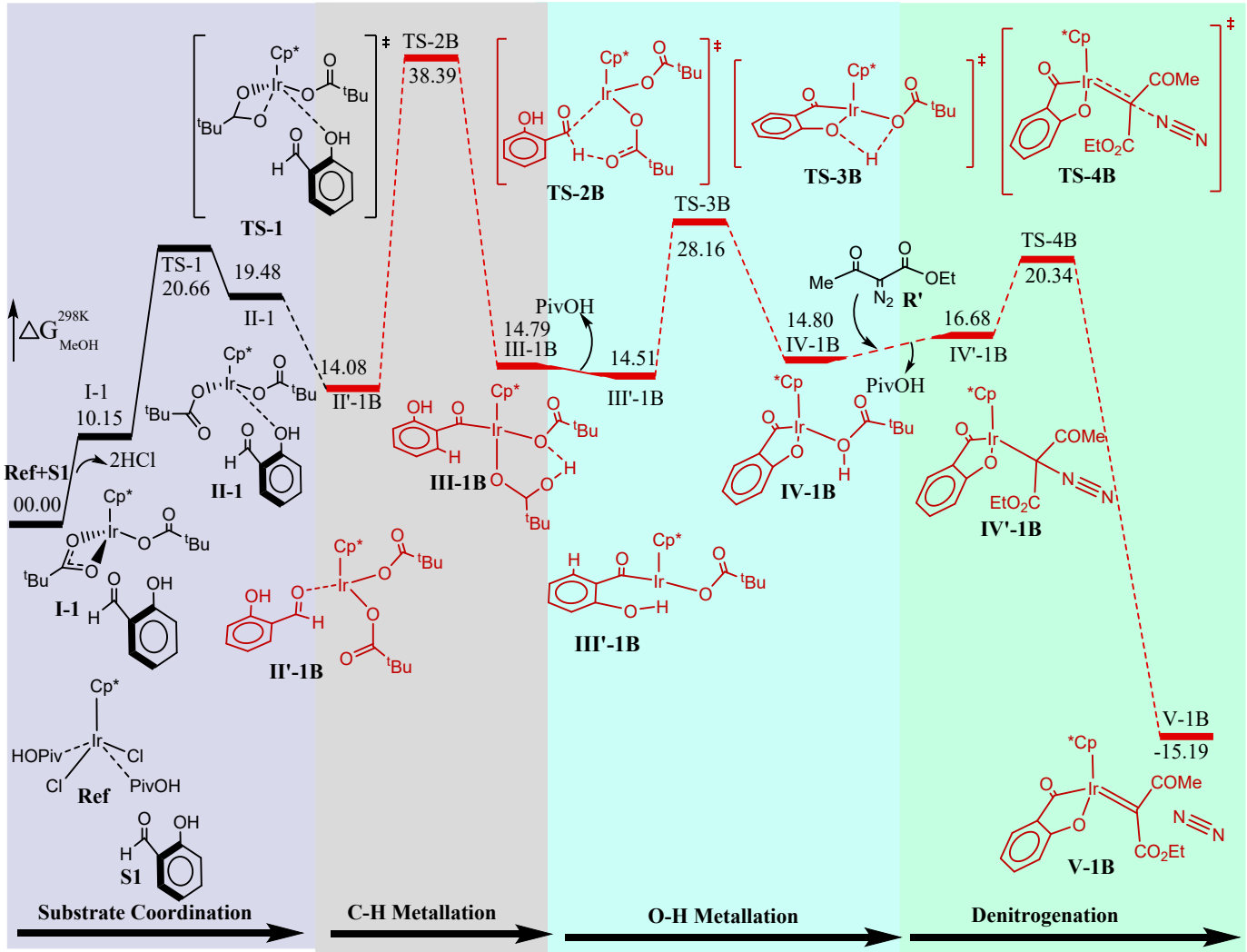


Fig-6: PES with Gibbs free energy (kcal/mol) and the structures of the stationary points for S1 using M06L functional & 6-311++G(d,p) basis set for non-metals and triple-zeta SDD for metal (red and black colours represent path-B, and common path respectively) (Detailed path)

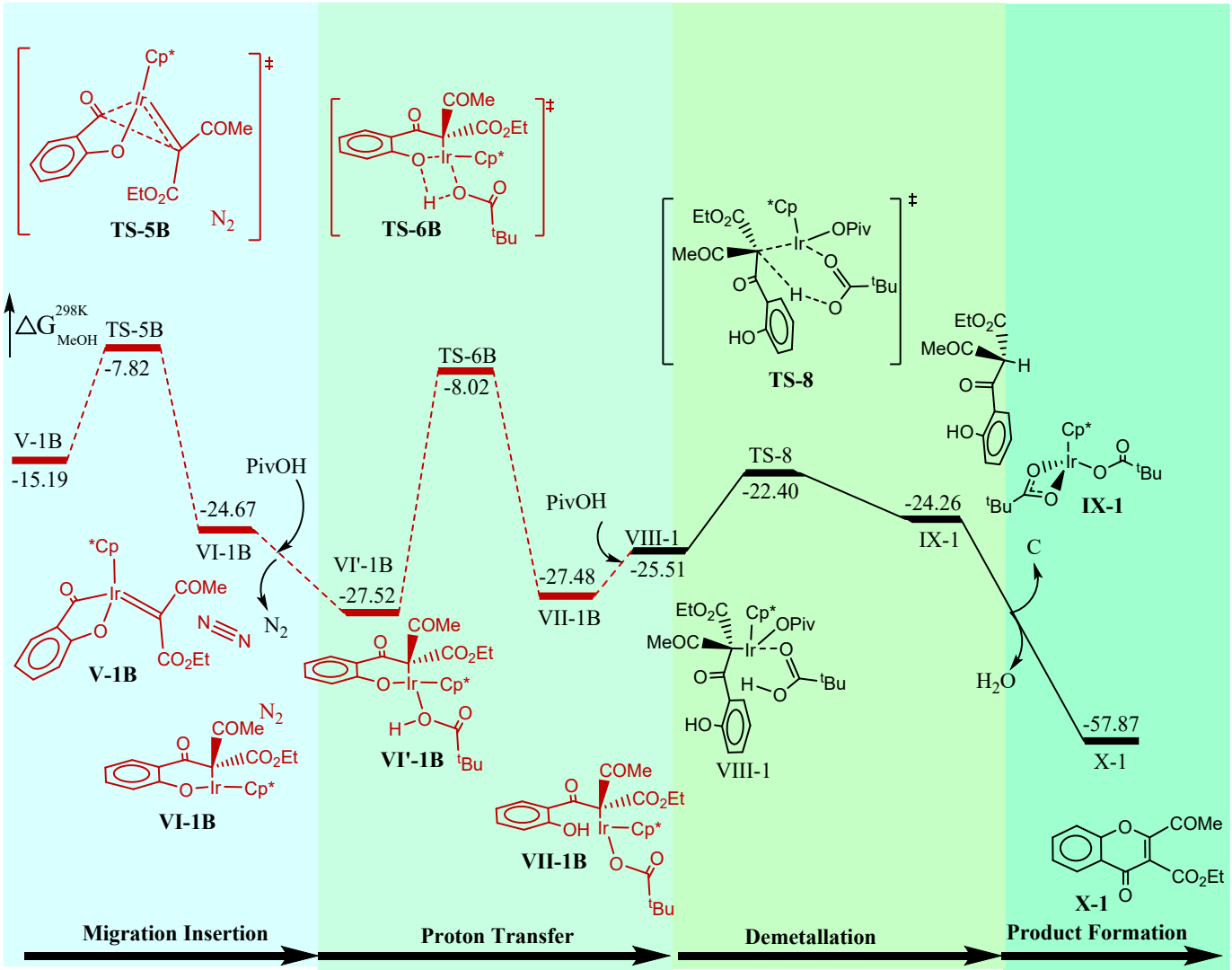


Fig-6A: PES with Gibbs free energy (kcal/mol) and the structures of the stationary points for S1 using M06L functional & 6-311++G(d,p) basis set for non-metals and triple-zeta SDD for metal (red and black colours represent path-B, and common path respectively) (Detailed path)

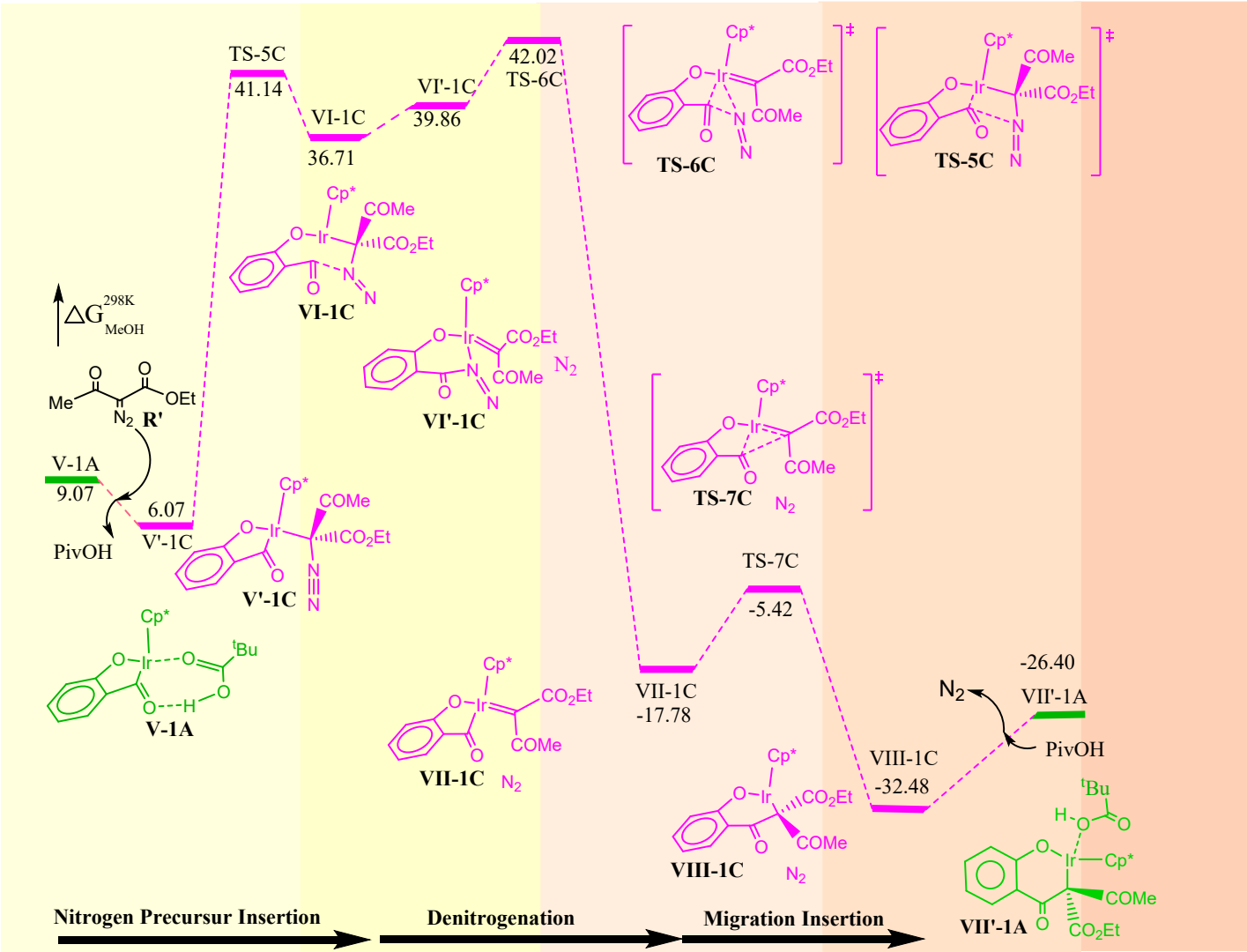
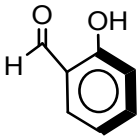
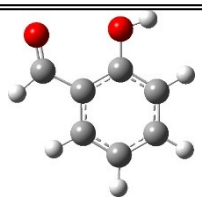


Fig-6B: PES with Gibbs free energy (kcal/mol) and the structures of the stationary points for S1 using M06L functional & 6-311++G(d,p) basis set for non-metals and triple-zeta SDD for metal (green, pink and black colours represent path-A, path-C and common path respectively) (Details of path-C)

St.Pt.	General Structure	Ball & Stick model
S1		

Cartesian co-ordinate

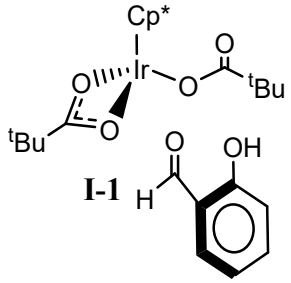
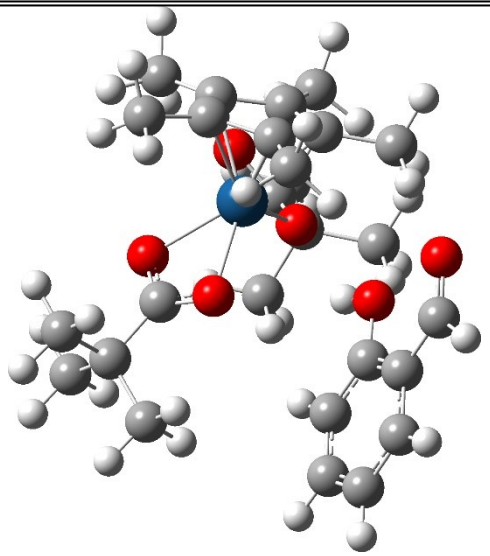
Atoms	X	Y	Z
C	-0.01946	0.85724	0.00008
O	-0.98850	1.78803	0.00040
C	1.33244	1.20679	-0.00014
C	2.31566	0.22773	-0.00030
C	-0.38096	-0.50492	0.00026
C	1.97465	-1.12238	-0.00019
C	0.63319	-1.46736	0.00019
H	0.33776	-2.51660	0.00042
H	2.74506	-1.88767	-0.00029
H	3.36135	0.52627	-0.00052
C	-1.77286	-0.98506	0.00053
H	-1.82981	-2.10381	0.00242
O	-2.77830	-0.31496	-0.00110
H	1.60805	2.26137	-0.00031
H	-0.58400	2.66361	0.00124

Frequencies

94.4723	194.1531	195.2168
264.0076	394.7275	414.7653
420.3882	447.7625	553.2002
575.7265	668.0339	726.5674
760.5006	775.5017	849.3556
883.1663	950.6734	982.2974
1024.9241	1071.3042	1125.9927
1166.2432	1186.0961	1233.0601
1320.3752	1344.0107	1388.0075
1417.0381	1493.2463	1542.7352
1654.1962	1676.6399	1853.6786
2830.8546	3155.1590	3159.9234
3184.0258	3209.4341	3876.9588

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.114055 Electronic Energy = -420.525646372
Internal Energy (E)= -420.404091372 Enthalpy (H)= -420.403147372
Gibbs Free Energy (G)=-420.443605372 Gibbs Free Energy of Solvation=-420.788232072

St.Pt.	General Structure	Ball & Stick model
I-1		

I-1

Cartesian co-ordinate

Atoms	X	Y	Z
C	2.55289	-1.44400	-1.04720
C	3.08317	-1.17515	0.26210
C	2.24927	-1.84830	1.24532
C	1.19872	-2.52609	0.52078
C	1.37269	-2.27106	-0.89269
C	-2.99208	-0.66700	-0.78623
C	-0.66556	2.13624	2.83575
C	-0.03525	1.22368	1.80488
O	1.15448	1.41499	1.40882
O	-0.64388	0.18943	1.38737
C	2.44042	-1.81926	2.72199
H	2.74663	-0.82127	3.05614
H	1.50797	-2.06389	3.24166
H	3.20427	-2.53750	3.04567
C	0.05994	-3.27381	1.11485
H	-0.83627	-3.17887	0.49053
H	0.30256	-4.34079	1.19808
H	-0.17996	-2.89772	2.11478
C	0.55752	-2.82585	-2.00551
H	-0.46735	-3.05584	-1.69814
H	0.49316	-2.10931	-2.83169
H	1.02553	-3.74131	-2.39155
C	3.12324	-0.98373	-2.34015
H	2.33561	-0.85771	-3.08997
H	3.61949	-0.01664	-2.23385
H	3.83972	-1.72292	-2.72208
C	4.23053	-0.27192	0.54315
H	4.23400	0.05518	1.58720
H	5.18424	-0.77398	0.33698
H	4.16223	0.62307	-0.08586
C	0.90056	1.84034	-1.71025
O	0.14331	0.90608	-1.18590
O	2.12032	1.86530	-1.63464
C	0.10821	2.98196	-2.35590

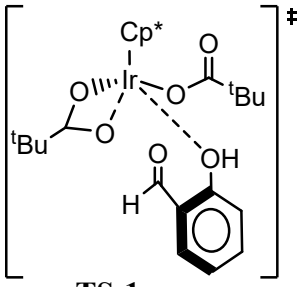
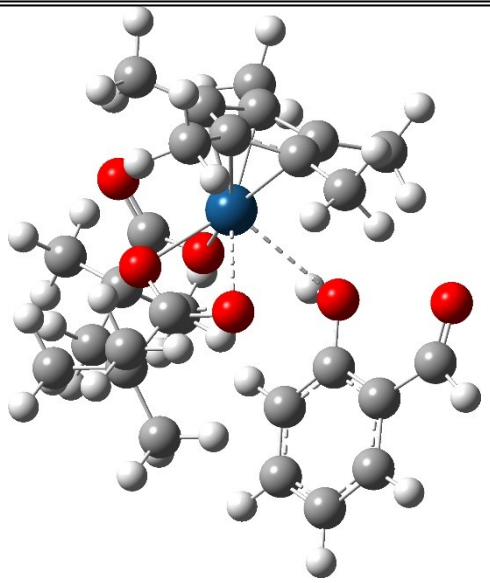
Frequencies

51.6079	28.1309	34.7439
52.5756	56.3493	66.7943
69.0710	76.9197	87.0538
94.6869	97.2889	107.4083
118.0438	120.7329	130.2100
139.9257	145.3027	157.9879
161.1420	168.1612	178.8521
182.2570	184.8991	188.5767
206.2971	210.1494	211.3584
214.9082	217.2842	222.2903
227.7934	234.8346	245.9057
249.8370	264.0739	268.1630
281.5761	302.5202	307.4830
311.2727	317.6298	320.4014
322.3440	329.3533	339.3044
345.3543	352.6512	372.0432
379.2397	393.0748	395.4703
396.2418	419.1042	422.3040
437.2475	450.8555	452.1050
459.7739	466.1400	467.5273
535.0898	539.2001	547.4836
549.5664	555.8297	568.5519
580.1195	581.9695	591.8892
604.6424	622.7568	632.1236
668.5417	744.9809	771.5329
784.6527	787.6322	800.3392
807.4475	812.7127	814.3421
832.2907	862.6810	888.1815
907.4028	915.2455	933.7003
940.6729	948.8382	951.2333
954.3401	957.1701	959.1515
962.7277	967.6265	977.6534
1010.3965	1021.0550	1033.9736
1037.1666	1038.5057	1039.6716
1041.0520	1041.7211	1042.6664
1046.6019	1047.2923	1077.1764
1093.1003	1099.2287	1106.8967
1136.4229	1173.4941	1185.4977

O	-1.81819	-0.94833	-1.34697	1190.8425	1219.0695	1230.9573
C	-1.04946	2.46342	-3.20629	1235.2077	1239.9161	1247.2159
H	-1.79041	1.91610	-2.61368	1262.6663	1264.4517	1269.6728
H	-1.56378	3.30619	-3.68654	1350.5970	1355.0046	1371.9496
H	-0.69212	1.79612	-4.00077	1375.4789	1378.3337	1380.9815
C	1.03690	3.83268	-3.21342	1383.1063	1384.8864	1389.4724
H	0.48900	4.69005	-3.62552	1396.9551	1399.8790	1404.4929
H	1.88369	4.20092	-2.62669	1407.6014	1408.7343	1413.8046
H	1.44311	3.25175	-4.04998	1416.8922	1429.8589	1436.2993
C	-0.42579	3.82250	-1.18959	1440.8124	1442.0565	1449.0380
H	0.40515	4.19302	-0.57416	1449.7679	1451.3841	1453.3524
H	-0.99030	4.68576	-1.56565	1456.2077	1457.1745	1459.0847
H	-1.08725	3.22866	-0.54387	1463.7843	1466.4617	1470.8405
C	-2.18284	2.15753	2.68580	1471.1208	1475.6390	1477.1635
H	-2.60760	1.15100	2.75641	1479.7652	1483.9162	1485.1620
H	-2.62207	2.78096	3.47508	1488.4170	1495.8962	1497.9142
H	-2.48281	2.58052	1.71755	1499.4960	1501.3507	1515.8253
C	-0.09540	3.54590	2.72512	1521.6152	1522.6767	1545.3461
H	-0.52902	4.18192	3.50721	1550.2207	1604.8224	1645.0432
H	0.99310	3.54707	2.83742	1679.0879	1782.1465	1825.5667
H	-0.33316	3.99333	1.75229	2835.9379	3012.9162	3025.2660
C	-0.28729	1.52595	4.19386	3030.3548	3031.2442	3035.3746
H	0.80281	1.48553	4.31312	3036.8915	3037.8583	3039.0419
H	-0.69986	2.13746	5.00615	3040.2771	3043.5471	3043.8931
H	-0.68634	0.50868	4.29126	3098.8212	3111.0067	3112.4945
Ir	1.09130	-0.41663	0.16062	3115.5089	3116.2124	3116.7111
C	-3.33860	0.64326	-0.43182	3119.4101	3120.9340	3121.4161
C	-4.59258	0.92721	0.08189	3123.8403	3124.9466	3128.3620
C	-5.54130	-0.08213	0.26327	3129.9696	3137.0204	3138.5744
C	-3.92673	-1.70462	-0.56858	3140.2020	3141.9299	3148.7177
C	-5.19348	-1.38016	-0.06009	3149.3032	3150.5595	3161.6071
H	-4.83586	1.95491	0.34636	3162.1351	3168.8776	3172.7810
H	-6.52654	0.14805	0.65866	3191.4148	3208.7772	3517.6612
H	-5.90693	-2.19152	0.08715			
H	-1.24273	-0.15079	-1.37939			
H	-2.58678	1.42241	-0.55365			
C	-3.65092	-3.12272	-0.79655			
H	-4.56130	-3.75711	-0.64866			
O	-2.59287	-3.64870	-1.08275			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.613254 Electronic Energy = -1607.51296776
Internal Energy (E)= -1606.86176676 Enthalpy (H)= -1606.86082376
Gibbs Free Energy (G)=-1606.96596576 Gibbs Free Energy of Solvation=-1607.01993298

St.Pt.	General Structure	Ball & Stick model
TS-1	 **TS-1**	

Cartesian co-ordinate

Atoms	X	Y	Z
C	2.38422	-1.81566	-0.71295
C	2.53638	-1.64567	0.71940
C	1.38066	-2.25879	1.36472
C	0.52933	-2.77975	0.34230
C	1.13602	-2.49642	-0.95157
C	-2.49444	0.02872	-1.47894
C	-1.54644	1.51995	2.81254
C	-0.79819	0.68671	1.77742
O	0.45165	0.87562	1.62248
O	-1.40551	-0.21121	1.15188
C	1.12764	-2.27086	2.83111
H	1.33637	-1.28761	3.26969
H	0.08238	-2.51348	3.04498
H	1.76106	-3.01187	3.33444
C	-0.77714	-3.45223	0.55058
H	-1.47873	-3.22536	-0.25795
H	-0.63736	-4.54075	0.58424
H	-1.23664	-3.13364	1.49066
C	0.59786	-2.94392	-2.26498
H	-0.49678	-2.91820	-2.27751
H	0.95798	-2.30575	-3.07947
H	0.92360	-3.97038	-2.47915
C	3.35366	-1.35712	-1.74228
H	2.84261	-1.11236	-2.67950
H	3.87241	-0.45610	-1.40289
H	4.09033	-2.14331	-1.95215
C	3.68656	-1.00476	1.40337
H	3.46886	-0.82940	2.46115
H	4.57527	-1.64599	1.33706
H	3.90028	-0.03995	0.93163
C	2.08218	1.89683	-0.86368
O	1.04992	1.12475	-1.04878
O	3.13593	1.56784	-0.33286

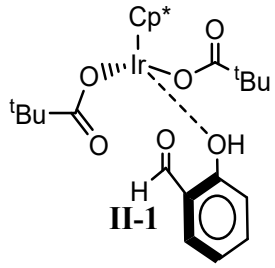
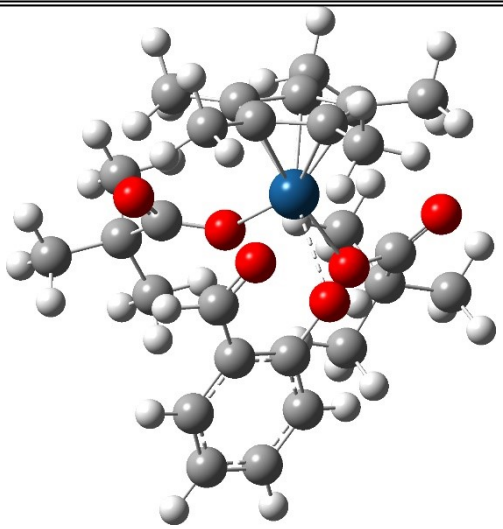
Frequencies

-83.6957	-15.8790	34.2642
40.1901	49.6033	58.9359
66.5499	71.8783	76.3379
84.2039	92.0166	94.3179
101.6384	120.9951	126.1571
130.2053	133.8015	138.2052
149.6825	159.9025	169.4928
172.4304	179.3840	190.6777
192.2781	204.8918	207.0696
212.5553	217.4412	223.8139
230.8396	239.6244	257.9019
270.8203	276.1075	286.5988
289.8072	297.3502	305.0321
307.9266	316.8843	320.6073
328.3746	336.7414	341.2969
352.7555	360.7547	364.4949
381.5074	386.1231	394.4219
402.2678	418.5195	425.2723
431.9148	438.8505	441.0021
452.0478	454.3511	467.2680
533.1435	539.8679	545.7284
547.4642	556.0261	566.0444
578.7409	580.6148	587.8258
602.8930	618.1729	624.8060
666.7287	679.5329	745.0505
768.7286	785.3305	788.5175
794.2391	807.6346	808.9897
811.6606	827.0803	882.6258
887.4961	907.9506	928.6874
936.1241	948.9221	950.5995
950.9716	954.8474	960.0134
965.3938	969.1873	976.7164
992.3250	1025.3715	1034.5011
1035.1349	1036.5454	1038.0626
1041.4379	1044.4393	1044.5787
1046.1415	1053.8192	1068.6867
1097.3462	1099.7735	1110.5590

C	1.83645	3.33662	-1.33784	1131.4783	1161.8183	1185.4509
O	-1.37271	-0.69531	-1.67207	1190.8749	1212.8452	1236.2002
C	1.24452	3.35575	-2.74602	1238.4834	1240.2449	1246.5563
H	0.29464	2.81289	-2.79392	1259.8155	1264.2969	1271.5519
H	1.06354	4.39162	-3.06260	1324.1347	1348.4866	1356.5131
H	1.93146	2.90136	-3.47163	1372.9072	1373.3577	1374.9844
C	3.14042	4.12371	-1.31696	1376.4731	1384.7259	1387.9471
H	2.95835	5.16046	-1.62975	1392.8652	1396.8379	1400.7506
H	3.58048	4.13117	-0.31505	1402.2072	1411.4839	1414.7257
H	3.87884	3.68379	-1.99736	1416.1270	1426.1100	1436.4933
C	0.84566	3.95531	-0.34546	1441.6300	1447.1167	1447.9157
H	1.25342	3.93230	0.67346	1449.5125	1454.4813	1457.9976
H	0.64195	5.00109	-0.61189	1459.7102	1462.3250	1465.8192
H	-0.10441	3.40486	-0.33643	1467.6916	1470.6981	1471.8459
C	-2.87060	1.99596	2.21840	1473.6377	1476.9772	1479.4673
H	-3.45392	1.15879	1.81881	1480.5841	1484.4463	1486.6654
H	-3.46274	2.50878	2.98777	1487.7419	1491.7520	1496.0157
H	-2.70170	2.70413	1.39619	1499.4153	1502.7634	1513.6571
C	-0.71867	2.71167	3.27656	1517.2466	1524.4248	1537.9251
H	-1.27357	3.27688	4.03691	1540.5884	1652.8764	1668.6073
H	0.23535	2.39089	3.70777	1675.9224	1774.4676	1828.7232
H	-0.49430	3.38864	2.44314	2847.2806	3015.1439	3021.8151
C	-1.81825	0.58171	3.99369	3026.3714	3030.8127	3034.9229
H	-0.87765	0.21204	4.42463	3035.6992	3035.8321	3038.0779
H	-2.36293	1.11555	4.78312	3040.1829	3042.6343	3044.1388
H	-2.41729	-0.27995	3.67727	3093.0333	3106.8529	3107.2300
Ir	0.78324	-0.63807	0.08419	3112.8217	3116.4161	3117.9663
C	-2.44287	1.42144	-1.41511	3118.3903	3122.0584	3122.3882
C	-3.60213	2.15333	-1.21302	3123.9609	3125.6610	3130.4585
C	-4.83405	1.51486	-1.05724	3131.4284	3131.7254	3139.5938
C	-3.72745	-0.63502	-1.34355	3141.5237	3145.2537	3148.9077
C	-4.87946	0.13377	-1.12415	3154.0615	3159.4677	3160.4819
H	-3.54053	3.23876	-1.16286	3160.6136	3166.2344	3167.5761
H	-5.73891	2.09237	-0.89146	3183.0780	3209.5605	3722.1464
H	-5.83045	-0.38893	-1.01979			
H	-0.65835	-0.08633	-1.93115			
H	-1.47025	1.90968	-1.49766			
C	-3.90211	-2.08242	-1.47927			
H	-4.96831	-2.39330	-1.34444			
O	-3.05582	-2.91727	-1.72979			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.612573 Electronic Energy = -1607.48858504
Internal Energy (E)= -1606.83856604 Enthalpy (H)= -1606.83762304
Gibbs Free Energy (G)=-1606.94156904 Gibbs Free Energy of Solvation=-1607.00197397

St.Pt.	General Structure	Ball & Stick model
II-1		

II-1

Cartesian co-ordinate

Atoms	X	Y	Z
C	2.99693	-1.04339	-0.42956
C	2.75319	-0.65891	0.95015
C	1.78065	-1.58849	1.50963
C	1.39048	-2.49945	0.47951
C	2.12298	-2.13522	-0.72384
Ir	0.92370	-0.43471	-0.08342
O	-0.78119	0.35453	0.81314
O	0.76121	1.47832	-0.99681
O	-1.30447	-2.99991	-1.65500
C	-2.33589	-2.51374	-1.24132
H	-3.05486	-3.12201	-0.64287
C	-2.81392	-1.14936	-1.50079
C	-1.98560	-0.10631	-1.94513
C	-4.17526	-0.89219	-1.30957
C	-2.53584	1.14496	-2.21830
C	-4.72917	0.34789	-1.58755
H	-4.80201	-1.70452	-0.94082
C	-3.89621	1.36578	-2.04955
H	-1.88018	1.94811	-2.55060
H	-5.79123	0.52470	-1.44274
H	-4.30547	2.34951	-2.26791
O	-0.65463	-0.31903	-2.09944
H	-0.21083	0.55370	-2.17792
C	-1.65401	-0.37540	1.44170
C	-2.66556	0.43409	2.26604
C	1.56477	2.47390	-0.71678
C	0.84786	3.74714	-0.25474
O	2.78822	2.41464	-0.70095
O	-1.68251	-1.60517	1.45386
C	1.94837	-2.80423	-2.03855
H	0.88325	-2.93697	-2.25541
H	2.39658	-2.21963	-2.84695
H	2.42425	-3.79342	-2.02614
C	3.98793	-0.41377	-1.34104

Frequencies

40.6149	48.5044	57.9979
60.8622	73.4442	74.8910
79.7966	88.7682	94.7574
98.7943	104.3108	105.3959
118.2619	120.7031	127.7824
133.3251	146.2700	149.6669
154.5577	165.1036	171.4179
186.4679	189.1770	202.7953
205.4991	219.6833	222.0991
231.3173	231.8146	235.2078
240.6357	242.8403	252.0088
270.8597	280.3898	282.1565
290.2250	297.6508	302.1868
307.9084	310.7100	316.4268
322.8258	327.6728	330.1680
336.2803	342.2589	378.2482
387.7461	392.3882	405.6824
407.6885	415.5423	422.9535
432.0194	436.0668	447.1880
452.1010	463.5364	475.9256
537.1811	538.8201	547.4630
549.4092	568.3326	570.0353
574.5955	579.5875	580.5452
601.8607	604.0491	634.2846
664.6758	730.8704	759.4637
779.9740	794.6453	799.2024
802.4493	812.4896	814.2918
817.7807	829.3520	866.4485
885.8390	908.3842	912.1382
943.0547	945.7741	948.0678
950.6117	957.7433	960.1328
961.1712	975.5619	980.3487
982.6657	1021.5591	1032.5878
1034.8888	1038.6824	1039.6102
1043.3883	1044.8899	1047.3691
1048.8858	1049.5552	1071.7193
1097.0271	1100.5665	1121.3920
1132.8010	1162.2758	1186.3152
1192.5371	1221.6044	1229.4300

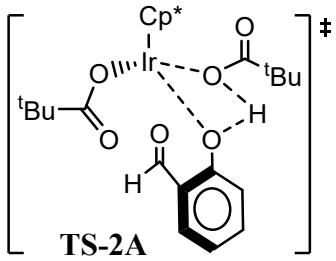
H	3.95462	0.67575	-1.24763	1238.3896	1242.6722	1245.4551
H	4.99826	-0.76902	-1.09857	1251.6053	1265.7594	1277.7969
H	3.78435	-0.67041	-2.38519	1306.4682	1351.5523	1362.2043
C	3.45943	0.42612	1.67684	1365.9413	1371.3564	1374.2424
H	2.91454	0.72061	2.57976	1376.4458	1380.5021	1381.3336
H	4.45943	0.08709	1.97918	1384.9525	1390.5348	1392.9204
H	3.57055	1.30752	1.03463	1397.7914	1408.8632	1413.5442
C	1.26931	-1.59110	2.90468	1419.8648	1423.8720	1428.5771
H	0.24492	-1.97626	2.93490	1432.9185	1438.4366	1441.7868
H	1.90357	-2.22036	3.54242	1445.9039	1448.2380	1450.0692
H	1.26313	-0.58037	3.32732	1459.8829	1461.0182	1461.7690
C	0.51912	-3.68952	0.65609	1467.4245	1468.3373	1469.7350
H	1.08051	-4.47210	1.18444	1473.5380	1474.1430	1478.1409
H	-0.37144	-3.43101	1.23549	1479.9593	1481.7118	1483.7327
H	0.17988	-4.08185	-0.30471	1487.4324	1488.7420	1490.2463
C	-2.96261	1.79435	1.64319	1498.0702	1499.1775	1512.5177
H	-3.35164	1.68506	0.62211	1524.0489	1524.9617	1542.2015
H	-3.71953	2.31864	2.24214	1543.8925	1653.4938	1674.2236
H	-2.06759	2.42399	1.59408	1745.3344	1765.3676	1833.8281
C	-2.02381	0.62508	3.64527	2880.7526	3018.6329	3020.7237
H	-2.70053	1.18698	4.30249	3023.0029	3030.5079	3033.1355
H	-1.81824	-0.34416	4.11812	3037.7650	3039.8352	3040.2893
H	-1.08251	1.18507	3.57063	3042.1187	3043.1662	3043.5726
C	-3.95622	-0.36375	2.41311	3098.0878	3106.9363	3109.2400
H	-3.75832	-1.35538	2.83076	3111.4569	3111.9762	3114.6415
H	-4.65655	0.16851	3.07000	3120.8000	3123.5005	3124.4604
H	-4.44092	-0.49947	1.43766	3125.3377	3127.6685	3129.9448
C	1.68862	4.97766	-0.56887	3142.6838	3149.1851	3150.3962
H	1.76657	5.13809	-1.65162	3151.6542	3157.3942	3159.4713
H	1.23056	5.87206	-0.12670	3159.6606	3167.2942	3169.6841
H	2.70280	4.86664	-0.17402	3169.7925	3183.2396	3194.8211
C	-0.54913	3.88483	-0.84641	3199.0496	3209.6188	3566.9939
H	-1.17301	3.02359	-0.58374			
H	-1.02805	4.79509	-0.46146			
H	-0.51073	3.96765	-1.94175			
C	0.73720	3.55788	1.26716			
H	1.73471	3.49817	1.72270			
H	0.20167	4.40438	1.71801			
H	0.18947	2.63297	1.49649			

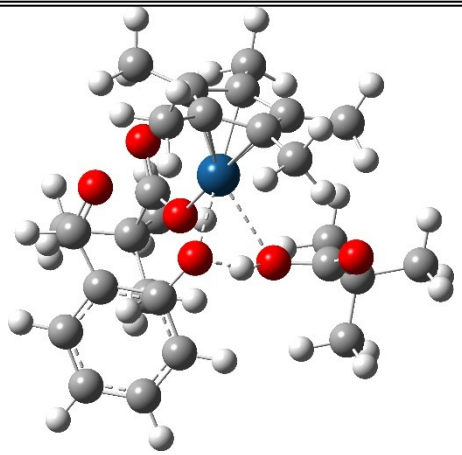
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.613824 Electronic Energy = -1607.50067969
Internal Energy (E)= -1606.84837569 Enthalpy (H)= -1606.84743169
Gibbs Free Energy (G)=-1606.95275969 Gibbs Free Energy of Solvation=-1607.00796234

St.Pt.	General Structure	Ball & Stick model

TS-2A





Cartesian co-ordinate

Atoms	X	Y	Z
C	2.54116	-1.29887	-1.02115
C	2.78051	-0.83450	0.32065
C	2.00438	-1.64056	1.24133
C	1.28241	-2.62192	0.45499
C	1.63023	-2.40340	-0.93956
Ir	0.66908	-0.65656	-0.09815
O	-1.00688	0.00090	0.82933
O	0.54890	1.73535	-0.64663
O	-1.53342	-2.45811	-1.20772
C	-2.59227	-1.88059	-1.37338
H	-3.55310	-2.43201	-1.22122
C	-2.79929	-0.49223	-1.76176
C	-1.75978	0.44136	-1.99580
C	-4.13572	-0.07497	-1.87942
C	-2.11724	1.76080	-2.32032
C	-4.47341	1.22194	-2.21341
H	-4.91663	-0.81334	-1.69312
C	-3.44359	2.14021	-2.43162
H	-1.32211	2.48335	-2.49240
H	-5.51370	1.52204	-2.30051
H	-3.68040	3.16960	-2.69284
O	-0.46276	0.12109	-1.95227
H	0.14721	1.08979	-1.55678
C	-1.53645	-0.48031	1.91921
C	-2.76364	0.29892	2.41230
C	1.61363	2.51250	-0.65890
C	1.58338	3.55218	0.46160
O	2.50721	2.44458	-1.48780
O	-1.13276	-1.45853	2.53695
C	1.14913	-3.18032	-2.11013
H	0.31845	-3.83609	-1.84620
H	0.79595	-2.51112	-2.90167
H	1.97546	-3.78234	-2.50958
C	3.10700	-0.70860	-2.26483
H	3.11168	0.38732	-2.21079
H	4.13431	-1.05760	-2.43154
H	2.50840	-0.99333	-3.13588
C	3.70698	0.26567	0.68805
H	3.42119	0.73588	1.63480

Frequencies

-153.4601	-109.0966	-94.0538
20.4660	35.9000	43.8799
60.1471	66.8406	72.9847
76.7317	85.3241	91.2175
95.5368	102.0951	116.0322
118.3480	124.3202	136.6265
141.6404	150.2476	155.8382
158.8309	174.2184	177.5373
183.0438	194.5247	199.7171
204.1449	213.8870	222.4590
233.6488	235.7225	241.7156
248.9573	255.6265	267.5287
277.7804	286.1589	287.0732
296.2217	301.2285	309.4846
310.4453	314.4177	323.1976
339.5347	340.8466	352.5519
370.9008	384.1558	386.1901
393.6372	413.0168	432.1994
436.2504	440.8129	448.0146
453.0269	463.9867	501.5741
533.9730	536.2109	542.9085
553.8474	570.2178	574.4916
579.6799	580.6570	594.2346
602.4960	626.8672	644.1203
679.4397	736.7791	751.8343
770.3710	784.0223	792.3230
796.4391	805.4160	808.9013
810.9366	817.4858	861.1343
894.8255	918.3004	925.4675
941.5089	941.8623	943.2461
948.0230	952.2081	953.7145
958.1658	962.0184	975.2279
983.2253	1024.1574	1028.3167
1032.3585	1035.0509	1036.4059
1037.2654	1039.6799	1042.3857
1044.3080	1046.1447	1076.2333
1095.4036	1099.3682	1109.6537
1141.1985	1170.8344	1184.1608
1192.1092	1230.5475	1232.4150
1234.4921	1239.6034	1244.5082
1263.7631	1266.7913	1268.8329
1337.3776	1357.5866	1366.9734
1372.9027	1374.3489	1376.5873

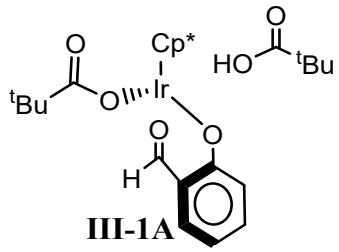
H	4.71883	-0.14220	0.81417	1377.6411	1381.5402	1387.2681
H	3.74634	1.03839	-0.08804	1390.6231	1393.6818	1394.8949
C	2.02380	-1.54769	2.72431	1401.7492	1412.7912	1415.2201
H	1.03160	-1.76323	3.12924	1420.5170	1422.7880	1429.0783
H	2.74926	-2.25715	3.14371	1430.9004	1433.4101	1436.4790
H	2.30631	-0.54177	3.05328	1438.4149	1451.0509	1453.0283
C	0.42583	-3.70534	0.99645	1453.6120	1457.5371	1458.2414
H	1.05054	-4.54831	1.32150	1459.4154	1462.6895	1464.2102
H	-0.15144	-3.33038	1.84666	1472.1607	1472.7307	1475.1128
H	-0.28422	-4.05797	0.24435	1477.7949	1484.1499	1485.3587
C	-3.10251	1.49598	1.53154	1488.9761	1492.3179	1495.1505
H	-3.40009	1.18026	0.52512	1499.3123	1501.1833	1503.6500
H	-3.93953	2.05172	1.97562	1510.4664	1514.8300	1524.4646
H	-2.25110	2.17974	1.42264	1533.6005	1624.6432	1640.9130
C	-2.45754	0.76644	3.83680	1676.0560	1768.6139	1810.3798
H	-3.32673	1.28893	4.25716	1814.2174	2848.8810	3018.2140
H	-2.21210	-0.08406	4.48100	3022.8922	3024.0553	3029.7134
H	-1.60916	1.46386	3.84893	3031.2628	3031.3492	3036.0515
C	-3.94369	-0.67485	2.43452	3038.1455	3039.5177	3042.4164
H	-3.71269	-1.55453	3.04445	3046.2025	3098.1475	3104.7605
H	-4.83359	-0.18161	2.84721	3109.8883	3110.8173	3114.2783
H	-4.19047	-1.01450	1.41862	3114.6600	3116.9357	3119.0964
C	2.94663	4.21551	0.59823	3120.3002	3123.8550	3130.3238
H	3.26464	4.66379	-0.34840	3130.9432	3135.7799	3137.1048
H	2.90951	4.99938	1.36524	3140.0422	3140.7392	3142.6416
H	3.71371	3.48715	0.89186	3147.7422	3150.6112	3156.1144
C	0.53024	4.59013	0.04877	3176.2117	3177.3382	3178.0744
H	-0.46092	4.12837	-0.04003	3189.3447	3193.7360	3209.1758
H	0.47470	5.38666	0.80191			
H	0.78789	5.05171	-0.91324			
C	1.15793	2.91467	1.78625			
H	1.89986	2.18659	2.14281			
H	1.06544	3.69121	2.55681			
H	0.19699	2.39609	1.68949			

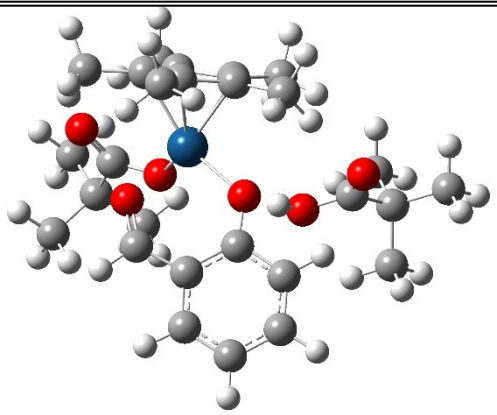
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.606888 Electronic Energy = -1607.48660451
Internal Energy (E)= -1606.84243351 Enthalpy (H)= -1606.84149051
Gibbs Free Energy (G)=-1606.94591551 Gibbs Free Energy of Solvation=-1607.00187442

St.Pt.	General Structure	Ball & Stick model

III-1A





Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.09345	-2.63152	-0.79404
C	-0.69044	-2.44297	0.58916
C	-1.82211	-1.88357	1.30492
C	-2.87712	-1.65610	0.36374
C	-2.42992	-2.13704	-0.94219
Ir	-1.15415	-0.53351	-0.24148
O	-0.26141	0.95442	0.91359
O	2.50078	-0.22103	0.33753
O	-2.22186	1.16888	-1.06968
C	-1.67710	2.15442	-1.59757
H	-2.34851	2.99745	-1.84741
C	-0.31122	2.34496	-1.95575
C	0.66763	1.30404	-1.90698
C	0.04186	3.62124	-2.45706
C	1.95907	1.60851	-2.40808
C	1.31368	3.90079	-2.88932
H	-0.73042	4.39072	-2.48294
C	2.27023	2.86786	-2.86631
H	2.69430	0.80656	-2.40221
H	1.57585	4.88927	-3.25448
H	3.27989	3.06600	-3.22154
O	0.45821	0.09874	-1.46735
H	1.68801	-0.18373	-0.22512
C	-0.94684	1.64637	1.77105
C	-0.17152	2.84339	2.34544
C	3.29247	-1.19266	-0.10311
C	4.61656	-1.23886	0.64671
O	2.98178	-1.96106	-0.99453
O	-2.11421	1.44530	2.09762
C	-3.24145	-2.09512	-2.18910
H	-3.74022	-1.12549	-2.29691
H	-2.61672	-2.24741	-3.07421
H	-4.01411	-2.87431	-2.18206
C	-0.19812	-3.14503	-1.86434
H	0.82273	-2.76316	-1.73542
H	-0.16049	-4.24141	-1.83826
H	-0.54592	-2.83785	-2.85541
C	0.59125	-2.87678	1.20924
H	0.93916	-2.13433	1.93721
H	0.46424	-3.83334	1.73350

Frequencies

32.9876	38.3672	43.9825
49.5508	54.8751	59.2671
64.7457	80.0797	85.6170
89.4263	97.9423	102.3048
107.6047	116.4807	124.2562
130.6576	145.4659	159.1311
168.7833	176.9905	181.6364
192.7274	194.9395	202.6912
208.6766	212.2640	224.4780
229.1106	233.9732	238.5920
242.6713	257.6041	265.5794
280.8059	287.8453	294.3629
302.0616	308.7653	311.8143
315.3598	318.9226	326.3119
334.3575	341.7597	349.8904
355.5197	360.1765	364.3570
378.6152	387.3257	391.6780
410.2044	414.6124	435.1215
445.9820	449.0981	454.8731
456.1584	475.2988	532.4201
538.5045	543.4925	544.2310
552.4953	555.1915	571.7038
586.8583	589.9027	597.6371
604.2452	610.0321	642.1716
679.2332	751.5341	757.2626
764.6692	774.8309	792.0965
800.3152	809.9842	817.1955
817.4660	854.6762	885.9336
893.0572	905.9581	916.4696
944.2090	945.3519	946.2260
953.1116	954.4072	957.5750
958.2877	959.7344	989.6733
992.9006	1015.6404	1038.8408
1040.1918	1041.5711	1043.7763
1044.7276	1046.3595	1049.6673
1052.8524	1058.2264	1068.4673
1098.8494	1099.9141	1118.3503
1149.1682	1172.3949	1187.6123
1192.7652	1221.3295	1235.9831
1239.0489	1243.3559	1249.5888
1255.2071	1268.6324	1271.2730
1294.0852	1367.8122	1372.1072
1381.8146	1382.3417	1382.5992
1383.8105	1385.9278	1387.2425

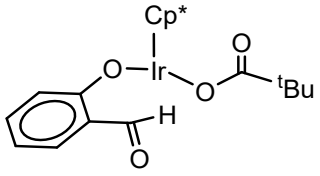
H	1.37637	-2.99884	0.45589	1399.0999	1400.2198	1405.7332
C	-1.85668	-1.58939	2.76094	1406.6950	1411.7615	1417.7890
H	-2.50489	-0.73708	2.97698	1429.7270	1430.7026	1434.6276
H	-2.21135	-2.47147	3.31038	1438.3689	1442.8783	1449.3780
H	-0.85738	-1.34039	3.13357	1449.8047	1451.2993	1455.6628
C	-4.18151	-1.00872	0.67049	1462.6056	1462.6942	1463.4127
H	-4.85367	-1.69714	1.19780	1466.2049	1468.2621	1469.3534
H	-4.01328	-0.12330	1.29436	1474.2662	1475.9223	1477.5454
H	-4.68203	-0.67917	-0.24510	1480.1359	1482.0548	1484.6991
C	1.31791	2.78772	2.02270	1490.4663	1496.6951	1498.0791
H	1.49869	2.84072	0.94194	1500.8799	1507.4236	1508.6502
H	1.83236	3.63352	2.49959	1510.5448	1523.2414	1529.7265
H	1.77398	1.85607	2.37939	1536.3014	1588.4253	1679.5583
C	-0.38654	2.87918	3.85662	1714.0457	1758.9394	1832.0945
H	0.07499	3.77776	4.28723	2985.6911	3017.8862	3024.0765
H	-1.45490	2.88036	4.09446	3024.9688	3028.8975	3030.4434
H	0.06808	2.00429	4.34032	3031.9038	3033.7283	3039.5130
C	-0.78997	4.09183	1.70832	3040.2473	3040.5215	3041.7098
H	-1.86276	4.14596	1.92491	3096.9256	3101.6932	3104.1915
H	-0.30558	4.99795	2.09630	3110.5788	3112.2890	3113.4448
H	-0.65322	4.08065	0.61680	3115.0175	3118.0582	3121.7443
C	5.48969	-2.34013	0.06141	3126.7842	3127.6553	3128.0592
H	5.70228	-2.15687	-0.99753	3132.8087	3138.4560	3138.7905
H	6.44180	-2.39014	0.60427	3139.8312	3141.7085	3143.8804
H	4.99570	-3.31529	0.13220	3144.6110	3146.7493	3149.5907
C	5.31162	0.11832	0.51143	3163.6646	3171.7331	3179.1671
H	4.70652	0.92219	0.94319	3198.5775	3214.9269	3465.6591
H	6.27839	0.09229	1.03029			
H	5.50313	0.36079	-0.54199			
C	4.32932	-1.52721	2.12336			
H	3.81822	-2.49156	2.24534			
H	5.27372	-1.57756	2.68008			
H	3.70645	-0.74509	2.57092			

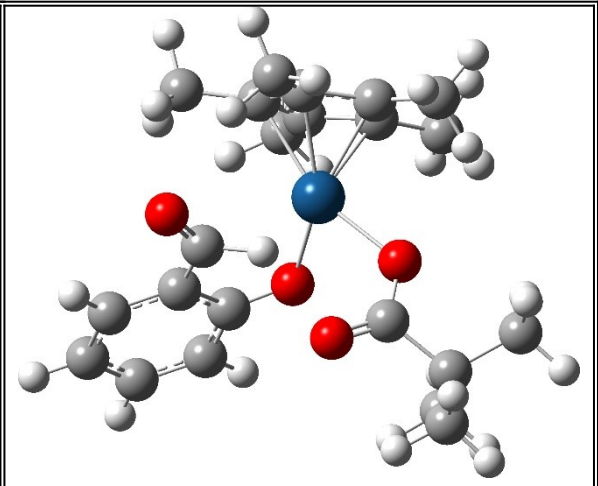
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.614307 Electronic Energy = -1607.51920504
Internal Energy (E)= -1606.86656204 Enthalpy (H)= -1606.86561904
Gibbs Free Energy (G)=-1606.97221204 Gibbs Free Energy of Solvation=-1607.02373876

St.Pt.	General Structure	Ball & Stick model

III'-1A





Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.81921	-2.44398	-0.92848
C	0.34475	-2.74183	-0.15693
C	0.07770	-2.34623	1.21916
C	-1.30124	-1.87617	1.28402
C	-1.84896	-1.92098	-0.03534
C	-1.82374	1.95580	-0.56892
Ir	-0.07594	-0.61663	0.01999
C	-2.85462	2.85797	-0.89533
C	-3.21954	3.85203	-0.01701
C	-1.16692	2.02475	0.69065
C	-2.54055	3.95543	1.21255
C	-1.54064	3.07555	1.56325
H	-1.02558	3.14655	2.51820
H	-2.81545	4.74674	1.90806
H	-4.01024	4.55380	-0.26758
H	-0.26721	0.65704	-1.42036
O	1.90867	-0.06590	-0.01978
C	2.28866	1.04219	-0.60190
C	3.66686	1.51880	-0.13245
O	1.61695	1.69711	-1.38666
H	-3.33278	2.74952	-1.86700
C	-1.39207	0.98141	-1.54096
O	-1.96440	0.61198	-2.54852
O	-0.27167	1.16014	1.08162
C	4.30547	2.39847	-1.19995
H	3.64374	3.22570	-1.47242
H	5.25417	2.80952	-0.83005
H	4.51574	1.82607	-2.11193
C	3.38337	2.34870	1.12646
H	2.87925	1.74080	1.88769
H	4.32147	2.73527	1.54666
H	2.73253	3.19938	0.88905
C	4.58955	0.35383	0.21214
H	4.76763	-0.28501	-0.66281
H	5.56133	0.73470	0.55365
H	4.16428	-0.27045	1.00507
C	1.65451	-3.25821	-0.63838
H	2.46218	-2.57095	-0.35628

Frequencies

26.1426	36.0912	40.7567
51.7030	57.3238	65.1664
88.0946	94.8566	122.3750
135.5231	145.4921	151.7764
160.6126	164.0593	173.1818
180.9843	186.2838	194.3523
201.3308	210.3163	211.7506
226.2545	232.7383	234.8520
245.4983	256.7006	263.2800
278.3295	285.7333	303.2614
308.0613	311.2186	313.8637
324.2998	348.1144	374.7217
388.1531	415.4425	426.1663
431.8421	444.4151	457.9589
468.0659	530.7877	532.8995
536.3634	542.0544	547.3010
571.8879	583.5255	584.7920
595.2583	603.3916	619.9606
641.7659	652.3503	747.7033
764.1777	790.9007	802.9908
807.9301	816.1121	824.4970
861.2866	877.3374	914.7142
946.4611	952.9866	953.6033
954.5086	961.8969	962.2979
979.1721	1036.7718	1038.3196
1039.7383	1043.3286	1043.6827
1044.0355	1045.8542	1050.6201
1082.9737	1088.8483	1097.1529
1103.9013	1118.9666	1142.4889
1180.5967	1185.6503	1205.1460
1235.5520	1245.5773	1268.5154
1273.3959	1341.5494	1354.7659
1373.3033	1374.9698	1379.6177
1382.9655	1392.2546	1397.3656
1401.0917	1405.6029	1409.1644
1435.5646	1435.9276	1436.5137
1439.5491	1444.0995	1449.7306
1450.9281	1451.8865	1454.0150
1458.3473	1459.7093	1465.4409
1467.7208	1469.3971	1474.4286
1478.0092	1483.8030	1488.4576
1495.9945	1497.8916	1508.4595

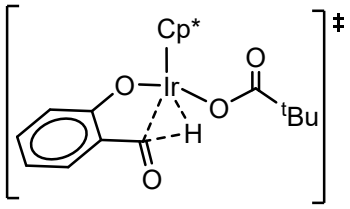
H	1.86771	-4.24224	-0.20282	1518.8678	1523.5907	1543.1374
H	1.66853	-3.35704	-1.72737	1604.2579	1671.1504	1779.9995
C	-0.99347	-2.59408	-2.39765	1805.7272	2277.9465	3023.7688
H	-0.04371	-2.81697	-2.89201	3025.6906	3029.4207	3032.5410
H	-1.69677	-3.40669	-2.61977	3035.6126	3036.7398	3038.9883
H	-1.39299	-1.66890	-2.83356	3044.6089	3104.2203	3107.7278
C	-3.23791	-1.56820	-0.43858	3111.3802	3114.9325	3115.8425
H	-3.26481	-1.16783	-1.45686	3118.5280	3119.6986	3126.1848
H	-3.88628	-2.45302	-0.39905	3129.3354	3136.4608	3142.1952
H	-3.66347	-0.80625	0.22302	3145.8014	3147.2195	3149.1518
C	-1.98213	-1.35961	2.50056	3149.2106	3149.3228	3174.8601
H	-2.71087	-0.58314	2.24584	3184.1272	3198.4756	3207.0416
H	-2.50932	-2.16725	3.02344			
H	-1.26387	-0.91254	3.19482			
C	1.03039	-2.50775	2.34930			
H	0.75215	-1.88069	3.20142			
H	1.06037	-3.55130	2.68953			
H	2.04174	-2.21860	2.04322			
H	-2.80335	-1.22132	2.48290			
H	-1.37192	-1.01392	5.58417			
H	-1.60493	-2.14965	4.22902			
Ir	1.06614	-0.33518	-0.31907			
H	-1.75239	0.62648	0.33798			
C	-3.38056	-0.40976	-0.65861			
C	-4.28232	0.51666	-0.11329			
C	-3.88073	-1.44938	-1.47227			
C	-5.64238	0.43691	-0.35231			
H	-3.87904	1.31567	0.50901			
C	-5.25399	-1.52911	-1.70883			
C	-6.12101	-0.59710	-1.15552			
H	-6.32438	1.16466	0.07673			
H	-5.63954	-2.33280	-2.33587			
H	-7.18654	-0.68124	-1.35624			
O	-3.02148	-2.33912	-1.99749			
H	-3.51662	-2.99637	-2.50049			

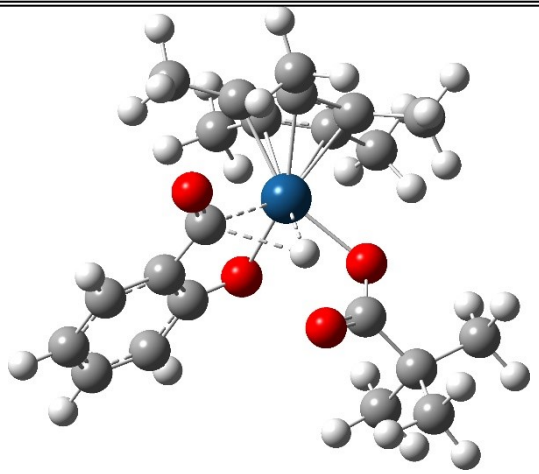
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.462130 Electronic Energy = -1260.64913599
Internal Energy (E)= -1260.15718999 Enthalpy (H)= -1260.15624699
Gibbs Free Energy (G)=-1260.24605199 Gibbs Free Energy of Solvation=-1261.31339186

St.Pt.	General Structure	Ball & Stick model

TS-3A





Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.95359	-1.76649	-0.89131
C	-0.97467	-2.53226	-0.18670
C	-1.00605	-2.13742	1.21911
C	-2.02351	-1.14434	1.36662
C	-2.58134	-0.87223	0.06660
C	-0.63507	2.52233	-0.48914
Ir	-0.41192	-0.41523	-0.03285
C	-0.96637	3.80971	-0.94348
C	-0.62833	4.91033	-0.18653
C	0.03241	2.32506	0.73908
C	0.05063	4.72139	1.03228
C	0.38186	3.46511	1.49610
H	0.90527	3.31981	2.43783
H	0.32289	5.59116	1.62796
H	-0.87355	5.91306	-0.52568
H	0.21619	0.44178	-1.33619
O	1.60306	-0.92193	0.05016
C	2.45998	-0.18335	-0.59853
C	3.90943	-0.41448	-0.15904
O	2.17428	0.67754	-1.42299
H	-1.47951	3.90495	-1.89804
C	-0.94457	1.33845	-1.26506
O	-1.61125	1.27029	-2.27379
O	0.30191	1.12189	1.16621
C	4.85879	-0.01710	-1.28189
H	4.64679	0.99794	-1.62899
H	5.89878	-0.06811	-0.93416
H	4.75602	-0.69165	-2.14090
C	4.10276	0.51173	1.04923
H	3.37671	0.27745	1.83740
H	5.11545	0.39409	1.45703
H	3.96414	1.56130	0.76152
C	4.15735	-1.86212	0.25316
H	3.97148	-2.54916	-0.58286
H	5.20316	-1.98751	0.56335
H	3.51199	-2.16061	1.08608
C	-0.04797	-3.55373	-0.74227
H	0.97766	-3.35822	-0.40547

Frequencies

-191.9673	15.7274	30.6674
39.6229	46.0375	55.8118
69.3879	86.5315	96.6943
133.0113	137.7155	146.4286
159.6379	162.5249	168.5527
172.1975	174.9609	177.8848
189.9071	192.0325	203.6136
209.7536	226.2221	247.9605
256.4651	261.4150	269.8632
274.2010	283.0996	288.9312
304.2119	307.0877	310.1645
321.2221	350.9059	351.9366
380.3235	391.1112	412.1395
426.1903	430.2801	440.1065
469.8418	495.5161	537.1969
540.9210	542.5178	552.6125
565.1215	568.8484	594.4048
596.7509	606.1040	626.2884
639.1099	653.4028	720.7664
762.1530	775.7061	791.6752
812.2329	817.0436	818.6954
843.6225	856.7250	881.2626
899.8172	922.2020	935.6541
944.8955	950.8802	951.6394
956.0720	965.1151	984.8029
1030.6651	1034.0292	1035.8324
1042.4097	1044.6116	1046.1131
1047.3934	1050.8617	1088.5628
1092.3082	1108.0654	1124.3908
1150.6662	1182.1816	1188.8914
1212.5258	1233.3184	1246.1850
1263.5094	1268.3532	1351.5455
1356.1392	1370.9465	1372.7688
1375.9575	1380.7405	1393.4935
1397.1577	1398.1652	1405.0858
1406.2422	1436.3866	1439.2234
1440.1730	1443.3579	1444.8811
1445.1157	1449.3513	1453.8461
1460.1506	1461.8811	1465.3151
1466.6762	1467.0751	1473.8420
1475.7663	1484.5707	1485.2104
1486.7514	1502.9242	1511.4942
1520.4088	1525.3637	1543.7429

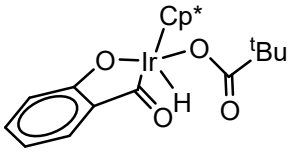
H	-0.33575	-4.55957	-0.41066	1614.8406	1666.5367	1745.6099
H	-0.04660	-3.53914	-1.83598	1788.4156	1878.9342	3023.6673
C	-2.29814	-1.84276	-2.33773	3026.8917	3035.3066	3036.6602
H	-1.62189	-2.51600	-2.87258	3037.3877	3039.8155	3041.0055
H	-3.32190	-2.21591	-2.46766	3041.9344	3106.4527	3113.2483
H	-2.23135	-0.84983	-2.79919	3116.2809	3116.4040	3116.6293
C	-3.71253	0.04880	-0.22074	3117.1752	3121.3848	3123.2180
H	-3.68196	0.39619	-1.25717	3127.2208	3129.7330	3142.1375
H	-4.67406	-0.45099	-0.04598	3148.0833	3149.8626	3151.8305
H	-3.67207	0.93509	0.42262	3154.0378	3166.0939	3168.9107
C	-2.36442	-0.40690	2.61073	3191.4141	3201.5460	3209.2786
H	-2.64767	0.62799	2.39036			
H	-3.20656	-0.88348	3.12824			
H	-1.51184	-0.37047	3.29515			
C	-0.13274	-2.71493	2.27695			
H	-0.13912	-2.10180	3.18275			
H	-0.45672	-3.72694	2.55259			
H	0.90424	-2.76976	1.92656			
H	-2.80335	-1.22132	2.48290			
H	-1.37192	-1.01392	5.58417			
H	-1.60493	-2.14965	4.22902			
Ir	1.06614	-0.33518	-0.31907			
H	-1.75239	0.62648	0.33798			
C	-3.38056	-0.40976	-0.65861			
C	-4.28232	0.51666	-0.11329			
C	-3.88073	-1.44938	-1.47227			
C	-5.64238	0.43691	-0.35231			
H	-3.87904	1.31567	0.50901			
C	-5.25399	-1.52911	-1.70883			
C	-6.12101	-0.59710	-1.15552			
H	-6.32438	1.16466	0.07673			
H	-5.63954	-2.33280	-2.33587			
H	-7.18654	-0.68124	-1.35624			
O	-3.02148	-2.33912	-1.99749			
H	-3.51662	-2.99637	-2.50049			

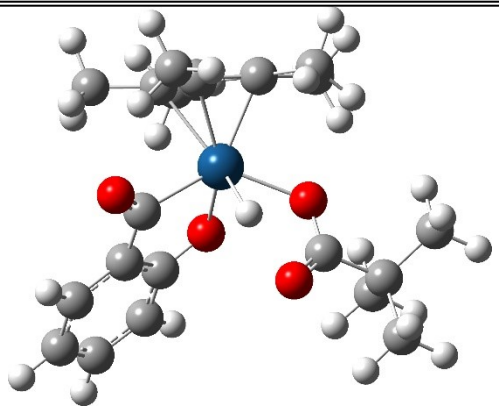
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.458396 Electronic Energy = -1260.64392691
Internal Energy (E)= -1260.15595091 Enthalpy (H)= -1260.15500691
Gibbs Free Energy (G)=-1260.24495791 Gibbs Free Energy of Solvation=-1261.30446716

St.Pt.	General Structure	Ball & Stick model

IV-1A





Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.56745	-2.49180	-0.67850
C	0.86979	-2.43177	-0.47523
C	1.13759	-2.28063	0.94454
C	-0.08968	-2.10913	1.59030
C	-1.16165	-2.17216	0.58226
C	-2.32904	1.36530	-0.60443
Ir	-0.08232	-0.42766	-0.16820
C	-3.37893	2.10035	-1.16918
C	-4.14342	2.92503	-0.36611
C	-2.03912	1.44072	0.76970
C	-3.85619	3.00336	1.00606
C	-2.82637	2.27932	1.57975
H	-2.60456	2.34287	2.64204
H	-4.45930	3.65215	1.63905
H	-4.95700	3.50922	-0.78758
H	0.60518	-0.41627	-1.59211
O	1.14070	1.24192	-0.06822
C	2.40892	1.12579	-0.32924
C	3.20083	2.40613	-0.02878
O	2.96869	0.10138	-0.71196
H	-3.56394	2.00292	-2.23677
C	-1.50427	0.44023	-1.38625
O	-1.67387	0.15997	-2.54951
O	-1.05754	0.71789	1.26513
C	2.50323	-2.22781	1.53159
H	3.00933	-3.19636	1.42488
H	3.10704	-1.47647	1.00944
H	2.47645	-1.97629	2.59561
C	1.90382	-2.77382	-1.48796
H	2.73966	-2.07147	-1.42608
H	2.27600	-3.79131	-1.30851
H	1.49329	-2.73248	-2.50155
C	-1.25060	-2.87576	-1.94396
H	-1.02893	-3.92128	-2.19089
H	-2.33542	-2.76960	-1.85595
H	-0.93833	-2.23874	-2.77838
C	-2.61343	-2.12914	0.91105
H	-3.22271	-1.95698	0.01840
H	-2.93633	-3.07298	1.36929
H	-2.82709	-1.31879	1.61660

Frequencies

22.2662	30.0753	36.2542
45.6310	57.7525	80.2531
94.1109	121.2146	128.4970
141.4676	157.8219	164.6265
169.8860	178.3314	181.7525
192.7819	206.2985	210.7402
218.9661	223.7833	240.6645
242.6141	247.2857	250.7498
259.6363	265.5475	276.3580
284.5940	290.4532	299.6233
301.1185	302.2028	314.5715
323.7881	335.9066	350.6608
378.8416	391.7167	414.0327
426.9393	444.5523	448.2749
473.5332	532.5571	534.1059
541.3901	552.5382	570.5422
572.3271	594.3947	604.3193
613.0662	621.6328	643.7646
649.5053	669.4126	756.3226
765.6532	782.1791	792.9702
810.8477	813.9814	820.4792
860.5346	866.7305	890.8890
921.0103	943.6655	944.9364
955.2137	955.7229	956.6887
958.5108	971.5986	982.4701
1021.3380	1031.3654	1041.4651
1042.9466	1043.7086	1045.5833
1049.0314	1052.3049	1087.7949
1093.4995	1110.4398	1117.0866
1147.7324	1176.8672	1189.0197
1205.4348	1239.4247	1249.1822
1266.2059	1266.7927	1341.0894
1361.7507	1363.0005	1370.8247
1380.2300	1385.2837	1390.3923
1392.3047	1393.8550	1401.4494
1417.8901	1423.6618	1430.8675
1440.7882	1444.4463	1450.1028
1451.0970	1452.3662	1458.7973
1461.9755	1462.7937	1464.2315
1465.7179	1469.2613	1476.1445
1478.3575	1482.6658	1486.3576
1487.3722	1489.5248	1502.2955
1518.0758	1531.1723	1586.4311
1628.3835	1662.1793	1756.8064
1816.8579	2205.5898	3018.4750

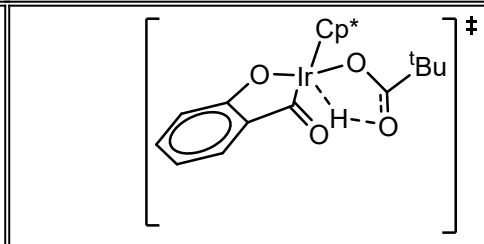
C	-0.34375	-1.78210	3.01374	3023.6893	3030.4207	3035.9906
H	-0.75177	-0.76249	3.07987	3037.2237	3039.3467	3043.4064
H	-1.08491	-2.46548	3.44603	3043.9595	3098.2099	3109.8019
H	0.56755	-1.83205	3.61564	3110.9453	3118.6322	3120.4330
C	4.52514	2.37594	-0.78262	3122.4426	3128.6345	3129.3150
H	5.11517	3.26813	-0.53526	3132.1277	3143.1684	3144.0160
H	5.10658	1.48544	-0.52472	3146.9267	3150.6300	3150.6753
H	4.36327	2.36374	-1.86707	3154.4056	3173.0657	3191.6669
C	2.40958	3.65598	-0.40261	3194.9575	3202.0361	3209.7896
H	1.46445	3.70717	0.14554			
H	2.99962	4.55246	-0.16991			
H	2.17916	3.67369	-1.47497			
C	3.46438	2.39312	1.48127			
H	4.02366	1.49382	1.77222			
H	4.05947	3.27016	1.76784			
H	2.52330	2.41529	2.04307			
H	-2.80335	-1.22132	2.48290			
H	-1.37192	-1.01392	5.58417			
H	-1.60493	-2.14965	4.22902			
Ir	1.06614	-0.33518	-0.31907			
H	-1.75239	0.62648	0.33798			
C	-3.38056	-0.40976	-0.65861			
C	-4.28232	0.51666	-0.11329			
C	-3.88073	-1.44938	-1.47227			
C	-5.64238	0.43691	-0.35231			
H	-3.87904	1.31567	0.50901			
C	-5.25399	-1.52911	-1.70883			
C	-6.12101	-0.59710	-1.15552			
H	-6.32438	1.16466	0.07673			
H	-5.63954	-2.33280	-2.33587			
H	-7.18654	-0.68124	-1.35624			
O	-3.02148	-2.33912	-1.99749			
H	-3.51662	-2.99637	-2.50049			

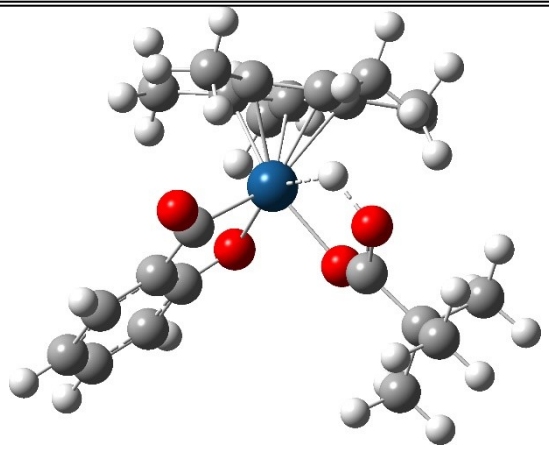
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.461420 Electronic Energy = -1260.65251733
Internal Energy (E)= -1260.16164433 Enthalpy (H)= -1260.16070133
Gibbs Free Energy (G)=-1260.24959133 Gibbs Free Energy of Solvation=-1261.30771862

St.Pt.	General Structure	Ball & Stick model

TS-4A





Cartesian co-ordinate

Atoms	X	Y	Z
C	0.39251	-2.31520	1.10412
C	-0.95230	-2.30024	0.57542
C	-0.88448	-2.48402	-0.87118
C	0.46080	-2.47007	-1.24389
C	1.27406	-2.28214	-0.03251
C	2.12889	1.57762	0.56236
Ir	0.11191	-0.44987	0.01711
C	3.00617	2.47662	1.18044
C	3.87194	3.22778	0.40759
C	2.11262	1.41492	-0.83487
C	3.85776	3.06882	-0.98738
C	2.99999	2.18191	-1.61320
H	2.98834	2.06305	-2.69380
H	4.53834	3.66108	-1.59710
H	4.55567	3.93553	0.86881
H	-0.91295	-0.02257	1.25448
O	-1.31384	0.97468	-0.60761
C	-2.19065	1.29790	0.27648
C	-3.30606	2.21614	-0.21480
O	-2.18589	0.86084	1.44295
H	2.97948	2.56272	2.26467
C	1.19450	0.73228	1.31375
O	1.11975	0.68556	2.52179
O	1.27975	0.55157	-1.37267
C	2.76436	-2.28992	-0.01725
H	3.15277	-1.91381	0.93466
H	3.16020	-3.30194	-0.17346
H	3.16202	-1.64358	-0.80781
C	0.75729	-2.37769	2.54542
H	0.44609	-3.33900	2.97266
H	1.83662	-2.27430	2.68701
H	0.28633	-1.56483	3.10914
C	-2.20470	-2.39608	1.37706
H	-2.50960	-3.44566	1.48396
H	-2.07314	-1.97045	2.37617
H	-3.02745	-1.85246	0.89987
C	-2.08730	-2.49965	-1.74797
H	-2.74687	-3.34206	-1.50405
H	-2.67005	-1.57711	-1.61543

Frequencies

-318.5904	24.8504	37.7195
44.5605	60.0966	80.4685
96.8214	109.2749	127.9629
135.9322	156.1192	161.8068
168.1338	172.6133	187.5000
197.0635	200.1854	205.6622
208.5358	209.8342	217.1976
233.5929	240.8037	246.2368
251.9776	264.4110	270.5701
275.4130	279.9711	290.4461
302.3124	305.8514	310.4537
329.1813	337.5722	353.8896
372.2321	394.1635	426.2561
427.9157	436.5972	445.5730
474.4309	510.2008	535.9878
538.1655	540.9596	554.0154
572.5412	595.8151	617.9012
618.4469	628.0600	633.1282
643.0311	656.1499	677.9615
760.5140	768.9191	791.4598
809.4649	815.9883	838.0814
860.8842	862.0313	881.3889
931.2458	945.3855	948.2946
954.6126	957.3228	958.3429
958.8520	964.3589	977.0093
1031.0603	1039.7448	1040.1517
1044.4787	1047.4207	1047.9827
1050.2473	1052.8218	1087.3414
1088.4157	1107.9675	1117.2895
1147.8640	1177.0773	1186.4113
1205.9153	1239.4628	1253.0223
1265.5488	1269.6733	1344.4382
1368.8696	1374.8795	1378.8791
1384.8707	1390.0921	1390.6979
1398.5030	1399.3994	1407.4801
1427.9405	1428.9375	1435.8807
1438.3510	1447.1251	1451.5560
1452.6790	1454.3407	1455.8354
1457.8060	1460.3263	1460.9137
1462.7709	1468.6414	1470.8559
1479.0535	1480.9657	1483.3838
1489.4966	1497.5080	1506.6254
1511.6175	1518.1353	1580.4341

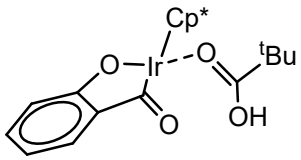
H	-1.82002	-2.57131	-2.80584	1593.6126	1627.0577	1662.1031
C	1.03568	-2.45320	-2.61314	1764.8781	1816.6192	3022.9560
H	0.27764	-2.64348	-3.37808	3024.2704	3030.3138	3034.5003
H	1.48098	-1.46740	-2.81090	3036.5254	3038.5573	3040.5765
H	1.82761	-3.20480	-2.71729	3040.9368	3099.6369	3101.2024
C	-4.17959	1.37192	-1.14983	3110.0920	3117.9077	3118.4677
H	-5.02455	1.97038	-1.51327	3122.0431	3125.2670	3128.2026
H	-3.60420	1.02250	-2.01492	3131.6981	3139.2051	3140.7982
H	-4.58855	0.49834	-0.62338	3142.9621	3146.9043	3149.8645
C	-4.13611	2.71504	0.96130	3150.2148	3151.0037	3172.2048
H	-3.52377	3.29462	1.66093	3189.9988	3200.3748	3205.3673
H	-4.94514	3.35976	0.59518			
H	-4.57650	1.88207	1.51882			
C	-2.71209	3.39492	-0.98389			
H	-3.52040	4.04439	-1.34374			
H	-2.05811	3.99734	-0.34179			
H	-2.12561	3.05576	-1.84261			
H	-2.80335	-1.22132	2.48290			
H	-1.37192	-1.01392	5.58417			
H	-1.60493	-2.14965	4.22902			
Ir	1.06614	-0.33518	-0.31907			
H	-1.75239	0.62648	0.33798			
C	-3.38056	-0.40976	-0.65861			
C	-4.28232	0.51666	-0.11329			
C	-3.88073	-1.44938	-1.47227			
C	-5.64238	0.43691	-0.35231			
H	-3.87904	1.31567	0.50901			
C	-5.25399	-1.52911	-1.70883			
C	-6.12101	-0.59710	-1.15552			
H	-6.32438	1.16466	0.07673			
H	-5.63954	-2.33280	-2.33587			
H	-7.18654	-0.68124	-1.35624			
O	-3.02148	-2.33912	-1.99749			
H	-3.51662	-2.99637	-2.50049			

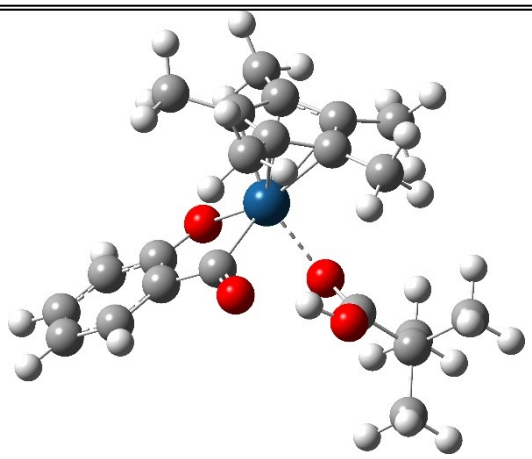
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.459311 Electronic Energy = -1260.65072759
Internal Energy (E)= -1260.16259359 Enthalpy (H)= -1260.16164959
Gibbs Free Energy (G)=-1260.24823559 Gibbs Free Energy of Solvation=-1261.3068256

St.Pt.	General Structure	Ball & Stick model

V-1A





Cartesian co-ordinate

Atoms	X	Y	Z
C	0.45931	-2.06640	1.35480
C	-0.89018	-2.08753	0.87420
C	-0.86450	-2.52356	-0.52957
C	0.46645	-2.65221	-0.93036
C	1.32161	-2.27695	0.20656
C	2.07282	1.68668	0.47114
Ir	0.24007	-0.48109	-0.09100
C	2.85259	2.65965	1.11153
C	3.85194	3.30670	0.41142
C	2.26138	1.37305	-0.89744
C	4.05081	2.99134	-0.94520
C	3.27647	2.05463	-1.60285
H	3.42769	1.82560	-2.65515
H	4.83634	3.50544	-1.49759
H	4.47611	4.05425	0.89415
H	-1.17183	1.21512	1.72965
O	-1.37357	0.91623	-0.67482
C	-2.21966	1.37855	0.10051
C	-3.54724	1.89904	-0.41747
O	-2.09835	1.43010	1.39923
H	2.64910	2.87987	2.15809
C	0.95039	0.98730	1.07622
O	0.43766	1.30034	2.16356
O	1.48415	0.48984	-1.46900
C	2.80953	-2.36301	0.20307
H	3.23983	-1.81615	1.04902
H	3.15439	-3.40434	0.25783
H	3.21625	-1.91573	-0.71104
C	0.87715	-1.83238	2.76372
H	0.76938	-2.74852	3.35807
H	1.92215	-1.51090	2.82059
H	0.27582	-1.04113	3.22455
C	-2.11950	-1.96880	1.70926
H	-2.40751	-2.93929	2.13670
H	-1.97288	-1.26739	2.53796
H	-2.97109	-1.60896	1.11910
C	-2.09002	-2.64775	-1.36592
H	-2.74743	-3.44455	-0.99372
H	-2.67018	-1.71373	-1.35261

Frequencies

18.8734	33.7064	59.5472
66.8916	79.1068	83.5237
104.6253	126.3718	129.6155
147.2791	152.3271	159.4640
169.6575	176.3475	180.8473
188.4529	197.1381	203.8278
211.5721	223.3910	227.6976
241.8458	252.7322	264.1363
265.9221	273.7274	276.3723
284.9809	296.2581	303.9757
309.9674	314.0410	324.4384
341.2129	368.9662	392.7757
396.5847	414.6553	419.6139
426.2533	445.6882	465.2976
486.4019	533.2305	537.1900
539.7705	547.7797	556.9302
568.9918	592.8122	601.9229
612.7471	623.9673	630.4002
660.2375	689.3923	761.6765
765.2527	781.4966	788.6964
802.3910	812.0628	856.6815
868.3538	896.3997	912.7404
947.9381	950.9288	951.3281
954.1202	957.9773	959.5241
965.5937	977.3441	1034.4842
1039.5182	1041.1113	1042.3330
1046.6632	1049.8433	1052.2790
1056.7546	1086.7959	1089.2490
1104.8876	1115.2311	1144.5643
1179.5468	1182.1943	1208.1185
1239.0748	1248.4011	1263.7369
1276.8931	1339.7961	1350.2689
1366.6126	1374.3936	1380.4945
1391.5894	1393.7598	1394.6950
1396.3521	1399.9691	1417.3470
1428.5177	1434.1931	1440.9895
1448.5724	1450.8282	1453.2953
1456.2571	1458.0668	1459.7786
1462.1979	1463.5180	1469.6024
1470.3223	1474.7453	1481.6574
1485.1453	1488.3064	1495.8551
1505.1630	1510.9514	1520.4603
1521.5694	1533.9806	1589.8440

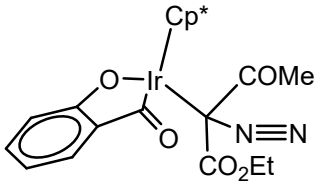
H	-1.84913	-2.86778	-2.41006	1613.2034	1657.8868	1668.8237
C	1.00250	-2.93281	-2.28977	1742.2187	3018.3892	3021.9813
H	0.20253	-3.09303	-3.01880	3026.3916	3028.9060	3031.7469
H	1.60833	-2.08647	-2.63874	3039.9485	3040.0483	3045.5617
H	1.64248	-3.82457	-2.28702	3084.2274	3088.4227	3098.7110
C	-4.62993	0.92749	0.07145	3103.5935	3109.1884	3113.9169
H	-5.60939	1.26266	-0.29081	3123.6733	3124.4879	3134.0904
H	-4.45904	-0.08570	-0.31933	3134.7103	3136.0598	3137.4713
H	-4.66282	0.87918	1.16519	3140.2030	3140.3013	3144.2242
C	-3.80767	3.29563	0.15022	3144.4847	3152.4007	3165.8787
H	-3.03093	4.00259	-0.16491	3183.3405	3197.7228	3203.5312
H	-4.77014	3.66664	-0.22270			
H	-3.84005	3.28599	1.24369			
C	-3.53762	1.93911	-1.94040			
H	-4.50272	2.31477	-2.30106			
H	-2.74749	2.59662	-2.31846			
H	-3.37186	0.94438	-2.36815			
H	-2.80335	-1.22132	2.48290			
H	-1.37192	-1.01392	5.58417			
H	-1.60493	-2.14965	4.22902			
Ir	1.06614	-0.33518	-0.31907			
H	-1.75239	0.62648	0.33798			
C	-3.38056	-0.40976	-0.65861			
C	-4.28232	0.51666	-0.11329			
C	-3.88073	-1.44938	-1.47227			
C	-5.64238	0.43691	-0.35231			
H	-3.87904	1.31567	0.50901			
C	-5.25399	-1.52911	-1.70883			
C	-6.12101	-0.59710	-1.15552			
H	-6.32438	1.16466	0.07673			
H	-5.63954	-2.33280	-2.33587			
H	-7.18654	-0.68124	-1.35624			
O	-3.02148	-2.33912	-1.99749			
H	-3.51662	-2.99637	-2.50049			

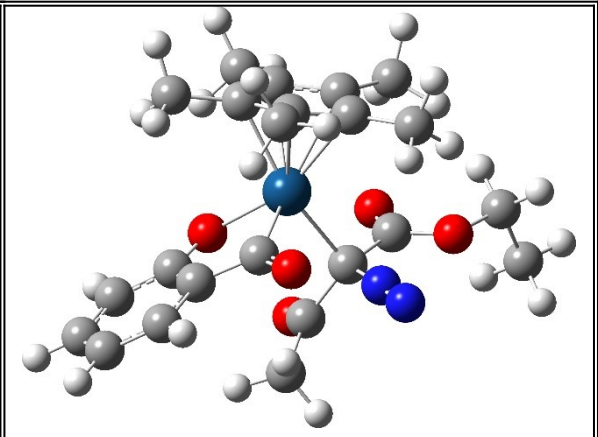
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.465016 Electronic Energy = -1260.68475717
Internal Energy (E)= -1260.19071417 Enthalpy (H)= -1260.18977117
Gibbs Free Energy (G)=-1260.27702417 Gibbs Free Energy of Solvation=-1261.32501423

St.Pt.	General Structure	Ball & Stick model

V'-1A





Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.30892	2.52206	0.81999
C	1.06986	2.12582	0.86410
C	1.57254	2.10696	-0.51289
C	0.49391	2.30824	-1.37895
C	-0.71056	2.50313	-0.56428
C	-2.74545	-0.69597	0.52002
Ir	-0.15003	0.49523	-0.01022
C	-2.54139	-0.84387	-0.86998
C	-3.57583	-1.41344	-1.64298
C	-3.93305	-1.11873	1.12967
C	-4.74726	-1.81045	-1.02444
C	-4.94096	-1.67097	0.36096
H	-4.02922	-1.00537	2.20819
H	-5.87220	-1.99814	0.81647
H	-5.53916	-2.25015	-1.62913
H	-3.42104	-1.53892	-2.71197
C	1.01441	-1.40696	0.13917
C	2.39886	-1.22088	-0.42624
C	0.22474	-2.57975	-0.48993
O	0.48564	-2.92874	-1.60950
N	1.04011	-1.48133	1.52319
N	0.99149	-1.53516	2.64525
C	2.99838	1.92508	-0.89473
H	3.10760	1.34534	-1.81663
H	3.47521	2.90254	-1.04627
H	3.56098	1.41494	-0.10495
C	1.88469	2.02944	2.10889
H	2.71998	1.32886	1.99410
H	2.30403	3.00150	2.40305
H	1.26580	1.66526	2.93794
C	-1.14352	2.87884	1.99845
H	-0.99282	2.17095	2.82019
H	-0.88620	3.88592	2.35110
H	-2.21057	2.86790	1.75380
C	-2.05331	2.84131	-1.11374
H	-2.84346	2.64158	-0.38242
H	-2.11141	3.89894	-1.40374
H	-2.27280	2.23534	-1.99957
C	0.49523	2.25669	-2.86589

Frequencies

21.0600	33.7471	43.4017
59.0822	76.6690	81.6615
84.2892	95.3306	100.5417
106.7825	117.1470	121.0116
137.6476	142.9207	149.5028
152.5925	159.1690	169.8884
184.7294	201.2578	207.3761
211.5672	218.4531	225.9389
230.1074	237.7014	244.7480
257.3906	263.6032	268.2277
276.3404	286.9720	305.1066
313.3393	321.6549	329.2075
333.0640	347.6185	370.4230
373.3087	385.6452	402.5573
413.2698	434.1066	445.7118
458.7948	481.0342	499.4317
502.9285	533.9865	537.1687
538.5612	542.4743	555.3004
567.5770	589.8533	595.5364
601.7262	607.7158	619.1292
626.0199	666.9880	676.8730
758.2027	765.6245	766.1471
774.1926	806.7707	818.2850
822.0220	859.1919	865.3192
876.0169	892.2524	952.6699
957.6405	959.4790	973.9472
977.8677	986.8847	1029.9120
1032.8362	1041.6897	1042.7574
1045.7582	1049.7075	1053.2239
1060.4056	1091.0818	1092.5436
1094.5836	1111.8106	1112.9165
1118.1292	1143.5525	1169.5956
1181.6950	1187.7428	1189.3326
1202.0243	1262.1572	1267.3238
1313.4313	1348.4048	1374.3937
1376.7151	1378.0166	1382.1134
1388.0169	1394.6763	1401.1068
1408.4013	1410.2887	1432.2167
1437.3075	1444.3444	1448.9242
1449.1830	1454.4104	1458.8678
1461.4355	1463.6637	1467.3257
1473.3923	1474.7443	1475.2889
1480.3772	1485.8599	1493.7920
1504.4804	1510.9001	1518.3384

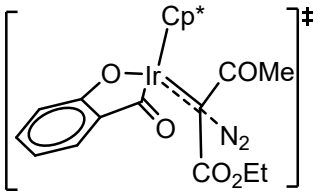
H	0.30667	3.24734	-3.30118	1519.0681	1522.5375	1582.3979
H	1.44993	1.88923	-3.25439	1616.3121	1660.9740	1740.7822
H	-0.28733	1.57943	-3.22852	1854.0698	1898.3945	2259.7636
C	-1.58156	-0.18778	1.25396	3027.1515	3029.6220	3032.2922
O	-1.39068	-0.50301	-1.39398	3039.4128	3039.9470	3051.8441
O	-1.48729	-0.17395	2.47477	3053.0241	3071.6599	3103.4180
O	2.63335	-1.09181	-1.59729	3103.6337	3113.9919	3120.2654
C	4.70197	-1.15550	0.12877	3122.0442	3123.7372	3130.2096
H	5.22162	-0.66620	0.95893	3135.8376	3140.6250	3141.3629
H	4.76788	-0.51995	-0.76043	3143.0404	3145.2502	3153.2363
O	3.32568	-1.22534	0.55144	3156.2184	3171.5862	3181.1620
C	5.23656	-2.53913	-0.14208	3191.2545	3196.7370	3202.1625
H	4.70472	-2.99914	-0.98106			
H	6.29943	-2.49025	-0.39995			
H	5.12610	-3.17939	0.73892			
C	-0.79366	-3.28475	0.36342			
H	-1.63014	-3.57605	-0.27860			
H	-0.33118	-4.20125	0.75134			
H	-1.17930	-2.70089	1.20152			
H	-1.60493	-2.14965	4.22902			
Ir	1.06614	-0.33518	-0.31907			
H	-1.75239	0.62648	0.33798			
C	-3.38056	-0.40976	-0.65861			
C	-4.28232	0.51666	-0.11329			
C	-3.88073	-1.44938	-1.47227			
C	-5.64238	0.43691	-0.35231			
H	-3.87904	1.31567	0.50901			
C	-5.25399	-1.52911	-1.70883			
C	-6.12101	-0.59710	-1.15552			
H	-6.32438	1.16466	0.07673			
H	-5.63954	-2.33280	-2.33587			
H	-7.18654	-0.68124	-1.35624			
O	-3.02148	-2.33912	-1.99749			
H	-3.51662	-2.99637	-2.50049			

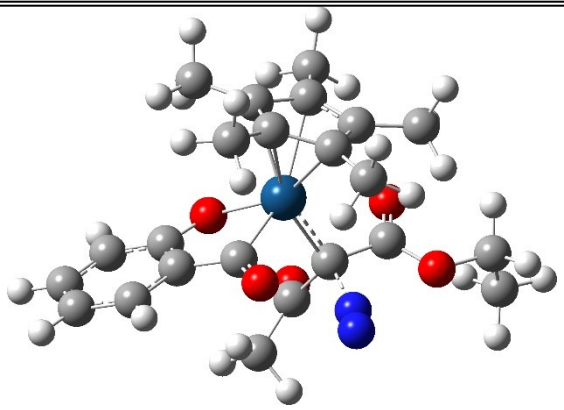
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.461151 Electronic Energy = -1482.11200971
Internal Energy (E)= -1481.61818971 Enthalpy (H)= -1481.61724571
Gibbs Free Energy (G)=-1481.71265471 Gibbs Free Energy of Solvation=-1482.93223842

St.Pt.	General Structure	Ball & Stick model

TS-5A





Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.88254	2.51139	0.52458
C	0.43802	2.27857	1.05521
C	1.35076	2.20252	-0.07214
C	0.60098	2.28760	-1.27584
C	-0.79269	2.43086	-0.90037
C	-2.66524	-0.87864	0.53503
Ir	-0.14699	0.44978	-0.05224
C	-2.46904	-1.03965	-0.85512
C	-3.49988	-1.63636	-1.61159
C	-3.84721	-1.30057	1.15881
C	-4.66465	-2.03173	-0.98050
C	-4.85471	-1.86951	0.40326
H	-3.94030	-1.16866	2.23538
H	-5.78266	-2.19334	0.86757
H	-5.45599	-2.48735	-1.57393
H	-3.35103	-1.77588	-2.67958
C	1.10653	-1.17428	0.05260
C	2.54516	-0.92544	-0.32988
C	0.59473	-2.46242	-0.62013
O	0.97215	-2.71427	-1.73798
N	1.18594	-1.54129	1.65894
N	0.90503	-1.45177	2.73798
C	2.83402	2.16581	0.04315
H	3.29906	1.76768	-0.86331
H	3.21891	3.18045	0.20871
H	3.16064	1.55303	0.89219
C	0.79863	2.28541	2.50119
H	1.80819	1.88850	2.65824
H	0.76805	3.29748	2.92628
H	0.10736	1.64941	3.06864
C	-2.10184	2.77290	1.33900
H	-2.06673	2.22493	2.28630
H	-2.18561	3.84294	1.56952
H	-3.01447	2.47031	0.81422
C	-1.91767	2.51761	-1.87173
H	-2.88858	2.42595	-1.37464
H	-1.89854	3.47423	-2.40924
H	-1.84780	1.71006	-2.60967
C	1.11542	2.23978	-2.67278
H	1.29160	3.24699	-3.07539

Frequencies

-406.2881	33.1976	36.2252
40.2585	58.0581	73.6964
84.6705	88.2114	101.1761
108.9350	118.8533	127.6333
136.7210	142.7227	145.8577
151.9946	171.1844	179.4424
185.6951	192.7917	203.5537
205.5448	221.1938	226.4721
229.1707	233.6912	238.7243
247.8004	256.1284	264.1308
266.8661	280.4115	286.8752
291.0814	296.8022	308.6201
316.1617	319.4512	329.9280
342.5102	358.8468	377.8200
401.8443	409.5265	415.1575
428.5488	435.3686	443.6902
480.5247	507.4253	534.3979
540.1587	541.8406	549.1093
564.6993	570.6738	589.3022
591.7130	601.4871	609.1775
624.5211	661.3057	673.2572
708.2319	747.7614	762.2591
765.1758	799.8081	813.5128
815.1294	858.5430	865.1094
877.7168	887.8854	899.1641
950.5668	952.8835	956.7803
969.0307	975.9346	1006.8921
1035.5488	1041.4364	1043.5021
1045.1792	1049.4754	1051.4912
1056.2587	1085.9030	1089.4858
1093.6688	1110.4244	1113.7482
1119.4477	1144.9938	1179.9677
1182.6374	1186.6478	1201.4841
1207.7652	1267.3393	1278.6695
1315.7693	1347.1313	1378.9814
1381.5144	1382.5854	1385.7437
1389.8100	1397.2183	1399.7253
1406.4575	1414.2765	1441.9590
1444.4419	1450.2703	1454.4043
1454.9616	1457.3605	1460.2529
1463.5356	1466.0717	1467.6223
1470.2368	1473.1141	1479.9313
1480.1056	1484.7727	1487.4858
1492.3237	1499.4371	1509.1142
1517.0306	1521.6517	1547.1297

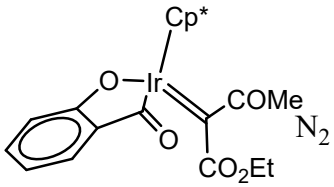
H	2.05055	1.67451	-2.73381	1614.9391	1660.9124	1731.5516
H	0.39798	1.73965	-3.33270	1837.8838	1877.8333	2265.4697
C	-1.50920	-0.33009	1.24712	3028.4144	3032.3077	3035.9123
O	-1.33259	-0.67678	-1.39523	3036.3069	3038.7763	3047.3945
O	-1.40701	-0.28079	2.46628	3055.1572	3075.0802	3107.0931
O	2.85949	-0.57164	-1.43752	3109.7230	3115.0836	3115.4334
C	4.80858	-1.00178	0.34043	3119.7607	3126.5530	3133.5551
H	5.29608	-0.78152	1.29476	3139.2385	3142.2411	3143.2938
H	4.92919	-0.14433	-0.33020	3146.5988	3150.2669	3161.7155
O	3.41275	-1.14221	0.67327	3171.7103	3174.2864	3181.0540
C	5.33292	-2.26837	-0.28839	3183.2872	3198.2653	3203.3735
H	4.83061	-2.45756	-1.24196			
H	6.40726	-2.17787	-0.47908			
H	5.17256	-3.12607	0.37262			
C	-0.32585	-3.36935	0.14655			
H	-0.85931	-3.99306	-0.57459			
H	0.27224	-4.02458	0.79339			
H	-1.04764	-2.83706	0.77308			
H	-1.60493	-2.14965	4.22902			
Ir	1.06614	-0.33518	-0.31907			
H	-1.75239	0.62648	0.33798			
C	-3.38056	-0.40976	-0.65861			
C	-4.28232	0.51666	-0.11329			
C	-3.88073	-1.44938	-1.47227			
C	-5.64238	0.43691	-0.35231			
H	-3.87904	1.31567	0.50901			
C	-5.25399	-1.52911	-1.70883			
C	-6.12101	-0.59710	-1.15552			
H	-6.32438	1.16466	0.07673			
H	-5.63954	-2.33280	-2.33587			
H	-7.18654	-0.68124	-1.35624			
O	-3.02148	-2.33912	-1.99749			
H	-3.51662	-2.99637	-2.50049			

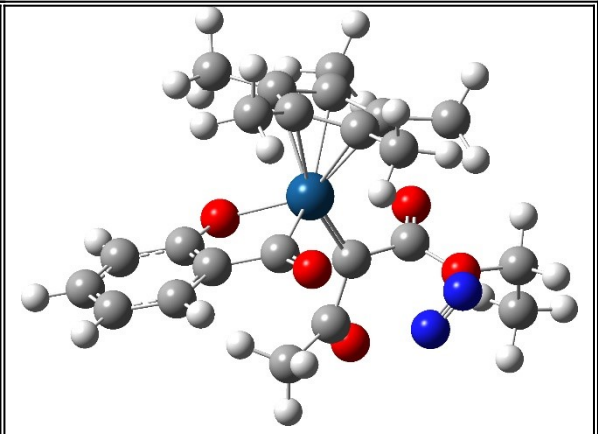
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.459126 Electronic Energy = -1482.10456030
Internal Energy (E)= -1481.6129093 Enthalpy (H)= -1481.6119653
Gibbs Free Energy (G)=-1481.7063383 Gibbs Free Energy of Solvation=-1482.92175086

St.Pt.	General Structure	Ball & Stick model

VI-1A





Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.19843	2.26442	0.73011
C	0.08697	2.03453	1.34587
C	1.10081	2.19999	0.32785
C	0.44021	2.52278	-0.90721
C	-0.97185	2.54177	-0.65170
C	-2.58472	-1.15821	0.44832
Ir	-0.17672	0.38158	-0.14111
C	-2.59742	-0.92115	-0.93830
C	-3.72199	-1.32724	-1.68267
C	-3.65115	-1.80179	1.08881
C	-4.77055	-1.95438	-1.03385
C	-4.74982	-2.19755	0.34976
H	-3.58648	-1.97268	2.16141
H	-5.59074	-2.69183	0.82884
H	-5.63457	-2.27078	-1.61576
H	-3.73378	-1.15241	-2.75548
C	1.12627	-0.95329	-0.49858
C	2.55429	-0.55042	-0.70312
C	0.99153	-2.40394	-0.87489
O	1.85435	-2.86685	-1.60582
N	1.55570	-1.96420	2.73418
N	1.98230	-1.05920	3.20310
C	2.56839	2.26343	0.57900
H	3.13748	2.07118	-0.33603
H	2.84147	3.25910	0.95183
H	2.88235	1.52806	1.32972
C	0.32416	1.85336	2.80541
H	1.39360	1.81378	3.03283
H	-0.10868	2.69119	3.36641
H	-0.13195	0.92404	3.16613
C	-2.50649	2.26432	1.44709
H	-2.46360	1.63131	2.33995
H	-2.77858	3.27854	1.76732
H	-3.31802	1.88252	0.81780
C	-2.01917	2.74089	-1.69005
H	-3.00862	2.45640	-1.31930
H	-2.06175	3.78949	-2.00928
H	-1.81205	2.12036	-2.56942
C	1.10790	2.80473	-2.20732
H	1.48730	3.83533	-2.23600

Frequencies

28.0312	45.6353	49.2787
58.7207	64.5846	81.6042
81.8076	95.8969	100.3461
106.9527	112.2438	126.3521
137.7107	144.8851	147.0569
155.5978	157.9459	162.3309
165.5779	177.2892	178.1968
184.5961	191.9687	196.3478
199.6785	217.8602	231.1888
238.5820	247.7208	259.6876
263.0844	276.2404	296.4705
301.6673	304.3796	312.9875
319.1313	322.3723	333.5463
353.3167	356.5731	360.6405
373.7619	389.5600	401.5038
424.7526	432.1348	458.3085
476.4102	490.8312	531.1299
539.5613	541.1442	550.2710
568.9257	579.7993	590.9778
600.1854	603.7469	626.7316
644.4911	670.6856	680.6179
736.3746	754.2317	758.5172
769.1941	812.7267	815.9757
817.2886	858.4135	861.0819
881.4906	888.5856	950.3014
956.0298	959.0043	962.2208
981.8622	1010.6251	1023.7681
1032.1492	1035.8592	1041.5030
1043.7075	1047.7125	1050.8874
1053.6311	1084.4382	1090.5408
1111.8534	1112.4911	1117.3549
1128.0007	1149.0700	1177.8319
1185.9804	1190.1569	1204.3479
1245.5977	1264.4979	1291.1551
1324.4635	1341.9443	1376.9401
1380.8446	1384.8388	1387.2416
1390.7016	1393.2451	1395.6669
1404.7549	1419.8582	1436.6760
1438.7802	1442.5738	1443.8862
1453.9256	1457.2532	1462.1949
1464.1267	1467.0139	1469.5671
1477.2904	1478.5522	1481.4781
1485.2156	1487.8491	1488.4251
1493.8846	1501.1933	1510.8163

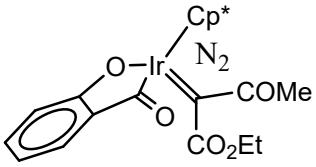
H	1.94876	2.12126	-2.36956	1514.5322	1524.1082	1532.2203
H	0.41016	2.68444	-3.04193	1624.2392	1660.1349	1777.0023
C	-1.37576	-0.71512	1.14696	1795.2841	1820.7440	2466.3705
O	-1.55626	-0.35849	-1.50824	3035.8459	3037.1273	3041.5567
O	-1.16399	-0.86842	2.33022	3041.9289	3044.0837	3053.5509
O	2.94733	0.12127	-1.63225	3057.0916	3065.6424	3116.5759
C	4.75601	-0.83174	0.10467	3117.2098	3119.8553	3122.9165
H	5.16669	-0.90171	1.11654	3125.6652	3127.4197	3137.9829
H	4.94357	0.17475	-0.28709	3145.0340	3145.1078	3146.4989
O	3.33814	-1.01182	0.27818	3151.4154	3155.6001	3159.1372
C	5.31066	-1.89607	-0.80942	3169.9501	3171.0664	3171.5824
H	4.90408	-1.78628	-1.81905	3190.9190	3203.0741	3206.9298
H	6.40174	-1.81897	-0.86399			
H	5.04818	-2.89235	-0.43993			
C	-0.14463	-3.24058	-0.37972			
H	-1.07484	-2.95602	-0.88450			
H	0.07527	-4.28728	-0.60147			
H	-0.30384	-3.10739	0.69612			
H	-1.60493	-2.14965	4.22902			
Ir	1.06614	-0.33518	-0.31907			
H	-1.75239	0.62648	0.33798			
C	-3.38056	-0.40976	-0.65861			
C	-4.28232	0.51666	-0.11329			
C	-3.88073	-1.44938	-1.47227			
C	-5.64238	0.43691	-0.35231			
H	-3.87904	1.31567	0.50901			
C	-5.25399	-1.52911	-1.70883			
C	-6.12101	-0.59710	-1.15552			
H	-6.32438	1.16466	0.07673			
H	-5.63954	-2.33280	-2.33587			
H	-7.18654	-0.68124	-1.35624			
O	-3.02148	-2.33912	-1.99749			
H	-3.51662	-2.99637	-2.50049			

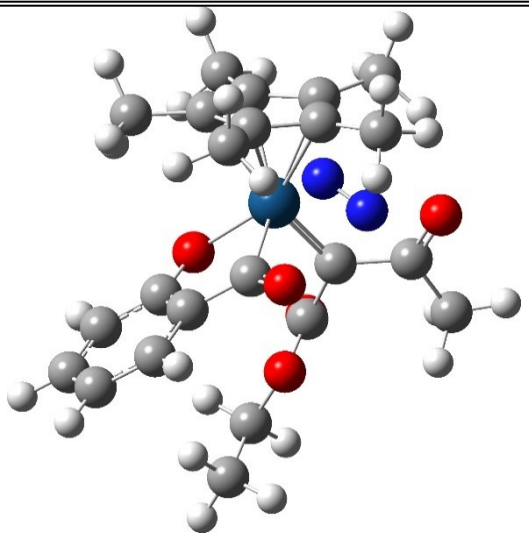
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.459950 Electronic Energy = -1482.15533580
Internal Energy (E)= -1481.6617658 Enthalpy (H)= -1481.6608218
Gibbs Free Energy (G)=-1481.7579488 Gibbs Free Energy of Solvation=-1482.97032634

St.Pt.	General Structure	Ball & Stick model

VI'-1A





Cartesian co-ordinate

Atoms	X	Y	Z
C	1.40660	-2.39486	-0.53404
C	2.27180	-1.32740	-1.00393
C	2.76877	-0.63268	0.15034
C	2.11982	-1.19854	1.31345
C	1.30495	-2.30268	0.87532
C	-2.22798	-1.11402	-0.45802
Ir	0.54583	-0.27986	0.00309
C	-2.15864	-0.68198	0.88306
C	-3.30473	-0.83535	1.69224
C	-3.40184	-1.66552	-0.99100
C	-4.44853	-1.39752	1.15641
C	-4.51274	-1.81794	-0.18431
H	-3.40561	-1.96586	-2.03682
H	-5.42653	-2.25748	-0.57516
H	-5.32458	-1.51496	1.79209
H	-3.25946	-0.50389	2.72702
C	0.23348	1.53143	-0.48203
C	1.10553	2.36701	-1.36258
C	-0.92269	2.25119	0.12663
C	-3.25105	2.53135	0.18225
H	-3.27253	2.17552	1.22100
H	-3.14819	3.62319	0.21022
C	-4.45433	2.07856	-0.59918
H	-5.36779	2.48721	-0.15497
H	-4.39524	2.41877	-1.63831
H	-4.52777	0.98498	-0.59728
O	-2.09059	1.97117	-0.45627
O	-0.78634	3.02928	1.04674
C	3.83769	0.40046	0.15454
H	3.90851	0.90306	1.12431
H	4.80901	-0.06911	-0.04906
H	3.65692	1.15556	-0.61800
C	2.69694	-1.14206	-2.41752
H	3.19798	-0.18129	-2.55079

Frequencies

-42.8306	-23.6871	24.3706
32.3683	40.7832	50.3152
58.4521	65.3812	80.5939
87.3917	102.0036	108.2722
115.2332	122.3005	127.3993
133.7333	137.0594	145.9494
152.3114	158.7015	167.0974
171.1667	180.2892	186.9837
189.3357	196.5312	209.4970
212.2970	217.7227	229.2541
240.6028	247.3633	257.4827
266.9274	271.7307	284.9682
289.0037	292.4830	297.6530
316.6163	317.6010	328.0172
369.4894	374.0938	395.5872
409.0958	412.3871	429.2227
464.0558	475.8741	535.5765
539.0818	539.7949	551.7352
561.8272	580.8556	584.1392
598.3950	604.3529	621.3699
631.5526	653.9414	666.5036
732.0769	759.9849	765.2603
807.0766	809.7169	810.0065
820.6133	846.9797	862.6757
876.8082	886.4561	930.2553
948.3453	958.3333	963.2800
974.6599	1019.8291	1023.9300
1031.3751	1035.7876	1041.1087
1043.2129	1043.5901	1048.5211
1059.3504	1086.4367	1087.9809
1109.7218	1110.5376	1119.4667
1142.0494	1142.1285	1170.9492
1180.6637	1186.5986	1206.3127
1236.7854	1266.7879	1279.5513
1316.5326	1343.8962	1364.5812
1375.3053	1377.4791	1383.2113
1387.7237	1391.2564	1394.6997
1397.4498	1421.5483	1431.1367
1437.9106	1438.8282	1442.3851

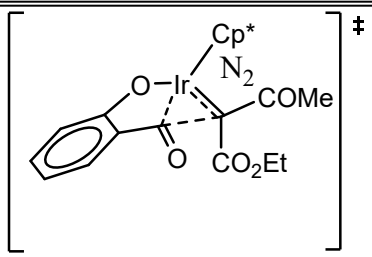
H	3.37243	-1.94939	-2.73151	1445.3216	1447.4841	1451.4813
H	1.82282	-1.14913	-3.07807	1456.8766	1459.2563	1462.3894
C	0.80044	-3.43191	-1.41058	1464.7210	1466.3375	1468.1306
H	0.53243	-3.01764	-2.38673	1472.2749	1482.3678	1486.8779
H	1.51879	-4.24644	-1.57129	1489.9260	1497.4418	1499.5712
H	-0.10615	-3.86219	-0.97144	1511.9151	1517.1029	1552.6910
C	0.46144	-3.12987	1.78229	1618.1850	1657.7555	1770.8050
H	-0.22840	-3.77047	1.22422	1821.6465	1828.6582	2465.5694
H	1.08229	-3.77509	2.41709	3034.6870	3037.4249	3038.0025
H	-0.13780	-2.49055	2.44256	3038.7032	3044.0553	3044.7858
C	2.29916	-0.81260	2.74059	3045.3126	3048.5078	3097.6363
H	2.92690	-1.54028	3.27241	3111.9555	3117.7037	3117.9587
H	2.76253	0.17248	2.84177	3122.6745	3129.4750	3134.9866
H	1.32862	-0.76925	3.24852	3142.0190	3142.1673	3142.6984
C	-1.02665	-0.90789	-1.25680	3149.1838	3163.9195	3166.4995
O	-1.05816	-0.14556	1.34882	3174.2036	3178.8421	3179.5178
O	-0.88960	-1.10623	-2.43693	3186.3767	3196.6739	3204.6018
N	2.24084	3.30904	1.54001			
N	2.32992	2.70467	2.46082			
C	0.69149	3.79270	-1.61721			
H	0.64765	4.35740	-0.68002			
H	1.40003	4.25595	-2.30635			
H	-0.31595	3.82068	-2.05293			
O	2.09856	1.90166	-1.90307			
H	-1.60493	-2.14965	4.22902			
Ir	1.06614	-0.33518	-0.31907			
H	-1.75239	0.62648	0.33798			
C	-3.38056	-0.40976	-0.65861			
C	-4.28232	0.51666	-0.11329			
C	-3.88073	-1.44938	-1.47227			
C	-5.64238	0.43691	-0.35231			
H	-3.87904	1.31567	0.50901			
C	-5.25399	-1.52911	-1.70883			
C	-6.12101	-0.59710	-1.15552			
H	-6.32438	1.16466	0.07673			
H	-5.63954	-2.33280	-2.33587			
H	-7.18654	-0.68124	-1.35624			
O	-3.02148	-2.33912	-1.99749			
H	-3.51662	-2.99637	-2.50049			

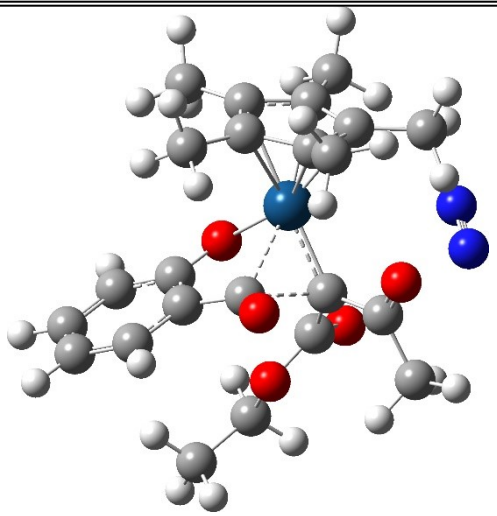
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.456606 Electronic Energy = -1482.16011681
Internal Energy (E)= -1481.66997981 Enthalpy (H)= -1481.66903581
Gibbs Free Energy (G)=-1481.76731481 Gibbs Free Energy of Solvation=-1482.97918586

St.Pt.	General Structure	Ball & Stick model

TS-6A





Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.66722	-2.15707	0.56558
C	-2.32292	-0.99202	1.15814
C	-2.88683	-0.22301	0.09775
C	-2.53756	-0.88528	-1.15415
C	-1.84519	-2.10912	-0.84005
C	2.03409	-1.04834	0.67411
Ir	-0.70644	-0.25657	-0.16118
C	1.97130	-1.09532	-0.74230
C	3.03328	-1.72725	-1.42475
C	3.09590	-1.63674	1.37681
C	4.07040	-2.30196	-0.71393
C	4.11405	-2.26896	0.69073
H	3.09346	-1.57259	2.46295
H	4.93755	-2.73500	1.22478
H	4.87247	-2.79704	-1.25918
H	3.00003	-1.75413	-2.51130
C	0.24819	1.34104	0.41364
C	-0.26643	2.23668	1.49041
C	1.32077	1.92719	-0.45613
C	3.61765	2.05074	-0.94390
H	3.40478	1.62501	-1.93401
H	3.60682	3.14266	-1.04810
C	4.90801	1.53462	-0.36498
H	5.75062	1.81676	-1.00450
H	5.07954	1.95057	0.63341
H	4.88555	0.44166	-0.28211
O	2.56604	1.65518	-0.05006
O	1.06769	2.64644	-1.39729
C	-3.71733	1.00144	0.25782
H	-3.85026	1.52641	-0.69362
H	-4.71460	0.74116	0.63591
H	-3.24989	1.69091	0.97101
C	-2.47819	-0.76033	2.61978
H	-3.04392	0.15210	2.81715
H	-3.00156	-1.61011	3.07760
H	-1.50586	-0.64099	3.10853
C	-0.95249	-3.20936	1.34016

Frequencies

-253.5910	-100.1113	33.3010
36.0907	49.1167	56.6910
79.6683	88.4806	90.6722
93.5775	98.9754	100.9239
111.9843	118.2653	123.8773
134.5307	139.2509	151.6981
159.4533	164.7969	167.7695
177.4192	179.6663	195.1765
202.3899	215.7729	223.4796
230.3061	236.0879	243.4707
247.2506	258.9213	282.7912
290.4765	299.4287	305.4860
314.5274	317.4774	320.8251
328.1096	356.0855	360.4947
380.6048	392.7605	399.4849
410.9347	419.6852	446.4920
458.1337	468.2061	526.7610
535.7414	542.4206	548.1323
555.6978	559.7568	580.7189
591.0881	597.2764	608.0271
616.4501	640.8050	683.2689
723.0976	754.7360	767.4792
799.2835	809.1232	810.2546
818.5773	820.9161	861.2414
875.1778	889.3430	932.8747
957.5790	964.5660	972.8329
982.1556	1022.4781	1028.1358
1032.7043	1033.6350	1038.2119
1041.1512	1043.4635	1044.9025
1047.8725	1093.1233	1095.5352
1108.9906	1113.1813	1118.5022
1137.0665	1145.6109	1180.6760
1183.8416	1186.7690	1199.8456
1240.5002	1260.4190	1291.8354
1306.7510	1345.9091	1371.8501
1376.4130	1379.4511	1380.9751
1390.3267	1393.5467	1394.4156
1401.4496	1419.2956	1429.1289
1437.9661	1440.5978	1447.3752
1451.1233	1456.2016	1457.8778
1458.1322	1459.8772	1464.8658

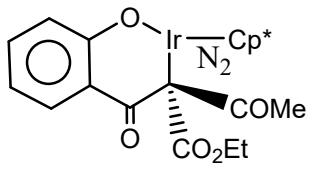
H	-0.63307	-2.82695	2.31430	1472.7670	1474.9366	1477.4117
H	-1.60445	-4.07478	1.51629	1481.5926	1486.3260	1493.0364
H	-0.05824	-3.55897	0.81258	1499.4776	1514.1015	1517.1449
C	-1.26506	-3.04214	-1.84492	1522.1142	1532.9635	1553.4895
H	-0.53631	-3.71871	-1.38722	1609.6051	1660.2344	1775.9316
H	-2.04514	-3.65246	-2.31700	1827.3603	1843.7514	2468.5217
H	-0.74333	-2.48794	-2.63409	3036.1499	3038.4437	3038.7445
C	-2.93515	-0.44932	-2.52066	3040.0755	3040.5383	3041.0847
H	-3.90041	-0.88975	-2.80591	3041.7286	3046.4009	3095.4862
H	-3.02939	0.63950	-2.58728	3118.2873	3118.6204	3120.3454
H	-2.19234	-0.75952	-3.26289	3120.7705	3124.0564	3131.1401
C	0.99534	-0.32364	1.39204	3139.7867	3140.8249	3140.8622
O	0.97744	-0.55141	-1.39532	3151.2131	3151.7290	3156.0015
O	0.82966	-0.24709	2.57910	3169.6759	3171.7895	3176.2120
N	-1.78088	3.64820	-1.02772	3189.6289	3200.1149	3205.5520
N	-2.17239	3.17939	-1.94849			
C	0.44769	3.54164	1.72250			
H	0.48508	4.13987	0.80498			
H	-0.06207	4.10002	2.50996			
H	1.48492	3.34404	2.02279			
O	-1.22272	1.91066	2.17577			
H	-1.60493	-2.14965	4.22902			
Ir	1.06614	-0.33518	-0.31907			
H	-1.75239	0.62648	0.33798			
C	-3.38056	-0.40976	-0.65861			
C	-4.28232	0.51666	-0.11329			
C	-3.88073	-1.44938	-1.47227			
C	-5.64238	0.43691	-0.35231			
H	-3.87904	1.31567	0.50901			
C	-5.25399	-1.52911	-1.70883			
C	-6.12101	-0.59710	-1.15552			
H	-6.32438	1.16466	0.07673			
H	-5.63954	-2.33280	-2.33587			
H	-7.18654	-0.68124	-1.35624			
O	-3.02148	-2.33912	-1.99749			
H	-3.51662	-2.99637	-2.50049			

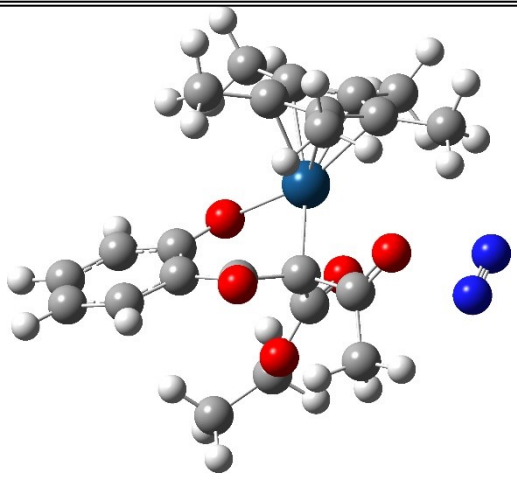
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.457899 Electronic Energy = -1482.14232105
Internal Energy (E)= -1481.65156905 Enthalpy (H)= -1481.65062605
Gibbs Free Energy (G)=-1481.74632805 Gibbs Free Energy of Solvation=-1482.96108879

St.Pt.	General Structure	Ball & Stick model

VII-1A





Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.32683	-2.17580	0.62696
C	-2.05518	-1.10938	1.28687
C	-2.84827	-0.44630	0.29157
C	-2.66708	-1.16493	-0.96605
C	-1.77534	-2.24637	-0.75935
C	2.48208	-0.49172	0.91371
Ir	-0.71449	-0.35593	-0.22708
C	2.25048	-1.07066	-0.36068
C	3.28661	-1.84253	-0.93004
C	3.68324	-0.74851	1.58793
C	4.47572	-2.05334	-0.25462
C	4.68522	-1.51258	1.01864
H	3.80215	-0.30528	2.57481
H	5.61816	-1.68736	1.54801
H	5.25137	-2.65942	-0.72031
H	3.10365	-2.27931	-1.91003
C	0.49398	1.11043	0.73840
C	-0.22693	2.18198	1.56198
C	0.85656	1.61061	-0.61082
C	2.52325	2.13948	-2.19960
H	2.04274	1.33196	-2.76304
H	2.17964	3.09634	-2.61019
C	4.02256	2.01516	-2.17149
H	4.42409	2.06004	-3.18870
H	4.47455	2.82181	-1.58585
H	4.31341	1.05785	-1.72372
O	2.07535	2.04759	-0.82671
O	-0.01738	1.52547	-1.49111
C	-3.83475	0.64088	0.53407
H	-4.07760	1.17496	-0.39034
H	-4.77103	0.22915	0.93452
H	-3.43705	1.36662	1.24877
C	-1.98013	-0.80892	2.74254
H	-2.44819	0.14916	2.97536
H	-2.47923	-1.60413	3.31194
H	-0.93925	-0.74812	3.08428
C	-0.39087	-3.12927	1.28159
H	0.12853	-2.65253	2.11993

Frequencies

32.9226	45.9883	52.1026
60.8856	69.4049	79.0231
85.4475	93.3594	100.2119
112.5803	115.3773	121.2333
129.3164	136.4440	144.3268
153.6977	169.2125	172.9024
173.7195	179.0331	181.9636
183.4226	193.3201	205.7237
209.2869	212.8617	219.1870
237.9086	240.9467	253.0480
263.8302	265.2256	277.6383
287.6441	291.2347	304.1437
308.0246	312.8177	321.6370
330.4828	358.6962	391.8000
401.8250	410.8301	420.8034
426.4884	445.1245	483.1059
499.4335	528.7436	538.0116
540.3095	542.7468	554.1090
558.1760	578.0268	588.2995
598.5206	611.8683	629.3832
654.8196	669.1315	729.1341
746.5298	761.1292	801.1565
811.7403	816.8622	817.8821
838.1501	858.3966	865.9204
882.0066	897.4200	959.4946
959.6428	972.2318	977.1009
996.9524	1018.4816	1036.9169
1040.2503	1044.9077	1046.3106
1052.2219	1053.9895	1061.5660
1085.5421	1093.9717	1101.5570
1116.9253	1125.6886	1131.7584
1151.6478	1164.2441	1181.1484
1183.9682	1191.3685	1212.3251
1255.2874	1283.6706	1291.6956
1344.2801	1352.4005	1367.4741
1377.2336	1378.2702	1382.5596
1392.8887	1398.2412	1398.6898
1404.7825	1428.0976	1437.9359
1443.6063	1444.7076	1445.2042
1448.0603	1451.7064	1456.9313
1458.0177	1460.6540	1462.2759
1468.7267	1474.8250	1476.2498

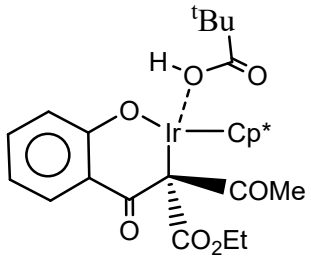
H	-0.92990	-4.00549	1.66613	1478.6779	1488.4282	1492.0952
H	0.37019	-3.47856	0.57533	1504.5597	1509.4774	1516.5770
C	-1.22240	-3.19606	-1.76241	1522.5321	1544.7114	1555.5251
H	-0.13024	-3.09230	-1.81790	1612.7688	1662.5418	1678.4588
H	-1.45437	-4.23409	-1.49283	1734.7546	1846.6699	2465.2595
H	-1.62586	-3.00986	-2.76202	3026.4063	3035.1635	3036.6532
C	-3.28410	-0.74486	-2.25371	3038.7577	3040.5319	3045.4371
H	-4.35104	-1.00100	-2.27801	3047.8080	3057.1623	3102.4564
H	-3.19921	0.34038	-2.38632	3113.6734	3113.7583	3115.6172
H	-2.79729	-1.22256	-3.10884	3118.2748	3130.8814	3136.4239
C	1.51683	0.40944	1.57153	3139.8381	3141.1537	3144.0716
O	1.13023	-0.94451	-1.04373	3145.4625	3149.4030	3168.7409
O	1.50818	0.57357	2.79135	3172.0694	3173.7483	3183.4953
N	-1.92067	3.64607	-0.64067	3187.5824	3189.6272	3202.4203
N	-2.73715	3.18200	-1.22292			
C	0.58601	3.41429	1.84261			
H	0.91038	3.87719	0.90185			
H	-0.00656	4.12688	2.42052			
H	1.48656	3.13246	2.39935			
O	-1.36416	2.06523	1.96140			
H	-1.60493	-2.14965	4.22902			
Ir	1.06614	-0.33518	-0.31907			
H	-1.75239	0.62648	0.33798			
C	-3.38056	-0.40976	-0.65861			
C	-4.28232	0.51666	-0.11329			
C	-3.88073	-1.44938	-1.47227			
C	-5.64238	0.43691	-0.35231			
H	-3.87904	1.31567	0.50901			
C	-5.25399	-1.52911	-1.70883			
C	-6.12101	-0.59710	-1.15552			
H	-6.32438	1.16466	0.07673			
H	-5.63954	-2.33280	-2.33587			
H	-7.18654	-0.68124	-1.35624			
O	-3.02148	-2.33912	-1.99749			
H	-3.51662	-2.99637	-2.50049			

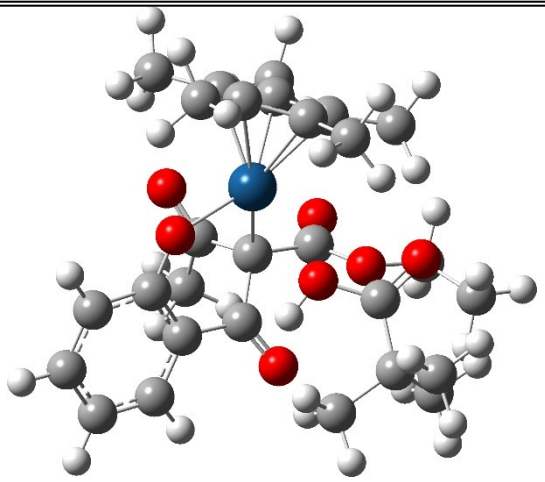
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.460870 Electronic Energy = -1482.18057354
Internal Energy (E)= -1481.68625754 Enthalpy (H)= -1481.68531354
Gibbs Free Energy (G)=-1481.78190754 Gibbs Free Energy of Solvation=-1482.99273624

St.Pt.	General Structure	Ball & Stick model

VII'-1A





Cartesian co-ordinate

Atoms	X	Y	Z
C	-2.60729	-0.30363	-1.97467
C	-1.87526	-1.50863	-1.76791
C	-2.03982	-1.93757	-0.38547
C	-2.87172	-0.97586	0.27112
C	-3.16516	0.07995	-0.69446
O	1.40877	-0.33037	-1.31351
C	2.29693	-1.34983	-1.22253
O	1.88375	-2.48303	-1.20476
C	3.78609	-1.00493	-1.21651
C	0.43540	2.66790	-0.56910
H	1.83866	0.54051	-1.27845
C	-1.05686	-2.24011	-2.76818
H	-0.13135	-2.61189	-2.31430
H	-1.61984	-3.09962	-3.15632
H	-0.78461	-1.60052	-3.61345
C	-1.52676	-3.21494	0.17790
H	-2.08119	-4.07047	-0.22976
H	-0.46346	-3.35026	-0.05441
H	-1.63927	-3.22761	1.26692
C	-3.98605	1.28938	-0.42928
H	-3.80797	2.05423	-1.19173
H	-5.05514	1.03814	-0.43475
H	-3.72522	1.71527	0.54499
C	-2.67582	0.51734	-3.21469
H	-2.08960	0.06718	-4.02135
H	-3.70992	0.61651	-3.56703
H	-2.27745	1.52393	-3.03659
C	-3.43067	-1.05997	1.64386
H	-4.35264	-1.65643	1.62761
H	-2.72858	-1.52131	2.34335
H	-3.66405	-0.06554	2.03191
Ir	-1.07379	0.01767	-0.39230
C	4.38248	-1.66730	-2.46326
H	3.98031	-1.22654	-3.38454
H	5.47004	-1.52601	-2.46880
H	4.16769	-2.74055	-2.47195
C	4.08092	0.49267	-1.22858
H	3.73362	0.97975	-0.30821

Frequencies

24.5292	41.6572	51.9283
63.1790	70.1069	74.2288
84.5747	88.6479	98.6768
102.3586	107.1075	114.5796
124.0636	133.2972	135.9009
137.8007	141.9224	150.9620
155.6876	161.8620	167.7159
174.2866	176.2305	188.3813
188.7501	198.7297	213.6105
222.9102	231.4393	240.5303
248.6516	249.5914	255.9153
260.2246	266.3550	274.1767
282.6026	285.9378	298.2980
301.0337	306.7761	309.1161
315.7370	328.9717	341.9788
345.8123	364.8196	370.9779
380.1096	389.7340	393.3131
396.3517	416.1437	426.4432
439.5374	444.6911	448.6299
455.9749	468.5219	494.8612
515.7713	531.9065	535.6083
540.9749	542.6156	551.0848
552.2782	576.6549	583.5532
592.6480	594.5482	606.5665
632.0201	652.0069	693.4734
721.0860	757.9443	766.4267
771.2210	772.6932	787.0270
812.6909	815.4355	819.6433
857.7892	873.0222	879.2186
885.6776	902.6585	919.1582
947.8066	952.5251	961.2206
964.3508	970.9058	978.4283
983.5973	994.4335	1011.5085
1020.6912	1034.0177	1034.8100
1043.5617	1046.1488	1046.2551
1047.4295	1056.4343	1062.9844
1096.9979	1098.1112	1104.6304
1114.0476	1115.8109	1137.7809
1138.7289	1146.2899	1153.0985
1173.9671	1185.8903	1188.0512
1191.9548	1222.1836	1232.5543
1241.5530	1268.4052	1271.9805

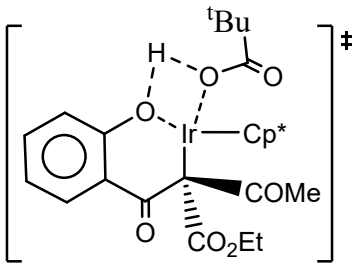
H	5.16534	0.64265	-1.28253	1288.0929	1304.9133	1335.4136
H	3.65486	1.00284	-2.10520	1344.7749	1372.7810	1377.5186
C	4.38987	-1.62833	0.04380	1380.3291	1383.9123	1384.4754
H	3.95116	-1.18200	0.94561	1387.6863	1390.2396	1392.9569
H	4.21634	-2.70947	0.05835	1397.8983	1407.8641	1415.1368
H	5.47175	-1.44686	0.05676	1426.0863	1432.4243	1433.7016
O	-0.45821	1.85120	-1.07787	1440.6213	1442.6149	1449.1382
C	1.35416	2.32790	0.45783	1452.5751	1454.9932	1458.7040
C	2.35405	3.24784	0.82612	1463.4618	1464.8998	1468.2943
C	0.55067	3.94974	-1.15579	1468.9439	1473.2367	1476.4231
C	2.44861	4.49420	0.24182	1477.9675	1483.2466	1483.7285
C	1.52732	4.83824	-0.75699	1485.6730	1491.8547	1494.0367
C	1.32141	1.04920	1.20857	1499.6088	1502.6485	1506.3627
O	2.35734	0.59283	1.68261	1511.6186	1521.8473	1537.2391
H	-0.15546	4.19820	-1.94469	1541.2430	1551.6237	1608.3311
H	1.58293	5.81688	-1.23066	1665.9593	1745.7567	1783.4384
H	3.21554	5.19742	0.55496	1832.4248	1871.5961	3022.2178
H	3.04641	2.93782	1.60761	3033.9884	3034.4021	3035.8905
C	-0.03206	0.42800	1.45869	3039.3357	3039.6411	3042.9925
C	-0.84586	1.41966	2.32686	3045.8807	3046.1321	3058.4824
C	0.03392	-0.85229	2.22671	3061.6777	3107.4978	3109.3453
C	1.02868	-2.95202	2.50635	3113.2610	3119.8115	3120.0440
H	0.07331	-3.49258	2.53106	3123.1785	3126.3289	3135.2464
H	1.25356	-2.66374	3.54018	3136.1742	3138.0684	3138.9486
C	2.12489	-3.78231	1.89547	3142.0708	3144.4882	3146.7023
H	2.19730	-4.74454	2.41336	3148.2778	3148.6826	3157.6860
H	1.93529	-3.96450	0.83162	3163.9246	3164.6751	3172.1972
H	3.08996	-3.27367	1.98308	3177.6457	3184.2329	3189.1691
O	0.87486	-1.76478	1.71599	3198.0426	3205.3057	3759.6760
O	-0.64598	-1.07940	3.21403			
O	-1.98777	1.74505	2.07936			
C	-0.12379	1.98076	3.52396			
H	-0.84497	2.42988	4.20998			
H	0.46360	1.21125	4.03331			
H	0.57311	2.75865	3.18474			

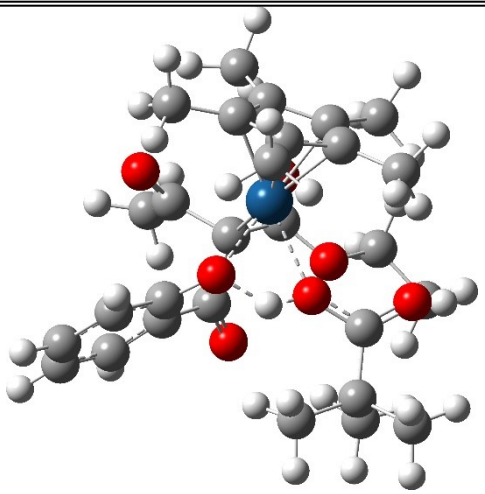
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.603275 Electronic Energy = -1719.55036718
Internal Energy (E)= -1718.90807518 Enthalpy (H)= -1718.90713118
Gibbs Free Energy (G)=-1719.01395018 Gibbs Free Energy of Solvation=-1720.41498918

St.Pt.	General Structure	Ball & Stick model

TS-7A





Cartesian co-ordinate

Atoms	X	Y	Z
C	-2.17627	-1.19446	-1.98761
C	-1.40387	-2.26771	-1.47764
C	-1.63449	-2.36414	-0.03897
C	-2.63229	-1.38238	0.31332
C	-2.90176	-0.59845	-0.86884
O	1.33238	-0.26604	-0.99174
C	2.47605	-0.94660	-1.07735
O	2.49930	-2.14391	-0.89514
C	3.72777	-0.11256	-1.33646
C	-0.07009	2.60189	-0.90244
H	0.98629	0.68646	-1.40249
C	-0.43419	-3.11914	-2.21548
H	0.53443	-3.13529	-1.70080
H	-0.80761	-4.14950	-2.28078
H	-0.26821	-2.75393	-3.23324
C	-1.06818	-3.41872	0.84453
H	-1.62608	-4.35935	0.74272
H	-0.02138	-3.61626	0.58210
H	-1.10235	-3.10702	1.89456
C	-3.83855	0.55118	-0.97818
H	-3.48241	1.26714	-1.72807
H	-4.83652	0.20919	-1.28319
H	-3.90912	1.08781	-0.02858
C	-2.19647	-0.67727	-3.38257
H	-1.34104	-1.04444	-3.95804
H	-3.11243	-0.98243	-3.90443
H	-2.15104	0.41727	-3.39283
C	-3.30250	-1.26859	1.63486
H	-4.02171	-2.09102	1.74405
H	-2.57961	-1.33518	2.45479
H	-3.84016	-0.32290	1.73231
Ir	-0.82649	-0.41500	-0.39656
C	4.59272	-0.84463	-2.36014
H	4.10912	-0.87703	-3.34480
H	5.55288	-0.32619	-2.47296
H	4.78522	-1.87310	-2.03991
C	3.41827	1.30327	-1.81392
H	2.88817	1.88548	-1.04853

Frequencies

-913.6295	-124.5750	-120.5385
28.1771	37.5527	38.3347
49.6200	65.1903	71.9455
76.2990	82.8660	90.3160
102.9983	105.7637	115.5011
117.7794	122.1947	126.9955
131.1749	133.6267	143.4092
149.1105	152.4253	160.1335
164.0605	182.2332	183.9067
195.3021	201.1863	206.4329
213.2327	217.3853	224.1447
238.8509	244.5397	251.0218
261.8928	266.9112	289.6281
294.0021	297.5075	300.7371
313.0966	319.8889	320.6903
337.2441	352.0940	367.4983
377.0914	380.2506	387.0538
401.8053	406.1322	412.9386
422.1966	428.1959	436.1814
443.2336	462.3076	491.4458
523.1559	534.8124	536.4730
549.3352	552.6602	559.7218
569.1636	578.1639	588.8285
596.4607	602.9434	610.6794
639.4447	648.7846	686.3567
726.7045	766.3116	775.3723
776.4384	793.4700	805.1068
808.5230	812.9273	826.5911
860.5303	873.2008	884.5467
891.4115	909.9073	938.8078
946.8176	949.9677	952.8088
957.9544	965.4606	975.3739
977.0200	989.3014	1011.8820
1026.4976	1030.8006	1032.3057
1036.4793	1043.1955	1046.8108
1049.4766	1052.8617	1057.7117
1088.2311	1090.9003	1101.4088
1111.1766	1111.8102	1131.6553
1146.9828	1155.7015	1169.9770
1173.6754	1183.7475	1187.6620
1194.1334	1221.9041	1235.8314
1242.4493	1265.6373	1283.2669

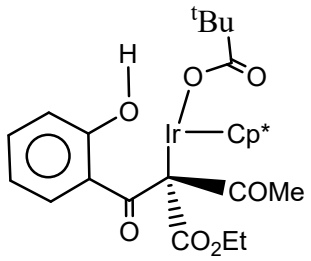
H	4.35839	1.82719	-2.02418	1286.9966	1311.0586	1322.6255
H	2.82606	1.30987	-2.73897	1347.9226	1365.8555	1371.8102
C	4.45910	-0.04355	0.01113	1372.6533	1379.1990	1379.7229
H	3.81986	0.39548	0.78832	1380.7849	1383.3328	1391.3399
H	4.76418	-1.04533	0.33430	1395.5398	1401.4843	1410.6769
H	5.35668	0.57905	-0.09322	1420.7597	1429.3414	1429.9191
O	-0.16115	1.39455	-1.48986	1436.0075	1438.1529	1444.2880
C	0.54397	2.75582	0.35331	1446.3674	1446.9488	1451.1186
C	0.76902	4.04040	0.85782	1455.2948	1456.9962	1457.4809
C	-0.50063	3.73504	-1.59765	1460.5160	1466.5181	1467.2042
C	0.34052	5.16208	0.16396	1470.5324	1472.6373	1481.3010
C	-0.30426	5.00042	-1.06234	1482.8213	1484.2339	1486.5049
C	0.92552	1.60144	1.21012	1490.0528	1500.9777	1503.7263
O	1.97993	1.61480	1.82544	1508.1967	1512.8140	1514.4062
H	-0.96740	3.59220	-2.56997	1534.5388	1552.8945	1631.2222
H	-0.64627	5.87356	-1.61440	1663.9219	1770.0113	1779.8303
H	0.49930	6.15561	0.57506	1828.0218	1832.8426	2106.6288
H	1.26881	4.13153	1.82084	3025.3419	3027.4648	3033.4730
C	-0.15120	0.54840	1.43353	3034.0259	3035.4267	3036.7551
C	-1.28921	1.33608	2.11131	3037.3677	3037.7948	3041.3052
C	0.27696	-0.59537	2.29844	3049.4141	3049.7436	3095.4305
C	1.89556	-2.22248	2.78321	3105.9829	3111.1842	3111.7740
H	1.18278	-3.04709	2.65203	3115.6402	3115.7085	3117.5804
H	1.85933	-1.93472	3.84115	3121.4701	3126.1882	3128.4507
C	3.28303	-2.60350	2.34229	3135.3519	3136.6997	3137.7044
H	3.63301	-3.46617	2.91914	3139.6039	3139.6919	3143.2232
H	3.29503	-2.86056	1.27703	3145.3410	3149.0648	3160.6949
H	3.98025	-1.77503	2.50746	3166.7533	3168.3420	3173.9330
O	1.47162	-1.10788	1.98621	3181.3004	3189.6393	3201.3907
O	-0.42561	-1.08254	3.17292			
O	-2.30740	1.65452	1.53151			
C	-1.04872	1.77833	3.53195			
H	-1.65928	2.65917	3.74460			
H	-1.34522	0.96226	4.19961			
H	0.01034	1.98164	3.72842			

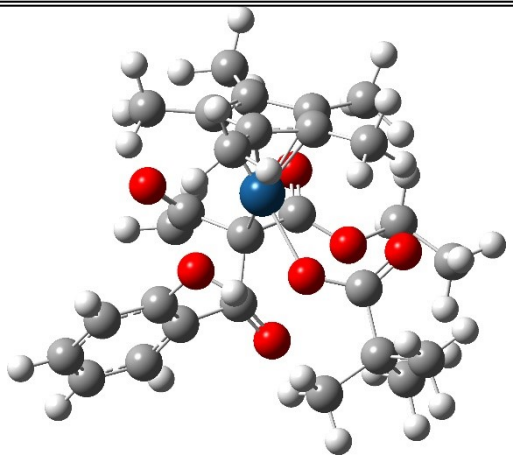
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.595881 Electronic Energy = -1719.54118318
Internal Energy (E)= -1718.90713818 Enthalpy (H)= -1718.90619418
Gibbs Free Energy (G)=-1719.01262818 Gibbs Free Energy of Solvation=-1720.40677711

St.Pt.	General Structure	Ball & Stick model

VIII-1A





Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.15583	-2.65519	-1.69809
C	1.14545	-2.55463	-1.14854
C	1.01994	-2.58621	0.30616
C	-0.37639	-2.84149	0.62838
C	-1.10673	-2.79828	-0.59707
O	0.90114	0.78859	-1.12692
C	2.16302	1.10884	-1.02211
O	3.02653	0.39958	-0.52401
C	2.50527	2.50055	-1.57369
C	-2.38680	1.41345	-1.09983
H	-0.66258	0.97583	-1.85729
C	2.42058	-2.40259	-1.89587
H	3.12501	-1.77907	-1.34061
H	2.87262	-3.38825	-2.06970
H	2.26021	-1.92867	-2.87030
C	2.14867	-2.59701	1.27246
H	2.58249	-3.60330	1.34912
H	2.93251	-1.90139	0.95430
H	1.80427	-2.29370	2.26790
C	-2.57472	-2.96204	-0.76992
H	-2.93986	-2.35227	-1.60380
H	-2.81849	-4.01014	-0.99009
H	-3.11654	-2.64554	0.12392
C	-0.53415	-2.60494	-3.13616
H	0.29614	-2.25590	-3.75723
H	-0.82964	-3.59931	-3.49588
H	-1.38171	-1.92994	-3.29883
C	-0.89814	-3.17653	1.97866
H	-0.63683	-4.21671	2.21570
H	-0.46315	-2.53300	2.75028
H	-1.98473	-3.07776	2.02587
Ir	-0.08686	-0.89920	-0.33530
C	3.61686	2.33456	-2.60938
H	3.26627	1.77165	-3.48522
H	3.96039	3.31725	-2.95804
H	4.46738	1.79842	-2.17579
C	1.30589	3.20643	-2.19617
H	0.51604	3.37615	-1.45347
H	1.61656	4.18534	-2.58449

Frequencies

37.9373	48.6949	58.3627
66.4677	73.5183	79.0521
86.1137	93.6694	100.5565
112.6316	114.8491	120.4616
126.7216	131.0284	136.0008
138.7447	144.6350	147.7879
154.1177	159.0827	167.0211
173.0165	177.6009	189.0136
199.7838	203.8885	205.8347
215.6621	219.3462	230.1049
233.7686	242.0851	252.8145
268.2971	272.5069	275.9035
291.1526	300.5601	306.9284
307.6344	315.8161	323.7750
336.5021	339.4050	346.0905
366.7456	370.8555	375.1094
384.5681	390.7996	400.9277
406.7933	416.9944	421.6374
425.7715	429.7604	443.5448
468.5070	473.2441	504.4156
530.8618	537.7933	541.0229
549.1485	557.6960	566.3032
576.9312	582.0462	584.2001
593.2176	602.6416	629.2158
646.4817	679.3152	716.0283
754.6580	778.0629	789.7875
794.4101	804.4319	806.2914
812.4207	820.0064	824.4932
854.4635	874.8023	885.0001
889.0608	913.3776	926.0993
946.0349	952.8075	957.3732
960.8350	966.7360	976.9296
988.0538	989.7705	1019.1567
1023.4307	1030.6672	1033.9886
1041.6882	1042.3685	1050.6793
1052.0148	1053.9465	1065.2409
1091.8209	1097.1984	1099.3840
1113.9222	1115.5560	1136.4964
1152.0246	1165.9449	1174.7157
1185.4752	1190.1099	1200.2817
1234.5205	1237.9694	1244.1857
1257.2037	1267.4887	1288.8215
1290.8308	1322.7155	1349.9277

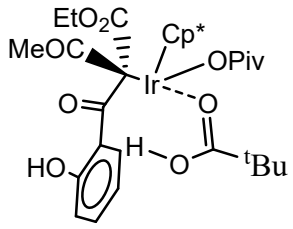
H	0.88807	2.63515	-3.03562	1367.1910	1368.9303	1374.5544
C	3.01538	3.32928	-0.39179	1375.1854	1376.8311	1382.8422
H	2.26039	3.37390	0.40426	1385.1149	1387.8688	1390.0028
H	3.93013	2.89096	0.02121	1396.1373	1399.1590	1415.7313
H	3.23853	4.35212	-0.72313	1424.2816	1428.4195	1434.3586
O	-1.51587	0.51096	-1.68262	1438.7433	1443.6480	1451.2076
C	-2.00435	2.14097	0.02879	1452.6171	1454.8728	1457.6792
C	-2.87298	3.12345	0.50941	1460.7534	1463.1894	1466.1619
C	-3.62551	1.60470	-1.69343	1468.9903	1470.3934	1472.4658
C	-4.11645	3.32498	-0.07544	1477.2749	1483.0020	1484.3206
C	-4.49768	2.55199	-1.16845	1486.8535	1489.5112	1491.4865
C	-0.75680	1.87770	0.82415	1496.9994	1500.6748	1516.4327
O	-0.05377	2.81446	1.15356	1520.8073	1529.0540	1536.1157
H	-3.87892	1.01956	-2.57390	1543.8613	1557.3942	1644.6733
H	-5.47147	2.69948	-1.62931	1679.1265	1768.4045	1777.1267
H	-4.78996	4.07911	0.32337	1792.7084	1831.3031	3022.2333
H	-2.55739	3.71038	1.37000	3025.7154	3029.7735	3037.3487
C	-0.59557	0.45294	1.31287	3038.3990	3038.7761	3039.0772
C	-1.94710	0.07193	1.94279	3040.0445	3048.8036	3051.4424
C	0.49699	0.23850	2.31225	3053.7290	3103.7178	3104.4377
C	2.70886	0.62479	2.97115	3106.9641	3115.3880	3115.6314
H	2.90563	-0.45432	2.99553	3120.0700	3120.2311	3123.4512
H	2.39178	0.91492	3.98086	3126.2218	3131.0467	3137.8403
C	3.91192	1.39364	2.49907	3141.1055	3141.9896	3146.0561
H	4.76522	1.18748	3.15407	3147.8381	3156.9805	3165.8067
H	4.16254	1.09857	1.47448	3166.4686	3168.7038	3176.5492
H	3.71818	2.47122	2.51425	3180.3491	3185.6826	3186.8672
O	1.63220	0.88379	2.05777	3198.5236	3205.6986	3453.2357
O	0.37725	-0.52181	3.26454			
O	-2.74818	-0.66389	1.40270			
C	-2.28109	0.72330	3.26229			
H	-3.36626	0.81155	3.35829			
H	-1.89863	0.08419	4.06492			
H	-1.80125	1.70256	3.37723			

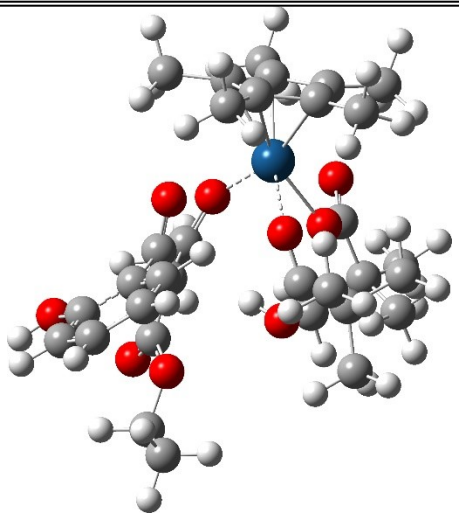
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.604079 Electronic Energy = -1719.55421561
Internal Energy (E)= -1718.91154561 Enthalpy (H)= -1718.91060161
Gibbs Free Energy (G)=-1719.01583961 Gibbs Free Energy of Solvation=-1720.4144679

St.Pt.	General Structure	Ball & Stick model

VIII'-1





Cartesian co-ordinate

Atoms	X	Y	Z
H	1.13122	1.21312	0.29858
C	-2.16797	-2.55799	-1.13049
C	-1.84210	-2.80565	0.23678
C	-2.71810	-1.99656	1.07596
C	-3.60262	-1.26000	0.21091
C	-3.23426	-1.56182	-1.16431
C	-2.34916	2.17556	-0.27196
O	-1.57873	1.33007	0.34659
O	-3.25660	1.88593	-1.04637
C	-1.97122	3.64362	-0.01954
O	0.09651	-0.47710	1.53411
C	0.65242	0.52160	1.98992
O	1.20157	1.45681	1.25439
C	0.74738	0.75176	3.48727
C	-4.69406	-0.34362	0.62996
H	-5.64317	-0.89275	0.68798
H	-4.49033	0.08917	1.61524
H	-4.79361	0.48217	-0.08011
C	-3.89513	-1.00076	-2.37112
H	-4.88416	-1.45468	-2.51673
H	-4.00534	0.08331	-2.25773
H	-3.29765	-1.18606	-3.26809
C	-2.74100	-2.02368	2.56205
H	-1.72487	-1.97803	2.96867
H	-3.30146	-1.17471	2.96637
H	-3.21226	-2.94507	2.92828
C	-0.76231	-3.69586	0.73872
H	-0.43518	-3.38545	1.73656
H	-1.11866	-4.73205	0.80289
H	0.11221	-3.65195	0.08298
C	-1.48953	-3.14401	-2.31546
H	-0.44850	-3.38404	-2.08482
H	-2.00602	-4.05428	-2.64540
H	-1.47781	-2.43429	-3.14839
C	-0.68191	1.02768	3.96859
H	-0.68583	1.15646	5.05800
H	-1.08305	1.93986	3.51029

Frequencies

24.2498	30.7022	40.5669
50.2810	57.8804	59.8815
66.2967	71.6045	78.5479
85.8127	88.5451	94.6319
102.2510	110.1574	111.9561
118.8459	122.6341	126.1375
135.0109	141.6511	145.3428
151.1605	163.3822	166.7267
169.8357	176.8207	178.8205
187.7841	191.7137	194.5725
199.8072	203.4460	205.9884
214.0899	215.0569	219.3205
224.0405	232.6327	234.6693
242.2564	246.1531	249.7244
257.8478	265.7738	281.1248
289.5508	293.1813	298.1664
301.6302	304.3131	309.8967
313.1264	314.4471	315.2098
327.5453	329.5162	341.0388
342.5621	344.5464	350.8829
353.7725	378.6590	380.7488
387.6831	389.2842	400.4232
406.0534	411.8104	420.8206
428.4833	434.3732	443.2857
447.0509	450.3944	480.0197
503.6306	532.7124	535.5458
536.6632	539.9077	544.8822
555.2393	571.2058	578.7734
586.8186	593.6626	598.6106
601.1843	618.0827	626.6793
631.9589	672.0249	721.1028
764.8173	772.7286	780.2318
787.6851	792.5138	796.7469
803.6106	808.1546	808.3428
819.0851	829.5886	850.4316
856.7847	881.8832	899.0566
905.8172	911.8160	942.3374
949.1434	949.3922	950.8744
954.4546	956.2716	958.4908
965.6236	970.0740	979.9316
1009.4131	1016.0840	1031.3626

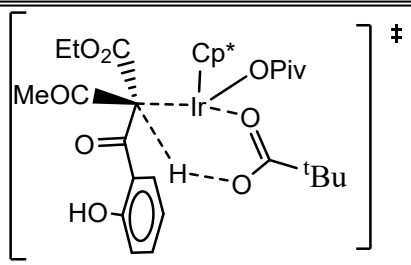
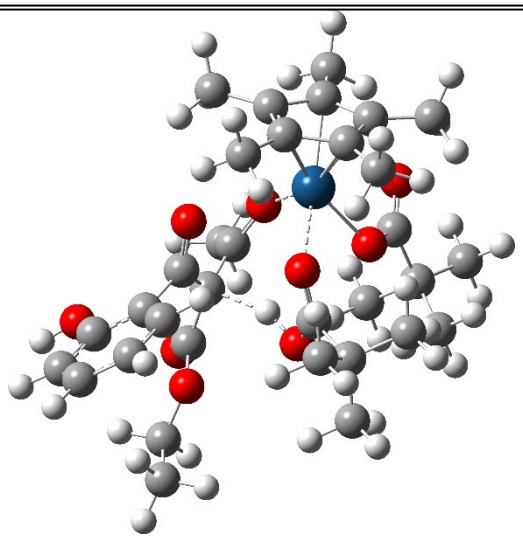
H	-1.34857	0.19796	3.70902	1034.9084	1035.2086	1038.0412
C	1.65013	1.92874	3.83764	1041.7788	1043.0583	1044.3758
H	1.68707	2.04588	4.92783	1048.3684	1051.3948	1051.8168
H	2.67217	1.77305	3.47430	1056.8596	1075.6770	1093.3636
H	1.27745	2.86362	3.40515	1096.2453	1105.9179	1108.3851
C	1.28137	-0.52949	4.13104	1131.1469	1146.9312	1157.1720
H	0.65013	-1.39179	3.88848	1177.2999	1179.1109	1184.4417
H	2.30188	-0.74577	3.78848	1187.8072	1195.5169	1235.9170
H	1.30721	-0.41262	5.22125	1239.1133	1242.7904	1247.7581
C	-3.16175	4.54390	-0.32614	1267.5440	1271.4182	1284.4001
H	-3.99623	4.33953	0.35619	1294.7925	1310.0666	1316.6870
H	-2.87830	5.59837	-0.21078	1327.8658	1335.0777	1363.1211
H	-3.52296	4.38386	-1.34612	1366.6886	1372.9996	1373.6394
C	-0.82890	3.94907	-0.99471	1375.8222	1378.5323	1380.9138
H	-0.50149	4.99170	-0.88850	1383.6332	1384.8127	1386.3262
H	0.03712	3.29877	-0.80612	1389.7800	1396.0892	1403.4049
H	-1.15548	3.79417	-2.03103	1412.5221	1415.8660	1418.3857
C	-1.49739	3.87720	1.41200	1422.6237	1428.6194	1432.0673
H	-1.25392	4.93856	1.55557	1435.8241	1443.0391	1445.5804
H	-2.28108	3.61492	2.13587	1447.9552	1449.4855	1450.7072
H	-0.60352	3.28527	1.63817	1455.9405	1458.4955	1459.4045
Ir	-1.58208	-0.69805	-0.19296	1460.9495	1461.1944	1465.2680
C	1.62546	0.42885	-1.57356	1467.6021	1468.1117	1473.1088
C	1.82287	-0.88535	-0.98785	1473.6727	1476.0896	1478.3637
O	0.92639	-1.73798	-0.92496	1479.1358	1480.6833	1483.7192
C	3.15046	-1.31246	-0.41837	1487.4562	1490.7698	1491.1240
C	4.35657	-1.29482	-1.12896	1494.9079	1497.1890	1498.5010
C	3.14656	-1.84189	0.87030	1512.4132	1515.0409	1523.5085
C	5.52949	-1.75753	-0.53815	1524.7456	1535.9521	1543.3415
C	4.31762	-2.28631	1.47728	1576.7750	1655.7973	1671.1145
H	2.19179	-1.88782	1.39486	1703.0401	1763.0719	1766.2786
C	5.51151	-2.24132	0.76687	1831.0632	3024.4186	3027.7325
H	6.45912	-1.74074	-1.10808	3031.7375	3032.7874	3034.0314
H	4.29463	-2.67630	2.49215	3034.1528	3037.3527	3039.3541
H	6.43572	-2.59416	1.21910	3040.9988	3042.4847	3044.5766
O	4.33166	-0.81863	-2.40056	3045.1183	3046.6950	3058.5953
H	5.22114	-0.83249	-2.76934	3085.8928	3101.0654	3111.9040
C	0.40237	0.69806	-2.26795	3114.2589	3117.5762	3119.8589
C	2.74075	1.38186	-1.72137	3120.1695	3121.2721	3121.6133
C	4.70919	2.13835	-0.65194	3127.6689	3128.5541	3129.9321
H	4.47650	3.19915	-0.81128	3134.3386	3134.8044	3137.0870
H	5.30044	1.80936	-1.51918	3139.9645	3142.8339	3145.1914
C	5.42319	1.89183	0.65252	3147.6561	3148.3812	3149.1518
H	6.37391	2.43394	0.68488	3149.7323	3153.8492	3157.8536
H	4.80583	2.22398	1.49423	3158.3142	3160.7464	3162.0953
H	5.62302	0.82070	0.78040	3167.4983	3181.3668	3193.8419
O	3.50130	1.38732	-0.60050	3203.8185	3450.6212	3897.8361
O	2.96786	2.13459	-2.64676			
C	0.35189	1.65471	-3.42578			
H	-0.67907	1.70466	-3.78578			
H	0.69885	2.64989	-3.13246			
H	1.03243	1.33403	-4.22061			
O	-0.70647	0.16363	-1.98774			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm

Zero-point correction= 0.752645 Electronic Energy = -2066.37750321

Internal Energy (E)= -2065.57673121	Enthalpy (H)= -2065.57578821
Gibbs Free Energy (G)=-2065.70136221	Gibbs Free Energy of Solvation=-2067.39371733

St.Pt.	General Structure	Ball & Stick model
TS-8		

Cartesian co-ordinate

Atoms	X	Y	Z
H	1.07929	1.00825	0.03746
C	-2.11321	-2.53717	-1.18817
C	-1.78834	-2.84139	0.16620
C	-2.70305	-2.10116	1.03007
C	-3.60945	-1.36041	0.18725
C	-3.21458	-1.57930	-1.19171
C	-2.48912	2.13566	-0.26108
O	-1.73371	1.31602	0.40732
O	-3.35899	1.81620	-1.06619
C	-2.14141	3.61547	-0.03308
O	0.01527	-0.50070	1.45128
C	0.58628	0.52936	1.85969
O	1.11777	1.41165	1.08644
C	0.68447	0.77655	3.35487
C	-4.71528	-0.48165	0.64788
H	-5.66148	-1.03778	0.65888
H	-4.52403	-0.11116	1.66060
H	-4.80962	0.38674	-0.01007
C	-3.86943	-1.01408	-2.39944
H	-4.68851	-1.66084	-2.74032
H	-4.24811	-0.01031	-2.19058
H	-3.14394	-0.91792	-3.21334
C	-2.72379	-2.18273	2.51421
H	-1.70669	-2.12616	2.91799
H	-3.30206	-1.36188	2.95010
H	-3.17064	-3.12796	2.84859
C	-0.68323	-3.71756	0.63845

Frequencies

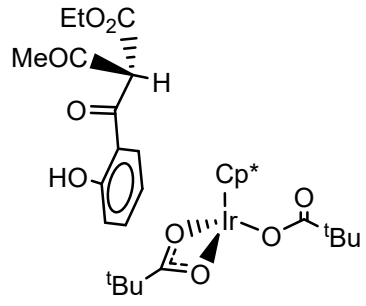
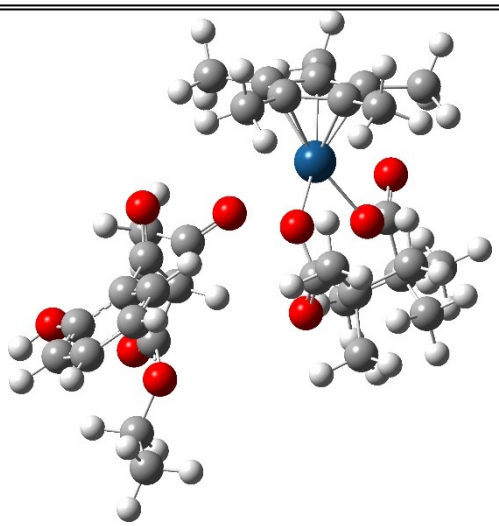
-503.8774	-124.3086	-52.4024
28.3974	32.5365	45.4639
54.8176	58.4007	61.3644
68.3632	69.8057	75.7784
85.0527	86.4374	88.6082
96.1388	101.0903	106.1435
113.2459	116.6663	119.5992
133.7857	141.1487	144.8088
146.8825	156.1957	160.4856
168.6817	176.3357	181.0674
189.2440	194.0885	196.0473
204.3684	207.2024	210.3007
215.5625	222.7016	229.9137
235.8118	236.8986	244.9676
259.9994	262.8677	269.6266
273.7078	279.4782	284.3464
294.5335	301.7473	304.5717
307.1898	313.0570	314.9949
320.5752	327.4219	333.5169
341.9463	342.8372	348.2139
354.8039	359.1784	370.7937
386.9168	391.3406	393.1383
406.6017	410.5799	421.4869
426.2756	434.9698	446.2302
448.6439	457.9229	468.8873
478.9348	527.5910	530.1100
536.3523	537.7733	544.8035
551.6368	569.8256	572.8874
586.7714	589.0640	596.4648
602.5422	608.5777	625.2853
632.4981	665.0499	703.1776

H	-0.35222	-3.41909	1.63898	743.3885	760.8559	777.3636
H	-1.01173	-4.76370	0.68746	790.6881	793.3174	801.6706
H	0.18339	-3.63947	-0.02491	802.6905	807.1166	808.4495
C	-1.43073	-3.06081	-2.39898	818.9859	827.8563	844.5522
H	-0.41020	-3.37522	-2.17144	853.5114	865.9667	899.9436
H	-1.98921	-3.91419	-2.80497	906.0213	912.9294	940.3156
H	-1.36925	-2.29537	-3.17827	944.5224	948.6675	951.5687
C	-0.74942	1.00223	3.84829	954.1501	958.5236	959.7018
H	-0.74386	1.19357	4.92856	960.6411	969.6548	981.9901
H	-1.21192	1.85850	3.34191	992.6839	1018.4064	1030.8869
H	-1.37068	0.12208	3.64889	1031.8805	1036.4310	1037.0452
C	1.55019	1.98855	3.67549	1041.6621	1043.3127	1045.6880
H	1.60058	2.12414	4.76317	1051.3232	1052.0435	1055.6572
H	2.57019	1.86059	3.29625	1056.6276	1071.6851	1092.2291
H	1.14203	2.90416	3.23418	1094.7511	1102.0152	1106.5782
C	1.27404	-0.47466	4.01046	1128.4467	1144.9126	1154.9661
H	0.67343	-1.36293	3.78309	1171.5595	1175.0124	1185.0439
H	2.30008	-0.65572	3.66284	1187.8423	1191.9553	1235.1210
H	1.30321	-0.34338	5.09920	1238.0093	1248.6341	1251.9508
C	-3.35472	4.48375	-0.34250	1271.5670	1274.3511	1278.4544
H	-4.17448	4.28002	0.35790	1282.9662	1292.6971	1312.2778
H	-3.09160	5.54631	-0.25690	1322.2655	1350.3627	1367.0116
H	-3.72657	4.29012	-1.35277	1370.5557	1376.0616	1376.4385
C	-1.01517	3.92710	-1.02548	1376.8194	1378.6717	1379.3185
H	-0.72178	4.98266	-0.95179	1380.8278	1384.2458	1389.1179
H	-0.12755	3.31313	-0.81679	1390.8757	1397.5307	1401.6072
H	-1.34115	3.73081	-2.05501	1407.1711	1411.3354	1415.1793
C	-1.65198	3.88522	1.38569	1419.1539	1420.5978	1427.8257
H	-1.42789	4.95374	1.50615	1429.5344	1432.2859	1439.8375
H	-2.41609	3.61893	2.12851	1444.7413	1446.3307	1447.1508
H	-0.74160	3.31585	1.60355	1451.1466	1454.2502	1455.3639
Ir	-1.59877	-0.70512	-0.14148	1459.9685	1461.7670	1462.4568
C	1.67053	0.50348	-1.41232	1465.9752	1467.9202	1471.5699
C	1.92583	-0.88229	-0.99446	1475.2498	1475.5093	1476.4762
O	1.07972	-1.77253	-1.07597	1478.3796	1480.7634	1483.9547
C	3.24982	-1.28848	-0.40564	1484.6034	1485.4917	1487.3390
C	4.45990	-1.21579	-1.10327	1490.6515	1497.8263	1499.4502
C	3.24171	-1.86385	0.86136	1500.4360	1506.3018	1512.4258
C	5.63785	-1.67142	-0.51880	1538.9648	1541.4030	1547.4796
C	4.41803	-2.30071	1.46453	1551.3991	1623.0774	1657.0579
H	2.28362	-1.95781	1.37293	1671.9875	1747.6293	1756.6687
C	5.61711	-2.20226	0.76843	1766.3081	1836.3744	3017.8264
H	6.57275	-1.61139	-1.07699	3023.6466	3026.9378	3032.4907
H	4.39391	-2.72694	2.46456	3035.7693	3036.7360	3037.7160
H	6.54457	-2.54972	1.21801	3038.8556	3039.6963	3040.9722
O	4.42648	-0.68915	-2.35528	3042.3900	3044.1572	3049.8598
H	5.31550	-0.67326	-2.72507	3057.8039	3090.7659	3100.7130
C	0.46328	0.73871	-2.18291	3101.8572	3110.3823	3110.7892
C	2.78615	1.46868	-1.55078	3112.7897	3120.8218	3123.4722
C	4.78099	2.19473	-0.52669	3124.3566	3126.1642	3127.7620
H	4.52670	3.25456	-0.65310	3129.0889	3129.7002	3133.1893
H	5.35385	1.89580	-1.41701	3139.1770	3140.5466	3141.7095
C	5.53606	1.92931	0.75025	3143.1265	3145.9267	3147.2028
H	6.48855	2.46929	0.75562	3148.6046	3149.1903	3151.7934
H	4.95144	2.25271	1.61767	3155.2271	3155.5977	3163.4043
H	5.73872	0.85671	0.85789	3168.6995	3170.0839	3171.5921
O	3.58563	1.42219	-0.46537	3185.0971	3200.3789	3898.8117
O	2.97243	2.26321	-2.44959			
C	0.45461	1.62214	-3.39437			
H	-0.55281	1.62123	-3.81812			
H	0.75804	2.64063	-3.13443			

H	1.19413	1.27937	-4.12499
O	-0.64664	0.23623	-1.88648

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.745743 Electronic Energy = -2066.36815662
Internal Energy (E)= -2065.57552562 Enthalpy (H)= -2065.57458262
Gibbs Free Energy (G)=-2065.69798962 Gibbs Free Energy of Solvation=-2067.38874485

St.Pt.	General Structure	Ball & Stick model
IX-1		

Cartesian co-ordinate

Atoms	X	Y	Z
H	1.38140	0.82831	-0.26935
C	-2.10996	-2.13511	-1.61642
C	-1.86867	-2.72109	-0.33863
C	-2.83112	-2.14771	0.59447
C	-3.68681	-1.23436	-0.15044
C	-3.22261	-1.20020	-1.50732
C	-2.46357	2.26695	0.05411
O	-1.77498	1.32908	0.63722
O	-3.37829	2.09926	-0.74793
C	-1.94423	3.67138	0.39000
O	0.03033	-0.69323	1.15630
C	0.50468	0.25608	1.91553
O	1.04405	1.28177	1.50729
C	0.36136	0.00595	3.42426
C	-4.81761	-0.45329	0.41525
H	-5.74156	-1.04580	0.39055
H	-4.61632	-0.17711	1.45661
H	-4.95711	0.47586	-0.14360

Frequencies

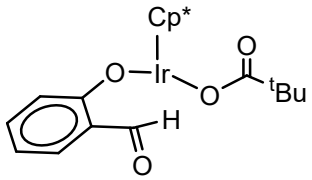
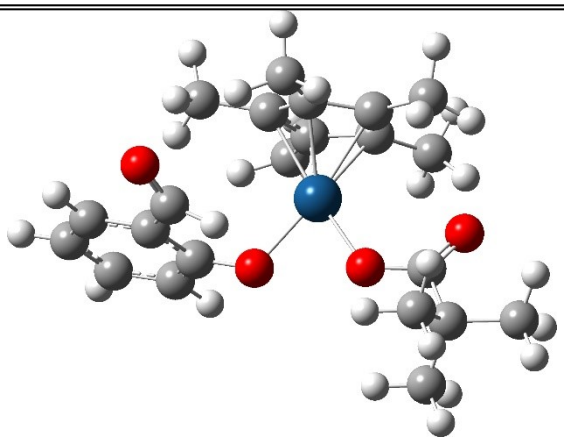
22.4475	31.0056	40.1175
45.2580	49.6974	52.4896
60.6852	66.8374	76.4786
79.1550	84.0113	90.2006
90.8618	99.6766	101.5965
106.8132	109.4689	115.9549
122.0259	139.2662	140.4628
146.7377	150.2664	160.4876
164.3740	167.2100	176.5195
181.9657	187.6955	189.3788
196.0109	198.3424	202.7506
207.1218	214.9296	221.6904
226.7206	228.6454	231.5379
232.1358	234.3435	246.5852
265.0790	276.1401	281.4546
286.4672	289.4792	294.2739
296.8542	303.5509	308.5448
310.8155	313.3661	316.0425
319.1851	330.6762	339.3172
345.0015	363.3923	366.5528
367.8350	375.5360	378.4540
389.2262	390.6645	392.5010

C	-3.81099	-0.40071	-2.61422	401.0155	418.8965	419.6679
H	-4.76422	-0.83492	-2.94289	426.4441	429.9611	438.4607
H	-3.97609	0.62766	-2.27625	442.7908	459.9973	471.8350
H	-3.13887	-0.36805	-3.47720	510.8284	516.9891	536.8028
C	-3.00908	-2.55789	2.01180	538.0824	547.1468	551.9566
H	-2.04616	-2.75062	2.49595	555.6627	568.0170	574.0323
H	-3.52621	-1.78694	2.59148	577.7004	589.9033	596.2010
H	-3.60493	-3.47867	2.06782	599.0752	601.7678	623.4548
C	-0.76880	-3.65450	0.02685	642.0118	667.9102	689.5768
H	-0.38570	-3.40949	1.02440	753.0530	767.3086	790.9120
H	-1.10969	-4.69743	0.03237	797.9121	800.8798	806.6107
H	0.07272	-3.55641	-0.66745	809.4605	811.3282	812.4089
C	-1.37592	-2.41026	-2.87853	818.4704	848.9293	853.3424
H	-0.42694	-2.91815	-2.69651	857.1371	862.4360	902.3495
H	-1.99700	-3.03515	-3.53356	904.2761	915.6400	943.5322
H	-1.15779	-1.47881	-3.41154	945.2133	947.3502	951.0265
C	-1.09906	0.30842	3.77765	956.3648	956.7275	965.8110
H	-1.27180	0.13236	4.84812	971.1537	973.8697	992.9591
H	-1.35197	1.35130	3.55101	1000.8163	1011.2476	1025.8339
H	-1.78113	-0.32877	3.20100	1036.0156	1039.3592	1040.1941
C	1.28545	0.93361	4.20300	1041.4654	1042.2164	1043.8812
H	1.15539	0.77830	5.28249	1045.8953	1048.9470	1052.4554
H	2.33584	0.74103	3.95109	1066.0705	1070.6071	1093.4931
H	1.07904	1.98323	3.97124	1099.2827	1110.7264	1112.2429
C	0.68250	-1.44620	3.77096	1116.5989	1143.6245	1162.5458
H	0.03201	-2.14096	3.22800	1168.1631	1176.6936	1184.5316
H	1.72440	-1.69206	3.52256	1188.8992	1230.8956	1235.2593
H	0.54952	-1.61461	4.84802	1239.2528	1244.9339	1250.6225
C	-3.00588	4.71462	0.06828	1258.7839	1263.6611	1274.1102
H	-3.89656	4.57775	0.69406	1275.1538	1280.1712	1286.4303
H	-2.61035	5.72228	0.25296	1310.4437	1320.9511	1356.1601
H	-3.32274	4.64570	-0.97697	1366.1341	1368.5056	1370.3646
C	-0.71963	3.86990	-0.51385	1373.5773	1375.2847	1376.3494
H	-0.29714	4.87266	-0.36506	1379.2962	1384.3647	1387.4573
H	0.05094	3.12697	-0.27276	1388.0135	1389.7024	1394.9344
H	-0.99434	3.76572	-1.57246	1397.5300	1400.6658	1414.4749
C	-1.51100	3.78076	1.84943	1418.0819	1428.6994	1429.3395
H	-1.15857	4.80029	2.05692	1431.2433	1435.7649	1436.1648
H	-2.34796	3.57263	2.53005	1443.6398	1444.7505	1446.3289
H	-0.69777	3.07938	2.06538	1452.4594	1453.1636	1456.5098
Ir	-1.65369	-0.57476	-0.15076	1461.2382	1461.8303	1462.7417
C	1.77795	0.61040	-1.29125	1464.1938	1470.9285	1471.8346
C	2.13287	-0.87122	-1.20183	1473.5436	1475.7497	1476.9341
O	1.39391	-1.69704	-1.70103	1476.9518	1480.7793	1482.7724
C	3.31200	-1.29787	-0.39298	1488.7275	1488.9072	1490.7079
C	4.61290	-1.13362	-0.87133	1494.2714	1496.3528	1497.4648
C	3.09979	-1.92918	0.82720	1502.4597	1509.5583	1515.2521
C	5.69555	-1.57277	-0.11783	1536.3957	1540.0013	1542.4379
C	4.17990	-2.35729	1.59405	1659.8519	1677.6800	1738.8153
H	2.07171	-2.05536	1.16624	1758.1187	1773.9388	1813.5782
C	5.47363	-2.17627	1.11805	1863.8782	2838.3843	3018.3888
H	6.70834	-1.44603	-0.50070	3021.0664	3023.1597	3024.8510
H	4.01079	-2.83752	2.55464	3029.7777	3030.5034	3033.6703
H	6.32454	-2.51303	1.70552	3036.5111	3039.5816	3044.5422
O	4.74201	-0.54330	-2.09020	3044.9691	3045.3761	3047.8982
H	5.67274	-0.47492	-2.32853	3048.5180	3098.4162	3101.3915
C	0.63389	0.75102	-2.26539	3102.0659	3102.1534	3109.7430
C	2.92715	1.58077	-1.45499	3110.1666	3113.0057	3115.3134
C	4.85170	2.36254	-0.35019	3122.6614	3125.1117	3126.3384
H	4.58554	3.41370	-0.51439	3128.5137	3128.8730	3129.8595
H	5.46963	2.04686	-1.20246	3137.9818	3138.1090	3138.2199

C	5.53081	2.13074	0.97347	3142.0615	3142.6648	3146.7351
H	6.47248	2.68645	1.02514	3149.2178	3152.2288	3155.9342
H	4.88756	2.45610	1.79667	3159.8975	3163.0974	3163.2507
H	5.74242	1.06336	1.11047	3177.2617	3184.4674	3184.5867
O	3.65827	1.57347	-0.34098	3198.9052	3215.5124	3897.6641
O	3.14601	2.29349	-2.40703			
C	0.92000	0.94807	-3.71343			
H	-0.00533	0.88337	-4.29044			
H	1.41585	1.91119	-3.86642			
H	1.63737	0.18240	-4.03787			
O	-0.52197	0.63428	-1.87363			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.750727 Electronic Energy = -2066.37371265
Internal Energy (E)= -2065.57443165 Enthalpy (H)= -2065.57348765
Gibbs Free Energy (G)=-2065.70102765 Gibbs Free Energy of Solvation=-2067.39194675

St.Pt.	General Structure	Ball & Stick model
III-1A’	 **III-1A'**	

Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.37318	1.77808	1.37375
C	0.87165	2.18711	0.75951
C	0.61974	2.35883	-0.63549
C	-0.80076	2.10180	-0.87076
C	-1.42238	1.79697	0.37892
O	1.66512	-1.00014	-0.19123
C	2.93126	-0.66717	-0.25860
O	3.35638	0.46282	-0.45686
C	3.86219	-1.86979	-0.06816
C	-2.87270	-1.63166	0.52633
H	-1.13403	-1.86347	1.82675

Frequencies

21.5850	30.3498	37.8055
48.9443	54.3443	60.2651
83.2318	86.9074	99.1462
108.6688	121.6373	130.5952
140.5421	146.9389	161.5570
165.0680	177.4193	181.3708
197.0403	201.1608	208.9105
224.8878	229.2426	237.2948
243.1618	254.7483	273.1599
276.2543	282.2224	292.5593
310.5394	316.0299	320.0518
336.5727	357.8256	367.5498
374.6668	386.6301	413.2678
426.2471	439.4774	451.8023
460.3225	463.8637	532.0391
534.9724	536.7545	539.0029

C	2.14714	2.41796	1.48825	564.4487	570.8701	577.6278
H	2.08922	3.35518	2.05735	580.4557	602.7043	608.3763
H	2.35151	1.60734	2.19712	642.1536	652.4595	740.6259
H	2.99374	2.46111	0.80217	781.4504	789.4002	804.2495
C	1.61049	2.77560	-1.66096	811.0691	814.4656	832.5698
H	1.74320	3.86517	-1.63865	868.2883	875.6412	915.6093
H	2.57148	2.28761	-1.47232	945.7825	949.3837	950.8991
H	1.28136	2.49943	-2.66766	956.7670	962.1937	975.8032
C	-2.87548	1.58772	0.61841	978.2523	1023.0740	1025.0718
H	-3.06518	0.99364	1.51790	1028.5237	1034.2856	1037.4078
H	-3.37115	2.55865	0.74777	1038.0687	1040.3132	1044.9263
H	-3.35604	1.07179	-0.21961	1047.8412	1090.2146	1097.6082
C	-0.55246	1.46543	2.81556	1106.2524	1110.0960	1148.6876
H	-1.33971	0.72270	2.98484	1188.4233	1189.9852	1200.7115
H	0.37443	1.07823	3.25000	1234.6070	1242.9466	1262.7045
H	-0.82459	2.37647	3.36519	1274.6190	1308.2543	1349.3001
C	-1.48544	2.17511	-2.18821	1364.3418	1374.0706	1375.8490
H	-1.77261	3.20914	-2.41886	1380.1488	1386.1165	1393.7772
H	-0.83265	1.82019	-2.99263	1399.3439	1406.0948	1411.0984
H	-2.39059	1.55808	-2.19912	1421.5410	1425.4670	1434.3725
Ir	0.13247	0.31141	-0.11855	1437.7047	1444.3326	1446.6891
C	3.58787	-2.48527	1.30635	1446.8914	1454.1955	1457.4815
H	2.55599	-2.84297	1.38119	1458.6464	1463.1339	1464.8205
H	4.26394	-3.33320	1.47724	1470.9702	1471.9397	1476.3428
H	3.76033	-1.75495	2.10850	1476.8727	1491.3959	1491.8411
C	3.57084	-2.90192	-1.15956	1498.2010	1500.5180	1502.2039
H	3.75707	-2.48366	-2.15712	1510.0718	1523.7558	1544.0446
H	4.22788	-3.77258	-1.03340	1622.4986	1660.0543	1778.1280
H	2.53045	-3.23892	-1.11738	1802.5600	2925.0446	3023.1599
C	5.31287	-1.41474	-0.15323	3027.4730	3035.9176	3036.4248
H	5.52647	-0.95531	-1.12443	3038.0408	3040.2638	3040.9891
H	5.53978	-0.67027	0.61800	3042.4103	3103.3996	3107.2998
H	5.98322	-2.27325	-0.01710	3113.7615	3119.1349	3121.5238
C	-2.09700	-1.49189	-0.64584	3122.8977	3123.7604	3126.0720
C	-2.75789	-1.44441	-1.88536	3135.9973	3136.2187	3141.2804
C	-4.26831	-1.70311	0.44338	3145.1473	3147.6743	3154.5152
C	-4.14045	-1.53367	-1.94582	3162.4960	3172.9859	3186.9189
C	-4.90868	-1.66293	-0.78248	3191.2477	3200.3369	3203.0339
H	-4.82209	-1.78962	1.37675			
H	-5.99142	-1.73191	-0.84579			
H	-4.63381	-1.49990	-2.91572			
H	-2.15141	-1.33937	-2.78324			
O	-0.77087	-1.40970	-0.58668			
C	-2.22580	-1.65111	1.84116			
O	-2.80887	-1.42994	2.88950			
H	-2.34796	3.57263	2.53005			
H	-0.69777	3.07938	2.06538			
Ir	-1.65369	-0.57476	-0.15076			
C	1.77795	0.61040	-1.29125			
C	2.13287	-0.87122	-1.20183			
O	1.39391	-1.69704	-1.70103			
C	3.31200	-1.29787	-0.39298			
C	4.61290	-1.13362	-0.87133			
C	3.09979	-1.92918	0.82720			
C	5.69555	-1.57277	-0.11783			
C	4.17990	-2.35729	1.59405			
H	2.07171	-2.05536	1.16624			
C	5.47363	-2.17627	1.11805			
H	6.70834	-1.44603	-0.50070			
H	4.01079	-2.83752	2.55464			
H	6.32454	-2.51303	1.70552			

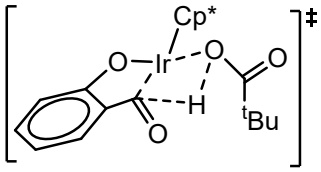
O	4.74201	-0.54330	-2.09020
H	5.67274	-0.47492	-2.32853
C	0.63389	0.75102	-2.26539
C	2.92715	1.58077	-1.45499
C	4.85170	2.36254	-0.35019
H	4.58554	3.41370	-0.51439
H	5.46963	2.04686	-1.20246
C	5.53081	2.13074	0.97347
H	6.47248	2.68645	1.02514
H	4.88756	2.45610	1.79667
H	5.74242	1.06336	1.11047
O	3.65827	1.57347	-0.34098
O	3.14601	2.29349	-2.40703
C	0.92000	0.94807	-3.71343
H	-0.00533	0.88337	-4.29044
H	1.41585	1.91119	-3.86642
H	1.63737	0.18240	-4.03787
O	-0.52197	0.63428	-1.87363

Statistical Thermodynamic Analysis

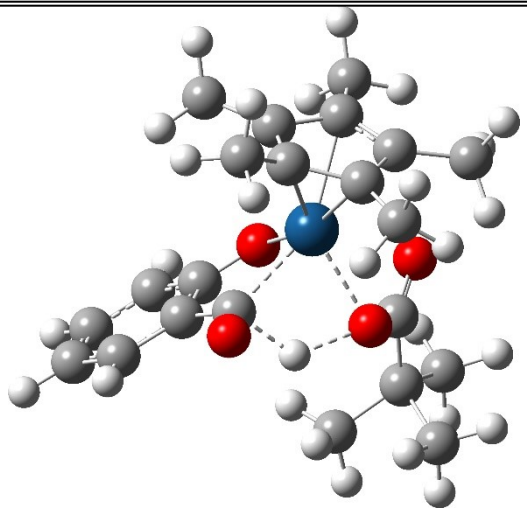
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.462498 Electronic Energy = -1260.66085688
Internal Energy (E)= -1260.16796788 Enthalpy (H)= -1260.16702388
Gibbs Free Energy (G)=-1260.25910088 Gibbs Free Energy of Solvation=-1261.32997517

St.Pt.	General Structure	Ball & Stick model

TS-3A’



TS-3A'



Cartesian co-ordinate

Atoms	X	Y	Z
C	-2.64348	-0.61927	-0.82870
C	-2.40447	-1.42562	0.35634
C	-2.21009	-0.56254	1.47037
C	-2.32603	0.80910	0.98832
C	-2.66444	0.75916	-0.41543
O	0.90889	-1.33180	-0.94624
C	1.51818	-2.04920	0.00915
O	0.94278	-2.42977	1.00621
C	2.98254	-2.34220	-0.29696
C	1.24791	2.17899	-0.52457
H	0.68993	-0.03640	-1.19738
C	-2.27475	-2.90658	0.34711
H	-3.26619	-3.37613	0.30629
H	-1.70815	-3.24049	-0.52899
H	-1.74498	-3.26746	1.23164
C	-1.85976	-0.94107	2.86631
H	-2.69604	-0.74775	3.55056
H	-1.59371	-1.99890	2.93671
H	-0.99292	-0.36827	3.21586
C	-2.97056	1.91340	-1.29903
H	-2.50535	1.79065	-2.28218
H	-4.05616	2.00314	-1.43234
H	-2.59986	2.85303	-0.87789
C	-2.94031	-1.11891	-2.19945
H	-2.53877	-0.43365	-2.95436
H	-2.48300	-2.09880	-2.36993
H	-4.02108	-1.21749	-2.36725
C	-2.20426	2.02402	1.83901
H	-3.14758	2.24534	2.35464
H	-1.42577	1.88298	2.59647
H	-1.92477	2.89944	1.24325
Ir	-0.67671	-0.06345	-0.05136
C	3.13885	-2.88617	-1.71674
H	2.76094	-2.17856	-2.46097
H	4.20032	-3.07399	-1.92363
H	2.60065	-3.83427	-1.84087
C	3.73118	-1.01018	-0.16465

Frequencies

-1368.0821	38.2268	40.5840
48.4325	58.6791	65.9437
99.2104	99.9722	120.3419
128.2405	139.6056	146.8736
151.5197	156.4889	162.4151
171.6865	176.4239	192.3402
197.7951	206.5586	212.4607
215.7771	227.1412	237.6000
240.4266	261.4878	273.3475
286.5085	296.3575	297.1148
303.5987	312.6312	319.8564
328.7242	337.0693	358.6192
384.3959	390.5166	410.9569
420.3946	421.6696	441.7303
449.5321	474.1755	528.2280
535.5930	537.5226	546.5642
553.3072	560.5647	571.5272
586.5100	591.9776	599.9941
603.7390	622.0788	668.3400
752.5205	764.0828	780.7560
797.4399	811.2505	815.5460
846.6782	859.8800	873.9696
900.6495	945.1909	952.2771
955.9089	963.4593	967.8447
972.1564	979.0862	981.0144
1033.7162	1037.1510	1037.5180
1038.3546	1039.2711	1044.6459
1048.0227	1050.9491	1091.3098
1098.9822	1110.4365	1117.6396
1144.7456	1182.2424	1186.7813
1198.4564	1212.3257	1242.0892
1266.1824	1268.1523	1321.2428
1345.2184	1377.3392	1379.1427
1383.2840	1388.4701	1397.3829
1398.6583	1399.8348	1406.6091
1412.4541	1434.2078	1436.8203
1439.1843	1446.5650	1448.0541
1451.4897	1453.9902	1455.9314
1462.8337	1463.4569	1470.9605
1473.9839	1474.4703	1481.5897
1482.8468	1483.5009	1487.7418

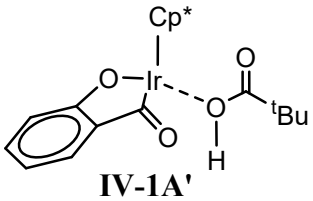
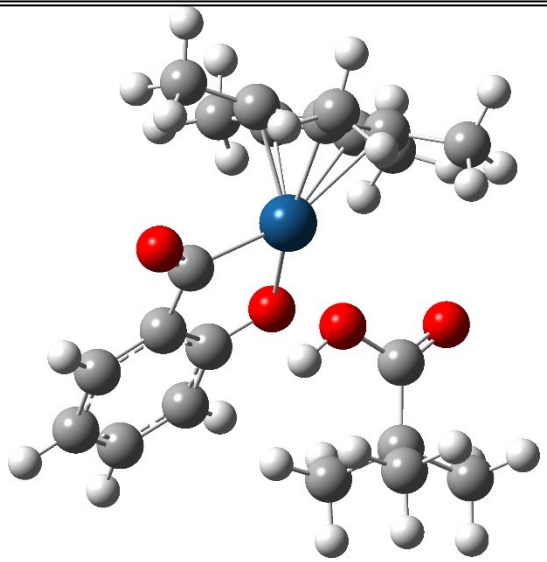
H	3.60670	-0.58522	0.83965	1494.4949	1503.5842	1513.7426
H	4.80291	-1.17031	-0.33902	1519.5122	1527.1883	1543.7332
H	3.37278	-0.27149	-0.89203	1592.7762	1616.1527	1666.3264
C	3.52500	-3.34324	0.71434	1790.9678	1818.8555	3025.2626
H	3.41723	-2.96717	1.73683	3032.5979	3032.9007	3038.4696
H	2.98883	-4.29729	0.65412	3038.6623	3039.0967	3039.8224
H	4.58829	-3.53176	0.51886	3041.0542	3110.2086	3113.9467
C	1.52631	1.63363	0.75358	3114.3049	3117.1156	3119.2433
C	2.49887	2.27963	1.54998	3121.9924	3124.4662	3124.5996
C	1.88964	3.34413	-0.97695	3127.1704	3136.9958	3138.9110
C	3.11787	3.42189	1.08494	3142.6361	3145.1408	3147.1736
C	2.82025	3.97146	-0.17725	3153.8655	3175.8769	3177.5430
H	1.63505	3.71782	-1.96704	3190.3328	3199.8603	3207.1874
H	3.32655	4.87256	-0.51278			
H	3.85913	3.91190	1.71430			
H	2.72949	1.85951	2.52625			
O	0.90787	0.56276	1.17739			
C	0.31292	1.42734	-1.34397			
O	-0.08907	1.72355	-2.45466			
H	-2.34796	3.57263	2.53005			
H	-0.69777	3.07938	2.06538			
Ir	-1.65369	-0.57476	-0.15076			
C	1.77795	0.61040	-1.29125			
C	2.13287	-0.87122	-1.20183			
O	1.39391	-1.69704	-1.70103			
C	3.31200	-1.29787	-0.39298			
C	4.61290	-1.13362	-0.87133			
C	3.09979	-1.92918	0.82720			
C	5.69555	-1.57277	-0.11783			
C	4.17990	-2.35729	1.59405			
H	2.07171	-2.05536	1.16624			
C	5.47363	-2.17627	1.11805			
H	6.70834	-1.44603	-0.50070			
H	4.01079	-2.83752	2.55464			
H	6.32454	-2.51303	1.70552			
O	4.74201	-0.54330	-2.09020			
H	5.67274	-0.47492	-2.32853			
C	0.63389	0.75102	-2.26539			
C	2.92715	1.58077	-1.45499			
C	4.85170	2.36254	-0.35019			
H	4.58554	3.41370	-0.51439			
H	5.46963	2.04686	-1.20246			
C	5.53081	2.13074	0.97347			
H	6.47248	2.68645	1.02514			
H	4.88756	2.45610	1.79667			
H	5.74242	1.06336	1.11047			
O	3.65827	1.57347	-0.34098			
O	3.14601	2.29349	-2.40703			
C	0.92000	0.94807	-3.71343			
H	-0.00533	0.88337	-4.29044			
H	1.41585	1.91119	-3.86642			
H	1.63737	0.18240	-4.03787			
O	-0.52197	0.63428	-1.87363			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm

Zero-point correction= 0.457910 Electronic Energy = -1260.60943938

Internal Energy (E)= -1260.12212038	Enthalpy (H)= -1260.12117638
Gibbs Free Energy (G)=-1260.20886438	Gibbs Free Energy of Solvation=-1261.27199892

St.Pt.	General Structure	Ball & Stick model
IV-1A’	 **IV-1A'**	

Cartesian co-ordinate

Atoms	X	Y	Z
C	2.62019	0.63158	-0.89256
C	2.46298	1.50742	0.27686
C	2.36789	0.71525	1.42059
C	2.44599	-0.69246	0.99488
C	2.76126	-0.71262	-0.42400
O	-0.99207	1.19410	-0.96969
C	-1.58822	2.11157	-0.12419
O	-0.88620	2.73446	0.61795
C	-3.09556	2.23980	-0.27435
C	-1.31249	-2.12874	-0.41067
H	-1.64015	0.63580	-1.42707
C	2.33481	2.98522	0.17475
H	3.31163	3.44150	-0.03643
H	1.65995	3.26468	-0.64261
H	1.93666	3.42715	1.09164
C	2.06097	1.14000	2.81340
H	2.89915	0.93342	3.49221

Frequencies

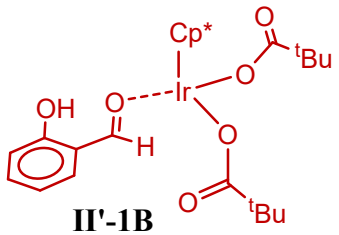
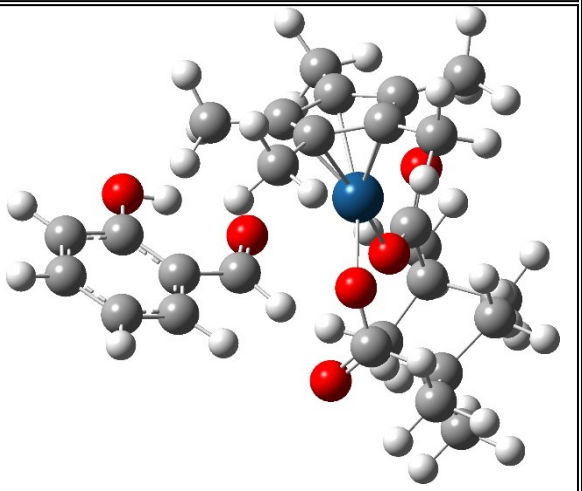
26.3715	33.7564	41.3834
49.5304	68.2301	73.0601
96.6619	99.1273	106.3511
119.5698	134.0411	139.1033
147.6048	151.5170	158.9772
168.4726	179.1288	186.2135
191.6916	206.5549	207.9375
216.5629	241.0144	245.2432
266.2383	269.7352	271.9967
285.4857	287.7071	299.5013
304.2191	308.6580	316.8548
327.5844	342.5579	355.8344
365.6087	390.1437	405.2841
415.4074	429.3265	469.5122
473.8081	521.6337	530.1466
537.0662	542.1055	548.3602
559.9824	571.4803	593.0447
600.4938	604.2482	618.8554
627.0489	654.9046	678.6222
756.2048	761.1396	764.0056
769.7617	803.9164	809.1158

H	1.83458	2.20926	2.86596	862.3122	866.6785	880.4364
H	1.18385	0.60063	3.19257	893.9358	942.5344	947.4171
C	3.12813	-1.88952	-1.25487	957.5221	959.6301	961.5524
H	2.53777	-1.90961	-2.17763	962.2958	972.8997	1031.0117
H	4.19469	-1.85831	-1.51164	1034.6344	1039.6043	1043.3194
H	2.93330	-2.82863	-0.72700	1043.8693	1044.4081	1046.1483
C	2.83339	1.08652	-2.29499	1050.6862	1087.0675	1088.4818
H	2.52395	0.30736	-3.00067	1097.8641	1104.7735	1113.2174
H	2.24159	1.98248	-2.51476	1147.5115	1176.2701	1186.1995
H	3.88783	1.32692	-2.49066	1197.8544	1225.7343	1238.9394
C	2.46191	-1.85074	1.93052	1255.6917	1263.7593	1318.1926
H	3.44460	-1.96752	2.40727	1345.2800	1365.8542	1375.4096
H	1.71399	-1.71441	2.71920	1383.0750	1386.1025	1392.2854
H	2.21862	-2.78231	1.40886	1393.3588	1394.7027	1400.2728
Ir	0.73394	-0.08534	-0.06010	1424.0656	1427.3678	1430.9956
C	-3.44416	2.61410	-1.71942	1438.3856	1443.8768	1447.3515
H	-3.16311	1.84047	-2.44469	1449.7097	1450.8911	1455.1138
H	-4.52867	2.75227	-1.80168	1457.6810	1459.1042	1460.2534
H	-2.96094	3.55158	-2.01885	1464.8916	1473.5364	1476.1460
C	-3.75180	0.90712	0.10617	1479.7523	1481.9966	1484.5345
H	-3.43148	0.57618	1.10067	1488.7681	1497.7748	1498.7264
H	-4.84083	1.03359	0.11149	1515.9853	1517.9062	1596.1358
H	-3.52623	0.09077	-0.59460	1618.7554	1658.4051	1756.3180
C	-3.57219	3.33541	0.67190	1921.2389	3024.9812	3026.2262
H	-3.33240	3.08801	1.71095	3028.4821	3031.1635	3032.2014
H	-3.09750	4.29472	0.43998	3035.4587	3036.1816	3046.1486
H	-4.65834	3.45217	0.58136	3100.2076	3102.9205	3106.6021
C	-1.58138	-1.53895	0.84484	3109.1856	3115.6829	3121.5832
C	-2.66890	-2.03475	1.59536	3122.1049	3131.2546	3133.8119
C	-2.11509	-3.15986	-0.91366	3137.2607	3138.3297	3140.9260
C	-3.45014	-3.05430	1.08047	3141.2070	3147.1031	3150.1378
C	-3.19078	-3.62295	-0.17724	3154.9796	3166.8270	3184.5151
H	-1.86260	-3.57688	-1.88725	3187.9314	3202.7188	3802.6555
H	-3.82294	-4.42209	-0.55605			
H	-4.28848	-3.42445	1.66918			
H	-2.87386	-1.59570	2.57013			
O	-0.84779	-0.53392	1.26142			
C	-0.15028	-1.57183	-1.12475			
O	0.18261	-1.92738	-2.24669			
H	-2.34796	3.57263	2.53005			
H	-0.69777	3.07938	2.06538			
Ir	-1.65369	-0.57476	-0.15076			
C	1.77795	0.61040	-1.29125			
C	2.13287	-0.87122	-1.20183			
O	1.39391	-1.69704	-1.70103			
C	3.31200	-1.29787	-0.39298			
C	4.61290	-1.13362	-0.87133			
C	3.09979	-1.92918	0.82720			
C	5.69555	-1.57277	-0.11783			
C	4.17990	-2.35729	1.59405			
H	2.07171	-2.05536	1.16624			
C	5.47363	-2.17627	1.11805			
H	6.70834	-1.44603	-0.50070			
H	4.01079	-2.83752	2.55464			
H	6.32454	-2.51303	1.70552			
O	4.74201	-0.54330	-2.09020			
H	5.67274	-0.47492	-2.32853			
C	0.63389	0.75102	-2.26539			
C	2.92715	1.58077	-1.45499			
C	4.85170	2.36254	-0.35019			
H	4.58554	3.41370	-0.51439			

H	5.46963	2.04686	-1.20246
C	5.53081	2.13074	0.97347
H	6.47248	2.68645	1.02514
H	4.88756	2.45610	1.79667
H	5.74242	1.06336	1.11047
O	3.65827	1.57347	-0.34098
O	3.14601	2.29349	-2.40703
C	0.92000	0.94807	-3.71343
H	-0.00533	0.88337	-4.29044
H	1.41585	1.91119	-3.86642
H	1.63737	0.18240	-4.03787
O	-0.52197	0.63428	-1.87363

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.463240 Electronic Energy = -1260.66090600
Internal Energy (E)= -1260.16748 Enthalpy (H)= -1260.166537
Gibbs Free Energy (G)=-1260.25706 Gibbs Free Energy of Solvation=-1261.31755767

St.Pt.	General Structure	Ball & Stick model
II'-1B	 **II'-1B**	

Cartesian co-ordinate

Atoms	X	Y	Z
H	-0.65968	-2.08813	0.48507
C	-1.48505	1.86403	-0.96703
C	-0.90936	2.72525	0.03715
C	0.42124	3.03582	-0.39400
C	0.65216	2.39117	-1.69108

Frequencies

33.1256	41.3877	52.5753
55.1285	56.2166	65.7940
72.4723	85.4785	86.8041
89.7630	91.2174	100.9884
110.1391	115.0188	116.0093
148.6927	152.0504	161.5145
168.9975	170.8272	178.7985
184.9856	190.6609	196.3346
206.3588	213.3444	218.4978

C	-0.53712	1.67969	-2.04400	224.2211	229.2739	245.9407
C	1.59994	-1.30604	-1.57756	251.3122	253.0671	255.8636
O	1.21412	-0.85557	-0.40049	261.9006	277.3728	281.2238
O	1.57718	-0.65137	-2.60805	297.9413	306.5498	312.4895
C	2.19562	-2.71591	-1.53369	316.1989	323.7414	325.4120
O	0.55294	0.46971	1.79226	329.0222	332.5905	333.8509
C	1.11668	-0.62021	2.28612	345.3131	355.3526	375.2929
O	0.50472	-1.65572	2.49035	381.7347	393.7435	394.9869
C	2.56503	-0.43879	2.75465	410.4271	420.2169	428.0018
C	1.89251	2.48219	-2.50217	434.6924	445.0708	454.4335
H	1.79908	3.26867	-3.26228	456.4288	459.5110	469.3155
H	2.75907	2.71946	-1.87615	534.4982	540.4196	547.7522
H	2.08353	1.52298	-2.99178	551.0281	554.2763	569.6562
C	-0.82321	0.91038	-3.28525	570.7009	575.6049	582.6774
H	-1.61182	1.41192	-3.86193	595.3731	605.2577	649.4858
H	0.06794	0.80725	-3.90526	671.9661	741.1508	780.5852
H	-1.16064	-0.10550	-3.04656	790.9515	796.8612	798.3896
C	1.40951	3.85614	0.35495	802.7991	811.9434	814.0479
H	1.30769	3.70365	1.43513	817.7279	840.5553	877.6731
H	2.43551	3.59307	0.07775	890.9894	898.2520	916.7625
H	1.26658	4.92360	0.14422	941.2038	946.1342	947.8431
C	-1.56049	3.11805	1.31641	949.7136	954.1713	959.9942
H	-0.81595	3.36552	2.07923	963.9933	976.9271	980.9831
H	-2.21605	3.98730	1.18185	998.9365	1023.2969	1031.5148
H	-2.16158	2.29092	1.71181	1033.7010	1036.4495	1038.9416
C	-2.86807	1.32997	-0.95740	1040.1296	1042.7625	1045.7837
H	-3.23287	1.14517	0.05805	1052.1062	1053.6533	1091.7737
H	-3.53697	2.06620	-1.42431	1098.7321	1099.5937	1108.9598
H	-2.95267	0.40110	-1.53058	1132.4496	1156.4642	1190.1860
O	-1.51124	-2.28526	-1.35277	1190.4877	1209.3694	1227.4058
C	3.22686	-1.80168	2.92134	1234.3181	1236.0724	1240.1114
H	4.23821	-1.68243	3.33147	1262.3983	1265.3746	1279.1840
H	2.64488	-2.43968	3.59306	1327.0117	1342.2901	1344.1874
H	3.30839	-2.32454	1.95928	1366.4762	1377.8111	1379.1075
C	2.47636	0.25871	4.11868	1380.1048	1381.4830	1382.5333
H	3.48220	0.40298	4.53454	1386.6995	1392.4178	1401.0675
H	1.99616	1.24073	4.02786	1403.0613	1408.1206	1414.6416
H	1.89666	-0.34550	4.82743	1426.0858	1430.2053	1436.7554
C	3.37937	0.42747	1.79621	1437.7979	1443.7704	1445.3980
H	3.40981	-0.00911	0.78940	1446.5227	1452.2386	1453.6609
H	2.96198	1.43857	1.71755	1457.1870	1458.4786	1460.0032
H	4.41069	0.51381	2.16326	1463.3140	1465.5270	1466.6393
C	2.01950	-3.37501	-2.89790	1469.2203	1471.5590	1472.9264
H	2.48080	-2.77820	-3.69058	1475.9711	1477.8819	1480.2175
H	2.48089	-4.37098	-2.89190	1488.8441	1491.0319	1499.5259
H	0.95538	-3.49134	-3.13652	1505.1088	1507.4917	1508.3337
C	1.56499	-3.58945	-0.45339	1511.4095	1521.4082	1530.9068
H	2.07109	-4.56374	-0.43048	1541.1518	1643.7430	1685.6477
H	1.63692	-3.13870	0.54345	1743.1232	1782.1236	1782.8225
H	0.50517	-3.76860	-0.67360	3019.6623	3023.7337	3026.2537
C	3.68910	-2.52375	-1.24212	3030.6971	3032.9477	3033.9390
H	4.19709	-3.49686	-1.23375	3037.1641	3039.1265	3039.6130
H	4.16135	-1.89676	-2.00877	3040.1321	3040.6804	3043.3512
H	3.84500	-2.05117	-0.26311	3109.0974	3113.0509	3115.0733
Ir	0.28807	0.92257	-0.15499	3117.2247	3119.0636	3119.0751
C	-1.56910	-2.03456	-0.14328	3120.3156	3121.6700	3122.2716
C	-2.78693	-1.64713	0.54488	3122.5111	3123.6260	3128.7169
C	-2.72183	-1.26961	1.89671	3132.7011	3135.1011	3138.7440
C	-4.02152	-1.60625	-0.14227	3139.5622	3142.7951	3146.5087
C	-3.86338	-0.85511	2.56044	3146.9902	3148.9023	3153.9714
H	-1.74529	-1.30154	2.38425	3157.3713	3179.0403	3182.6250

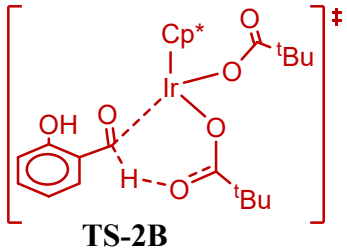
C	-5.17282	-1.20552	0.54046	3200.8252	3208.0241	3461.5780
C	-5.08393	-0.83540	1.87381			
H	-3.81830	-0.56123	3.60552			
H	-6.11591	-1.18589	0.00069			
H	-5.98655	-0.52104	2.39458			
O	-4.11241	-1.90718	-1.44195			
H	-3.20840	-2.16333	-1.74260			
H	5.67274	-0.47492	-2.32853			
C	0.63389	0.75102	-2.26539			
C	2.92715	1.58077	-1.45499			
C	4.85170	2.36254	-0.35019			
H	4.58554	3.41370	-0.51439			
H	5.46963	2.04686	-1.20246			
C	5.53081	2.13074	0.97347			
H	6.47248	2.68645	1.02514			
H	4.88756	2.45610	1.79667			
H	5.74242	1.06336	1.11047			
O	3.65827	1.57347	-0.34098			
O	3.14601	2.29349	-2.40703			
C	0.92000	0.94807	-3.71343			
H	-0.00533	0.88337	-4.29044			
H	1.41585	1.91119	-3.86642			
H	1.63737	0.18240	-4.03787			
O	-0.52197	0.63428	-1.87363			

Statistical Thermodynamic Analysis

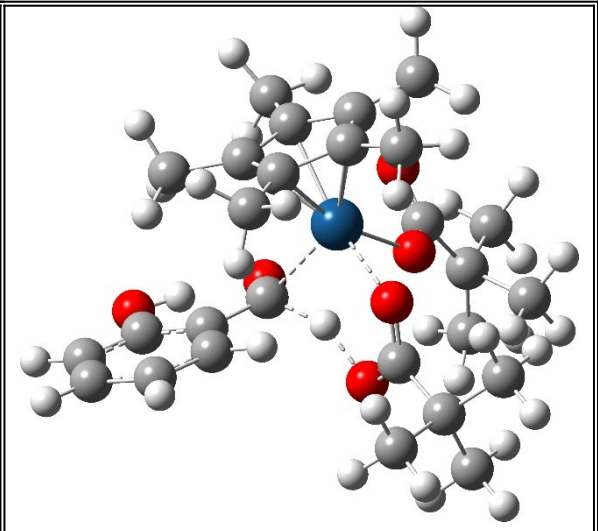
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.613850 Electronic Energy = -1607.50556410
Internal Energy (E)= -1606.8532241 Enthalpy (H)= -1606.8522801
Gibbs Free Energy (G)=-1606.9586691 Gibbs Free Energy of Solvation=-1608.29792319

St.Pt.	General Structure	Ball & Stick model

TS-2B



TS-2B



Cartesian co-ordinate

Atoms	X	Y	Z
H	-0.06985	0.88142	0.97364
C	-1.64940	-1.87116	-1.01219
C	-1.49761	-0.95895	-2.10477
C	-0.16903	-1.16908	-2.65630
C	0.48623	-2.18989	-1.88594
C	-0.41663	-2.60061	-0.82746
C	2.49716	-1.09707	1.00443
O	1.86752	-0.18083	0.32498
O	2.28932	-2.30259	0.95461
C	3.54315	-0.48649	1.94917
O	0.49121	1.55245	-1.14800
C	0.69510	2.40094	-0.21724
O	0.47105	2.16948	0.99526
C	1.13483	3.79734	-0.64139
C	1.85474	-2.71828	-2.12613
H	1.81973	-3.54369	-2.84894
H	2.51060	-1.94058	-2.53157
H	2.29784	-3.06707	-1.18988
C	-0.23076	-3.70128	0.15686
H	-0.85767	-4.56225	-0.11249
H	0.81327	-4.00975	0.21424
H	-0.50706	-3.36695	1.16234
C	0.39839	-0.44460	-3.82471
H	0.04145	0.58953	-3.86263
H	1.49128	-0.41342	-3.78145
H	0.10844	-0.93814	-4.76146
C	-2.51770	-0.02275	-2.65382
H	-2.05528	0.92468	-2.95590
H	-3.01245	-0.45018	-3.53557
H	-3.28713	0.21204	-1.91101
C	-2.88230	-2.11378	-0.21763
H	-3.57974	-1.27180	-0.25065
H	-3.39337	-2.99480	-0.62874
H	-2.65686	-2.33133	0.83195
O	-0.46893	-0.82553	2.30709
C	1.88910	4.47723	0.49669
H	2.18869	5.48754	0.19064

Frequencies

-1631.7852	38.5202	44.7562
47.4974	53.1360	64.2222
69.9254	78.7677	82.2429
89.9772	95.8196	107.4682
125.5414	132.9452	146.7358
150.5946	154.9307	165.6088
166.7049	173.6567	182.1756
186.4920	188.4412	196.8360
200.1531	213.5267	225.6928
227.2490	231.7971	244.4833
251.0790	252.7193	265.1809
273.8361	276.7877	281.8752
289.2039	303.9163	306.4044
308.5334	313.2025	324.0578
325.2771	326.7706	335.0101
343.2537	363.9972	371.5323
394.5017	398.4850	401.2455
413.1108	423.2408	431.3892
435.8589	437.8198	444.9998
452.4976	462.9340	477.0186
525.0513	535.3282	541.8731
547.9612	564.5591	571.2324
577.6365	587.5783	589.5310
601.7567	612.4864	635.3338
645.5318	684.8555	750.0021
779.0890	794.0820	795.0825
806.4944	817.3022	818.9598
819.9984	826.0434	829.5518
881.3507	901.1511	919.4130
927.3154	949.9639	952.0582
955.8205	956.6901	959.0555
965.4844	967.2090	971.2879
981.7439	992.4446	1037.4311
1038.6624	1041.9130	1043.5436
1044.4973	1046.6772	1050.7133
1052.0291	1052.5783	1060.8086
1087.0110	1095.2740	1109.5644
1133.3581	1155.4642	1182.1547
1188.4283	1212.5717	1236.0059
1240.1424	1246.8955	1249.1040
1259.8795	1266.3095	1268.3168

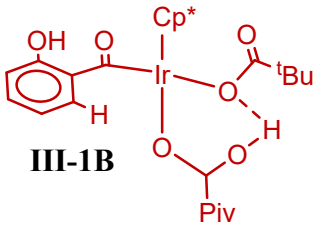
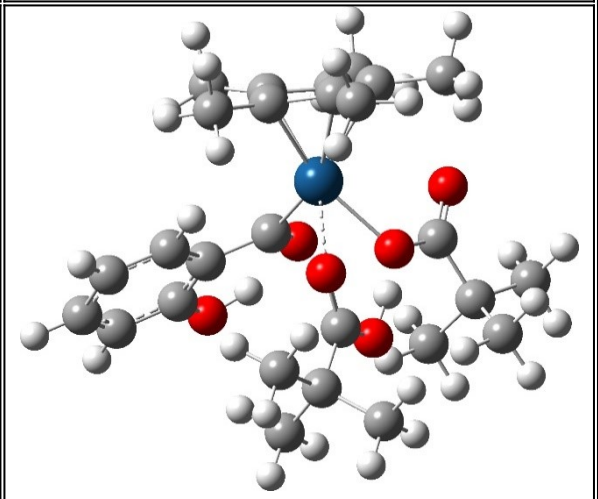
H	1.27107	4.55259	1.39631	1308.9943	1343.4811	1355.7857
H	2.79485	3.91713	0.76060	1366.8405	1375.4999	1379.6614
C	-0.15669	4.56582	-0.94774	1381.1539	1383.0348	1385.1543
H	0.08101	5.59328	-1.25087	1388.2574	1390.1031	1396.0691
H	-0.71306	4.08693	-1.76426	1399.6861	1400.9124	1412.5110
H	-0.80411	4.61132	-0.06273	1417.6177	1430.7761	1431.5842
C	2.01022	3.72460	-1.88838	1432.5689	1442.1123	1447.2044
H	2.92253	3.14714	-1.69474	1449.5414	1452.6021	1455.7917
H	1.48144	3.24890	-2.72058	1458.3190	1460.6354	1461.5156
H	2.30497	4.73693	-2.19252	1463.3258	1465.8600	1469.6227
C	4.48718	-1.57218	2.44825	1471.8863	1472.9989	1475.8123
H	5.03072	-2.03872	1.61764	1477.0160	1478.0881	1478.4196
H	5.22212	-1.14225	3.14174	1483.2772	1489.5415	1490.9857
H	3.93655	-2.36326	2.96683	1498.7547	1502.5803	1503.1239
C	2.76775	0.11511	3.12727	1513.3843	1520.7650	1525.6991
H	3.47019	0.52686	3.86481	1528.0030	1535.2595	1638.7526
H	2.10494	0.92134	2.79054	1673.1428	1691.5569	1703.7688
H	2.15366	-0.64659	3.62368	1778.4419	3022.4802	3023.0280
C	4.33292	0.61744	1.24830	3025.8446	3031.7158	3035.0648
H	5.06910	1.04721	1.94092	3036.4367	3038.6291	3039.9683
H	4.87723	0.23024	0.37695	3041.3367	3041.7067	3043.3095
H	3.66777	1.41867	0.90608	3104.6754	3107.8738	3113.5184
Ir	0.04871	-0.47580	-0.62134	3113.7208	3115.6876	3118.5342
C	-0.88996	-0.04959	1.43825	3119.6087	3119.6745	3122.5208
C	-2.26855	0.45693	1.46173	3124.7885	3125.9791	3132.8588
C	-2.70152	1.41057	0.52775	3133.1375	3136.9833	3141.5956
C	-3.19031	-0.03281	2.41696	3143.5624	3145.8207	3146.8350
C	-4.01026	1.85546	0.50819	3149.6272	3152.7753	3167.9155
H	-1.98564	1.77530	-0.20835	3179.1243	3185.3942	3185.7146
C	-4.51695	0.41487	2.39033	3200.1557	3206.6598	3427.0140
C	-4.91530	1.34601	1.44785			
H	-4.33163	2.59411	-0.22142			
H	-5.20754	0.01059	3.12584			
H	-5.94842	1.68709	1.44185			
O	-2.85274	-0.95011	3.32411			
H	-1.88297	-1.10893	3.22778			
H	5.67274	-0.47492	-2.32853			
C	0.63389	0.75102	-2.26539			
C	2.92715	1.58077	-1.45499			
C	4.85170	2.36254	-0.35019			
H	4.58554	3.41370	-0.51439			
H	5.46963	2.04686	-1.20246			
C	5.53081	2.13074	0.97347			
H	6.47248	2.68645	1.02514			
H	4.88756	2.45610	1.79667			
H	5.74242	1.06336	1.11047			
O	3.65827	1.57347	-0.34098			
O	3.14601	2.29349	-2.40703			
C	0.92000	0.94807	-3.71343			
H	-0.00533	0.88337	-4.29044			
H	1.41585	1.91119	-3.86642			
H	1.63737	0.18240	-4.03787			
O	-0.52197	0.63428	-1.87363			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm

Zero-point correction= 0.609519 Electronic Energy = -1607.47132519

Internal Energy (E)= -1606.82420719	Enthalpy (H)= -1606.82326419
Gibbs Free Energy (G)=-1606.92697119	Gibbs Free Energy of Solvation=-1608.25861711

St.Pt.	General Structure	Ball & Stick model
III-1B	 **III-1B**	

Cartesian co-ordinate

Atoms	X	Y	Z
H	0.10352	1.97114	0.74853
C	-0.82861	-2.63382	-0.81205
C	-0.42831	-2.81266	0.55278
C	-1.54813	-2.41939	1.41532
C	-2.56375	-1.90702	0.60181
C	-2.10070	-1.93820	-0.79413
C	-2.28057	1.85198	-0.23022
O	-1.23194	1.34520	0.37700
O	-3.15075	1.18340	-0.76194
C	-2.32649	3.38540	-0.22298
O	0.95613	-0.01443	1.58986
C	1.52997	1.08379	1.63332
O	1.04396	2.16657	1.10001
C	2.86799	1.25384	2.32457
C	-3.87266	-1.34642	1.02770
H	-4.68609	-2.01957	0.72553
H	-3.92580	-1.21831	2.11311
H	-4.04069	-0.37630	0.54780
C	-2.92947	-1.62765	-1.99049

Frequencies

17.4749	36.1898	37.1773
45.7714	55.7210	67.4460
71.9510	79.0937	83.5313
87.4317	96.8503	116.8214
134.3813	139.4658	145.5563
154.3377	156.2804	159.1911
166.7158	168.6314	173.2217
184.8167	188.0192	194.0854
198.6359	206.0558	213.5988
214.9871	221.5028	223.3290
233.3418	252.1426	256.2479
274.7657	283.9309	286.7616
292.8997	294.8958	309.4236
314.0551	319.7831	324.2793
332.0705	339.2324	339.6298
359.0122	369.6499	388.7591
395.2387	396.5888	403.8245
411.8410	427.3656	440.7800
448.6664	455.5928	459.4544
468.9831	486.3418	531.8555
536.0767	547.5967	548.2835
553.1139	570.0970	572.3785
593.3998	595.1632	608.7810

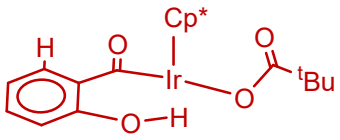
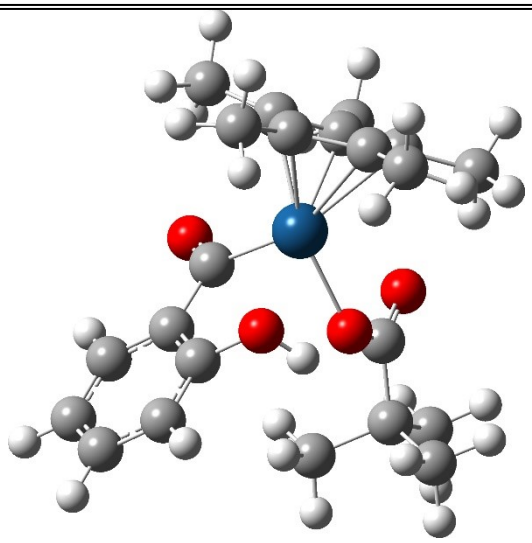
H	-3.48463	-2.51654	-2.32147
H	-3.62858	-0.81826	-1.77218
H	-2.29894	-1.28532	-2.81811
C	-1.49594	-2.48192	2.90219
H	-0.59157	-1.98721	3.27892
H	-2.35893	-1.98712	3.35722
H	-1.47683	-3.52078	3.25777
C	0.79400	-3.49792	1.06079
H	1.28310	-2.90871	1.84768
H	0.53434	-4.47447	1.49090
H	1.52657	-3.67081	0.26622
C	-0.10968	-3.08514	-2.03554
H	0.96952	-3.17183	-1.87391
H	-0.48489	-4.06610	-2.35514
H	-0.26440	-2.38454	-2.86310
O	-0.14965	0.81197	-2.23567
C	2.67060	2.19922	3.51490
H	3.63056	2.34962	4.02375
H	2.29594	3.17488	3.18904
H	1.96423	1.78207	4.24364
C	3.85390	1.87420	1.32688
H	4.82692	2.00240	1.81729
H	3.99812	1.22852	0.45013
H	3.50854	2.85391	0.98253
C	3.38515	-0.09698	2.80343
H	2.68282	-0.57146	3.49851
H	3.54235	-0.77917	1.95878
H	4.34363	0.03955	3.31844
C	-3.67411	3.85251	-0.76069
H	-4.49848	3.48943	-0.13630
H	-3.70916	4.94956	-0.77622
H	-3.84306	3.48142	-1.77627
C	-1.21081	3.89766	-1.13976
H	-1.25030	4.99358	-1.19381
H	-0.21422	3.61476	-0.78161
H	-1.32795	3.49894	-2.15435
C	-2.13111	3.92364	1.19572
H	-2.21094	5.01854	1.18874
H	-2.90110	3.53746	1.87577
H	-1.15188	3.66418	1.61106
Ir	-0.62047	-0.70041	0.11904
C	0.44977	0.11053	-1.40954
C	1.90963	-0.11000	-1.58743
C	2.63591	-0.98942	-0.76992
C	2.60983	0.57889	-2.61199
C	3.99264	-1.20281	-0.93980
H	2.09836	-1.50184	0.02419
C	3.99050	0.38014	-2.76469
C	4.66835	-0.50261	-1.94534
H	4.52578	-1.89788	-0.29505
H	4.49374	0.93083	-3.55537
H	5.73664	-0.65180	-2.08869
O	2.01470	1.42121	-3.45268
H	1.05248	1.40850	-3.22142
H	5.67274	-0.47492	-2.32853
C	0.63389	0.75102	-2.26539
C	2.92715	1.58077	-1.45499
C	4.85170	2.36254	-0.35019
H	4.58554	3.41370	-0.51439
H	5.46963	2.04686	-1.20246
C	5.53081	2.13074	0.97347

615.6021	630.2451	667.3907
681.5415	755.0906	774.8823
777.7149	780.7267	797.6113
807.3824	811.0591	825.1057
828.2728	836.1541	877.1069
909.5401	910.4717	922.7420
949.1204	949.5001	956.4951
958.4291	963.0780	964.1260
965.3139	973.3382	974.7890
1005.2320	1019.0084	1028.7629
1038.2647	1040.0222	1043.3890
1046.2170	1048.1612	1050.0209
1052.0324	1056.3592	1057.5310
1092.7049	1096.5707	1109.1298
1123.4683	1148.8136	1179.8832
1185.8706	1198.4577	1231.5500
1239.8671	1242.9703	1245.5936
1251.5781	1259.8602	1265.1859
1340.0279	1347.5918	1367.3621
1367.8059	1374.3983	1384.3408
1385.0869	1386.4198	1393.1119
1398.8778	1401.0315	1404.8278
1405.6789	1418.6724	1424.1888
1431.0614	1436.1315	1440.3465
1442.2153	1445.2958	1451.0762
1454.6213	1455.6432	1458.4247
1459.3893	1460.0950	1462.7307
1464.7095	1465.3925	1469.7513
1477.8316	1479.1348	1480.8188
1484.7126	1484.7895	1489.0925
1490.4354	1498.3548	1498.8002
1500.4560	1511.4769	1523.9497
1527.9437	1532.7367	1559.9898
1584.5852	1636.7364	1666.1568
1694.2450	1737.0597	1797.8011
2744.0497	3026.0415	3027.3537
3031.0360	3031.1363	3032.1810
3032.5010	3033.4930	3037.1656
3038.6096	3039.5714	3040.3105
3096.5818	3102.8541	3106.3152
3110.5443	3115.7208	3119.0493
3120.0196	3122.6439	3123.6508
3123.8202	3127.5543	3134.5753
3137.7306	3137.7683	3141.3999
3143.4635	3145.0552	3145.8602
3146.4669	3147.9931	3149.2488
3177.8911	3182.4671	3193.2568
3204.5624	3225.0654	3376.4826

H	6.47248	2.68645	1.02514
H	4.88756	2.45610	1.79667
H	5.74242	1.06336	1.11047
O	3.65827	1.57347	-0.34098
O	3.14601	2.29349	-2.40703
C	0.92000	0.94807	-3.71343
H	-0.00533	0.88337	-4.29044
H	1.41585	1.91119	-3.86642
H	1.63737	0.18240	-4.03787
O	-0.52197	0.63428	-1.87363

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.614433 Electronic Energy = -1607.52627565
Internal Energy (E)= -1606.87360765 Enthalpy (H)= -1606.87266365
Gibbs Free Energy (G)=-1606.97941465 Gibbs Free Energy of Solvation=-1608.29765982

St.Pt.	General Structure	Ball & Stick model
III'-1B	 **III'-1B**	

Cartesian co-ordinate

Atoms	X	Y	Z
C	2.77297	0.18142	-1.18543
C	2.55342	1.24483	-0.30639
C	2.28828	0.69361	1.03218
C	2.50460	-0.73683	0.96736
C	2.64840	-1.06598	-0.41954
O	-0.91900	1.11911	-0.55775
C	-1.25014	2.17360	0.14083
O	-0.52187	2.73170	0.94782
C	-2.68698	2.64015	-0.13378

Frequencies

23.8941	38.0846	39.1661
58.8586	63.5136	75.2894
86.5407	88.3792	111.2408
123.4282	130.9860	138.8976
145.3643	150.1157	152.4181
169.3669	178.8765	191.5268
203.0152	210.4114	217.1870
219.7765	239.5787	242.5713
245.3027	261.1779	262.0207
278.8402	283.6758	287.6607
298.6835	311.3791	321.8335
339.7828	349.2477	362.7055
378.5458	387.4357	417.3202
427.6652	430.8209	437.5720

C	-1.74882	-1.85668	-0.85784
H	-1.16433	-0.24857	-1.72144
C	2.45284	2.69419	-0.61919
H	1.51049	3.09109	-0.22169
H	3.27403	3.24738	-0.14464
H	2.48908	2.88559	-1.69584
C	2.12236	1.47333	2.28737
H	3.09261	1.64715	2.77337
H	1.63795	2.43117	2.08769
H	1.47628	0.92516	2.98204
C	2.84372	-2.42098	-1.00539
H	2.26821	-2.53029	-1.93210
H	3.90092	-2.60044	-1.24322
H	2.51255	-3.20454	-0.31707
C	3.00586	0.23303	-2.65524
H	2.30452	-0.41472	-3.19579
H	2.88682	1.24785	-3.04641
H	4.01989	-0.10617	-2.90662
C	2.53820	-1.64684	2.14228
H	3.47650	-1.51372	2.69592
H	1.70296	-1.43210	2.81883
H	2.46641	-2.69803	1.84444
Ir	0.70619	-0.16359	-0.08377
C	-2.85974	2.94770	-1.62174
H	-2.66120	2.06635	-2.24176
H	-3.88818	3.27784	-1.81945
H	-2.18335	3.75014	-1.94281
C	-3.63620	1.50811	0.27343
H	-3.47832	1.21976	1.32132
H	-4.67917	1.83415	0.16553
H	-3.49189	0.61405	-0.34621
C	-2.98759	3.88574	0.68906
H	-2.87108	3.68702	1.75947
H	-2.30435	4.70261	0.43226
H	-4.01675	4.21998	0.50317
O	-0.79158	-1.15122	-1.58941
C	-1.67043	-1.82629	0.53051
C	-2.63161	-2.51153	1.27360
C	-2.74971	-2.55161	-1.51882
C	-3.64435	-3.21078	0.63094
C	-3.69987	-3.23180	-0.76228
C	-0.57051	-1.04857	1.19345
O	-0.51872	-0.99448	2.41092
H	-2.77448	-2.55467	-2.60560
H	-4.49074	-3.78196	-1.26681
H	-4.39424	-3.74337	1.21071
H	-2.55634	-2.46981	2.35793
H	-2.21094	5.01854	1.18874
H	-2.90110	3.53746	1.87577
H	-1.15188	3.66418	1.61106
Ir	-0.62047	-0.70041	0.11904
C	0.44977	0.11053	-1.40954
C	1.90963	-0.11000	-1.58743
C	2.63591	-0.98942	-0.76992
C	2.60983	0.57889	-2.61199
C	3.99264	-1.20281	-0.93980
H	2.09836	-1.50184	0.02419
C	3.99050	0.38014	-2.76469
C	4.66835	-0.50261	-1.94534
H	4.52578	-1.89788	-0.29505
H	4.49374	0.93083	-3.55537

462.9473	515.9437	528.6432
537.7867	546.9462	553.5397
561.7833	580.6604	592.4856
597.0958	613.4700	623.5370
648.4553	668.5275	724.5470
772.8783	780.0940	782.3715
805.4687	808.0540	817.4957
836.5620	881.2115	893.5185
919.0399	942.3407	943.1877
946.3684	959.2788	959.8985
964.5674	993.8425	1027.5585
1034.8468	1036.0551	1042.8104
1043.4610	1045.0571	1047.7528
1052.1183	1085.6436	1089.4666
1104.0953	1107.1266	1152.3486
1176.4931	1184.8488	1189.5599
1224.3221	1238.3511	1245.0160
1263.1254	1271.3850	1330.4685
1359.3779	1364.9943	1369.8207
1372.8697	1376.5990	1386.3480
1388.3228	1390.3915	1394.9828
1413.0841	1427.2103	1431.0159
1440.0635	1442.8299	1444.4673
1449.1127	1450.1663	1453.9455
1455.9092	1457.6251	1463.3760
1467.9010	1469.3146	1470.4002
1472.7667	1482.0544	1483.1503
1485.2952	1493.5980	1504.9249
1509.2123	1526.2793	1587.6420
1649.5802	1667.1922	1762.9892
1790.5752	3023.6803	3026.3195
3029.3196	3030.5984	3034.9861
3035.8522	3036.7279	3037.4289
3099.6558	3108.4605	3109.5045
3111.1655	3119.0912	3119.2260
3119.5278	3123.4514	3123.5422
3124.7022	3137.6262	3139.7458
3142.1212	3143.4350	3150.5070
3183.3693	3195.1912	3198.7017
3203.9094	3208.7058	3523.6442

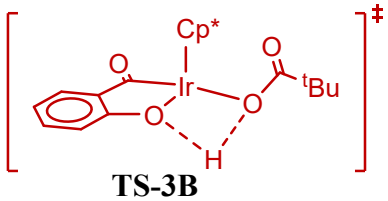
H	5.73664	-0.65180	-2.08869
O	2.01470	1.42121	-3.45268
H	1.05248	1.40850	-3.22142
H	5.67274	-0.47492	-2.32853
C	0.63389	0.75102	-2.26539
C	2.92715	1.58077	-1.45499
C	4.85170	2.36254	-0.35019
H	4.58554	3.41370	-0.51439
H	5.46963	2.04686	-1.20246
C	5.53081	2.13074	0.97347
H	6.47248	2.68645	1.02514
H	4.88756	2.45610	1.79667
H	5.74242	1.06336	1.11047
O	3.65827	1.57347	-0.34098
O	3.14601	2.29349	-2.40703
C	0.92000	0.94807	-3.71343
H	-0.00533	0.88337	-4.29044
H	1.41585	1.91119	-3.86642
H	1.63737	0.18240	-4.03787
O	-0.52197	0.63428	-1.87363

Statistical Thermodynamic Analysis

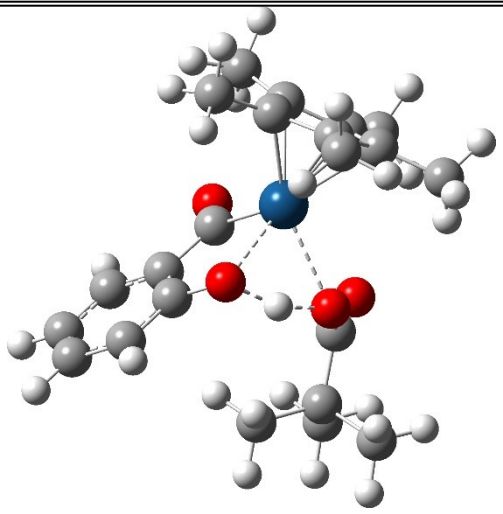
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.463220 Electronic Energy = -1260.66897530
Internal Energy (E)= -1260.1756233 Enthalpy (H)= -1260.1746803
Gibbs Free Energy (G)=-1260.2652063 Gibbs Free Energy of Solvation=-1261.31643198

St.Pt.	General Structure	Ball & Stick model

TS-3B



TS-3B



Cartesian co-ordinate

Atoms	X	Y	Z
C	2.86057	0.11212	-1.18208
C	2.66614	1.27317	-0.43265
C	2.37215	0.89209	0.95967
C	2.54390	-0.53314	1.06920
C	2.67714	-1.03509	-0.27984
O	-0.85113	1.47994	-0.76537
C	-1.62132	2.01301	0.20625
O	-1.13359	2.40991	1.23838
C	-3.09050	2.20061	-0.16548
C	-1.58329	-1.77252	-0.85169
H	-0.97489	0.29567	-1.25890
C	2.60396	2.67944	-0.90944
H	1.65760	3.14465	-0.60699
H	3.41512	3.27252	-0.46720
H	2.68130	2.75028	-1.99804
C	2.16689	1.83439	2.09312
H	3.12367	2.20295	2.48817
H	1.55638	2.68907	1.78550
H	1.62047	1.33693	2.90137
C	2.85642	-2.45364	-0.69260
H	2.34621	-2.64819	-1.64278
H	3.92014	-2.69393	-0.82507
H	2.44038	-3.14149	0.04996
C	3.08976	-0.01815	-2.64718
H	2.33487	-0.66650	-3.10921
H	3.04462	0.95157	-3.15143
H	4.07334	-0.45974	-2.85614
C	2.54359	-1.31176	2.33384
H	3.47471	-1.13299	2.88591
H	1.69487	-1.02329	2.96458
H	2.46093	-2.38646	2.14268
Ir	0.78456	-0.07020	-0.08376
C	-3.14579	3.27176	-1.26123
H	-2.59518	2.95661	-2.15427
H	-4.19015	3.45564	-1.54430
H	-2.71938	4.21869	-0.90728
C	-3.70120	0.90118	-0.68926

Frequencies

-1604.1331	29.2376	39.0928
46.5399	54.9564	67.8800
76.0370	87.3531	112.1411
122.8483	133.8280	142.0566
145.6835	157.8893	166.1331
168.5495	175.3893	178.1777
186.8151	204.5591	209.2383
216.5261	228.3988	247.8660
250.7261	255.2657	267.4512
282.0052	287.6837	294.6480
307.6945	310.9268	324.9863
330.0857	339.6060	349.5635
367.0666	375.8724	386.6437
403.7613	427.8264	436.1723
449.1683	463.3227	528.3095
537.1099	539.0330	551.3647
554.5717	569.2048	580.2909
592.7544	599.2673	601.2696
615.8411	649.2517	672.3539
761.7770	770.9631	784.1217
798.6796	806.5914	810.5467
852.3832	873.2722	892.6786
900.6220	946.8221	950.7734
952.9699	959.3729	959.8823
962.8624	979.2857	1028.5479
1036.1973	1039.7976	1040.0099
1043.7585	1044.1261	1046.3693
1052.8861	1086.0676	1089.3188
1103.4091	1106.8108	1145.9993
1174.6527	1180.2074	1189.7444
1195.0782	1242.1303	1249.4012
1265.1503	1297.5160	1317.6825
1366.1596	1366.4118	1373.3371
1380.1617	1386.9654	1387.9034
1397.6368	1401.1695	1401.8438
1417.4773	1428.9964	1435.6118
1439.6937	1446.3298	1447.3230
1449.9409	1450.9948	1455.8427
1457.3292	1461.5353	1464.2238
1464.8996	1470.7132	1470.9979
1480.2443	1480.9829	1481.7380

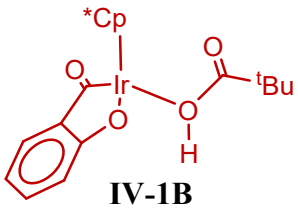
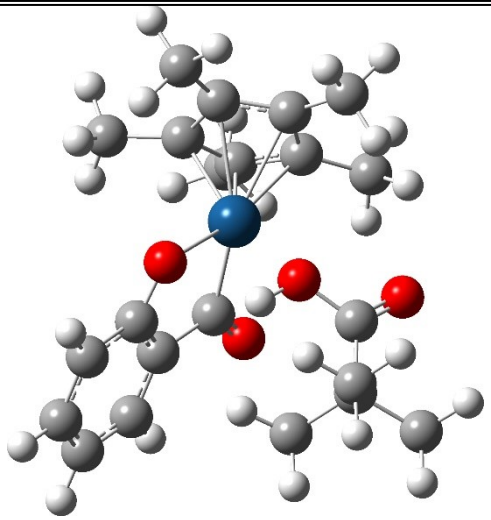
H	-3.62745	0.09046	0.04775	1486.3865	1499.2640	1506.9005
H	-4.76541	1.06229	-0.90277	1507.9833	1509.3645	1539.7227
H	-3.22728	0.56719	-1.62002	1591.6670	1640.1793	1655.3485
C	-3.85606	2.67442	1.06402	1769.5926	1842.7938	3028.5450
H	-3.81672	1.92707	1.86442	3028.8316	3030.6574	3031.1168
H	-3.43187	3.60270	1.45951	3032.8425	3035.2886	3037.6684
H	-4.90758	2.84997	0.80400	3039.7178	3099.5755	3108.8400
O	-0.69690	-1.01571	-1.54624	3113.8548	3115.4836	3116.5712
C	-1.55161	-1.76553	0.54797	3121.2823	3123.9703	3125.2789
C	-2.48416	-2.51033	1.27443	3126.7947	3137.6894	3139.5126
C	-2.53533	-2.53976	-1.52412	3139.9699	3141.1070	3143.7233
C	-3.43446	-3.26994	0.60954	3144.1218	3149.9475	3181.5491
C	-3.44921	-3.28351	-0.78852	3192.3543	3201.9860	3207.5958
C	-0.50856	-0.93744	1.21269			
O	-0.46620	-0.82465	2.42530			
H	-2.54649	-2.53209	-2.61127			
H	-4.19163	-3.88196	-1.31283			
H	-4.16135	-3.85488	1.16752			
H	-2.43197	-2.47198	2.36050			
H	-2.21094	5.01854	1.18874			
H	-2.90110	3.53746	1.87577			
H	-1.15188	3.66418	1.61106			
Ir	-0.62047	-0.70041	0.11904			
C	0.44977	0.11053	-1.40954			
C	1.90963	-0.11000	-1.58743			
C	2.63591	-0.98942	-0.76992			
C	2.60983	0.57889	-2.61199			
C	3.99264	-1.20281	-0.93980			
H	2.09836	-1.50184	0.02419			
C	3.99050	0.38014	-2.76469			
C	4.66835	-0.50261	-1.94534			
H	4.52578	-1.89788	-0.29505			
H	4.49374	0.93083	-3.55537			
H	5.73664	-0.65180	-2.08869			
O	2.01470	1.42121	-3.45268			
H	1.05248	1.40850	-3.22142			
H	5.67274	-0.47492	-2.32853			
C	0.63389	0.75102	-2.26539			
C	2.92715	1.58077	-1.45499			
C	4.85170	2.36254	-0.35019			
H	4.58554	3.41370	-0.51439			
H	5.46963	2.04686	-1.20246			
C	5.53081	2.13074	0.97347			
H	6.47248	2.68645	1.02514			
H	4.88756	2.45610	1.79667			
H	5.74242	1.06336	1.11047			
O	3.65827	1.57347	-0.34098			
O	3.14601	2.29349	-2.40703			
C	0.92000	0.94807	-3.71343			
H	-0.00533	0.88337	-4.29044			
H	1.41585	1.91119	-3.86642			
H	1.63737	0.18240	-4.03787			
O	-0.52197	0.63428	-1.87363			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm

Zero-point correction= 0.457794 Electronic Energy = -1260.63840056

Internal Energy (E)= -1260.15098956	Enthalpy (H)= -1260.15004556
Gibbs Free Energy (G)=-1260.23886856	Gibbs Free Energy of Solvation=-1261.29412208

St.Pt.	General Structure	Ball & Stick model
IV-1B	 **IV-1B**	

Cartesian co-ordinate

Atoms	X	Y	Z
C	-2.85566	0.04965	-1.12180
C	-2.64518	-1.22582	-0.59455
C	-2.33729	-1.10197	0.83809
C	-2.48142	0.27308	1.20254
C	-2.64261	1.01785	-0.03278
O	0.93909	-1.30407	-0.82974
C	1.62529	-2.22387	-0.07071
O	0.98654	-3.01353	0.56562
C	3.14116	-2.16155	-0.17316
C	1.34749	1.93206	-0.79453
H	1.46724	-0.61836	-1.28596
C	-2.56831	-2.52216	-1.32042
H	-1.60095	-3.00482	-1.12846
H	-3.35005	-3.21249	-0.97754
H	-2.67505	-2.39562	-2.40187
C	-2.14595	-2.23513	1.78470
H	-3.10875	-2.61492	2.15452
H	-1.60801	-3.06022	1.30870
H	-1.54885	-1.91716	2.64664
C	-2.81888	2.48995	-0.17170
H	-2.39507	2.83897	-1.12019
H	-3.87998	2.77287	-0.14684
H	-2.30028	3.02390	0.63150
C	-3.08334	0.44456	-2.53864

Frequencies

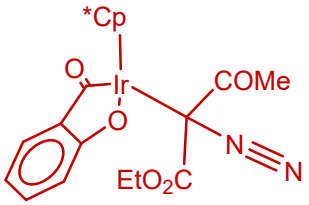
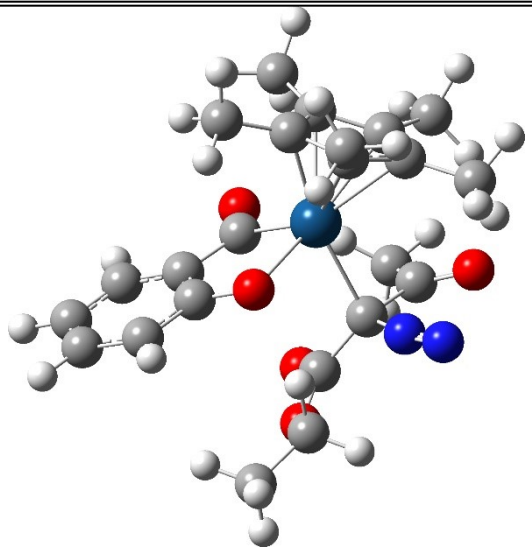
31.2463	38.2634	49.7780
52.5277	68.6763	73.7957
83.4397	98.8667	107.2791
122.4843	133.6506	150.5399
160.0928	163.8164	164.8486
177.6763	181.6404	186.8841
211.9659	214.0911	221.1845
234.1852	239.6161	242.8588
260.7249	270.0556	270.8021
293.9192	300.4950	306.4444
308.8306	312.2158	326.4773
331.5040	360.1901	365.0938
377.7043	390.0248	405.5715
415.2039	430.1462	469.0828
476.8947	518.6518	532.1207
539.4540	542.4077	550.1257
568.2140	592.9767	596.5578
600.6726	614.4831	621.9767
656.1601	679.3639	731.3947
763.5199	766.8862	768.3145
805.7264	806.3872	814.4349
860.8479	866.0178	885.6295
896.5357	945.4776	954.7954
956.0165	956.5197	963.0114
969.8793	975.4485	1019.0461
1033.2179	1038.0740	1043.2539
1044.1783	1045.4544	1045.7880
1048.6775	1064.6844	1089.9282

H	-2.30010	1.13496	-2.87733	1095.5309	1109.4992	1110.4655
H	-3.07299	-0.42193	-3.20669	1142.8474	1169.0779	1178.5605
H	-4.04922	0.95224	-2.66094	1186.5199	1199.1188	1240.1696
C	-2.43128	0.81108	2.58730	1256.3403	1264.3189	1309.2936
H	-3.35038	0.55359	3.12882	1339.3091	1368.3572	1375.1554
H	-1.57109	0.40121	3.12897	1377.0111	1388.8889	1391.5315
H	-2.32893	1.90111	2.59109	1393.7020	1396.2091	1404.2432
Ir	-0.75475	0.07540	-0.07981	1419.8370	1429.9830	1431.5872
C	3.54806	-2.47637	-1.61836	1437.9708	1446.8910	1451.1002
H	3.17887	-1.73224	-2.33462	1451.4721	1454.0944	1456.3922
H	4.64218	-2.48316	-1.68965	1458.4543	1461.5120	1466.8445
H	3.18288	-3.46219	-1.93026	1468.3521	1470.0260	1475.3705
C	3.64858	-0.77212	0.22767	1478.7909	1481.0399	1485.5284
H	3.31122	-0.49367	1.23364	1487.6830	1502.0556	1509.2451
H	4.74496	-0.78377	0.22790	1513.1991	1519.9300	1592.4143
H	3.33686	0.02475	-0.46107	1625.5594	1657.6871	1758.5093
C	3.72284	-3.21101	0.76694	1906.8469	3026.9558	3028.7500
H	3.44026	-3.00866	1.80525	3029.3511	3029.9234	3033.6109
H	3.36613	-4.21442	0.51338	3035.2456	3035.8581	3047.6665
H	4.81674	-3.19936	0.69585	3101.0879	3108.8462	3112.3725
O	0.46035	1.17680	-1.42232	3112.4005	3115.2208	3120.3111
C	1.46099	1.84381	0.60755	3123.4815	3124.8772	3128.7773
C	2.42489	2.57933	1.30187	3135.9414	3137.9814	3138.9482
C	2.22820	2.78165	-1.48935	3140.1954	3141.9371	3149.5517
C	3.28386	3.41838	0.61139	3160.1756	3170.8989	3182.8520
C	3.17306	3.51010	-0.78318	3191.8713	3201.8709	3668.4880
C	0.56288	0.86039	1.24567			
O	0.65317	0.54586	2.42313			
H	2.14749	2.85194	-2.57190			
H	3.84656	4.16883	-1.32946			
H	4.03653	3.99947	1.13831			
H	2.47995	2.46167	2.38293			
H	-2.21094	5.01854	1.18874			
H	-2.90110	3.53746	1.87577			
H	-1.15188	3.66418	1.61106			
Ir	-0.62047	-0.70041	0.11904			
C	0.44977	0.11053	-1.40954			
C	1.90963	-0.11000	-1.58743			
C	2.63591	-0.98942	-0.76992			
C	2.60983	0.57889	-2.61199			
C	3.99264	-1.20281	-0.93980			
H	2.09836	-1.50184	0.02419			
C	3.99050	0.38014	-2.76469			
C	4.66835	-0.50261	-1.94534			
H	4.52578	-1.89788	-0.29505			
H	4.49374	0.93083	-3.55537			
H	5.73664	-0.65180	-2.08869			
O	2.01470	1.42121	-3.45268			
H	1.05248	1.40850	-3.22142			
H	5.67274	-0.47492	-2.32853			
C	0.63389	0.75102	-2.26539			
C	2.92715	1.58077	-1.45499			
C	4.85170	2.36254	-0.35019			
H	4.58554	3.41370	-0.51439			
H	5.46963	2.04686	-1.20246			
C	5.53081	2.13074	0.97347			
H	6.47248	2.68645	1.02514			
H	4.88756	2.45610	1.79667			
H	5.74242	1.06336	1.11047			
O	3.65827	1.57347	-0.34098			
O	3.14601	2.29349	-2.40703			

C	0.92000	0.94807	-3.71343
H	-0.00533	0.88337	-4.29044
H	1.41585	1.91119	-3.86642
H	1.63737	0.18240	-4.03787
O	-0.52197	0.63428	-1.87363

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.463796 Electronic Energy = -1260.66460444
Internal Energy (E)= -1260.17101344 Enthalpy (H)= -1260.17007044
Gibbs Free Energy (G)=-1260.25932744 Gibbs Free Energy of Solvation=-1261.31570978

St.Pt.	General Structure	Ball & Stick model
IV'-1B	 **IV'-1B**	

Cartesian co-ordinate

Atoms	X	Y	Z
C	1.95563	-0.94866	-1.82951
C	2.72101	-0.03990	-1.08856
C	2.75985	-0.49745	0.30390
C	2.11256	-1.77201	0.36582
C	1.50285	-2.00738	-0.92186
C	-2.19731	-0.97647	-0.52153
Ir	0.55858	-0.27295	-0.07381
O	-1.22649	-0.36879	-1.17717
C	-1.99941	-1.33419	0.82569
C	-3.01152	-1.95669	1.56230
C	-3.43507	-1.26667	-1.12490
C	-4.22545	-2.24192	0.96163

Frequencies

29.8390	44.6685	49.0532
70.4230	79.3493	87.5869
98.7655	115.1890	120.7431
127.5623	136.1849	137.2642
143.8936	146.3649	159.3389
163.9959	171.3314	182.2709
186.5728	197.4826	204.6165
212.8763	222.1235	230.9688
241.0884	243.0448	252.2572
265.4104	266.6130	275.9804
282.9288	291.0289	296.7348
301.3333	312.5464	324.8624
327.9908	341.9179	346.8041
355.5422	358.9179	390.4924
397.4950	436.9197	441.6137
461.4193	475.5960	485.5534

C	-4.42312	-1.89360	-0.38221
C	-0.67857	-0.99272	1.37884
O	-0.36103	-1.19324	2.53955
H	-3.58720	-1.00178	-2.17008
H	-5.37636	-2.12066	-0.85725
H	-5.02008	-2.72916	1.52064
H	-2.81305	-2.20289	2.60355
C	-0.09019	1.84432	0.46391
C	1.05450	2.20449	1.43606
C	-1.52552	2.00399	0.93917
C	-2.50018	2.38651	-1.33100
H	-2.05652	3.33508	-1.66414
H	-1.92755	1.53278	-1.71540
C	-3.94503	2.29856	-1.75200
H	-4.02027	2.32125	-2.84403
H	-4.38178	1.36277	-1.38828
H	-4.52170	3.13451	-1.34401
O	-2.50437	2.35561	0.10857
O	-1.76823	1.85054	2.10792
N	0.21437	2.46407	-0.72350
N	0.64726	2.99905	-1.61221
C	3.63570	0.07394	1.36528
H	3.35421	-0.30987	2.35184
H	4.68340	-0.20647	1.18721
H	3.58476	1.16793	1.39652
C	3.37621	1.20526	-1.57058
H	3.12583	2.06184	-0.93201
H	4.46896	1.09712	-1.54309
H	3.09471	1.44402	-2.60159
C	1.53476	-0.85246	-3.25420
H	0.44606	-0.96273	-3.33726
H	1.80811	0.11335	-3.69196
H	1.99636	-1.64173	-3.86191
C	0.74502	-3.21703	-1.34782
H	-0.00799	-2.95885	-2.10036
H	1.41362	-3.97105	-1.78440
H	0.21779	-3.67428	-0.50406
C	2.09652	-2.67023	1.55008
H	3.08486	-3.12520	1.69394
H	1.82329	-2.11361	2.45286
H	1.36203	-3.47341	1.43637
C	0.91139	1.81947	2.87275
H	0.15466	2.44656	3.35339
H	0.57544	0.78257	2.99026
H	1.88393	1.98261	3.34471
O	2.02823	2.78957	1.00040
H	-1.15188	3.66418	1.61106
Ir	-0.62047	-0.70041	0.11904
C	0.44977	0.11053	-1.40954
C	1.90963	-0.11000	-1.58743
C	2.63591	-0.98942	-0.76992
C	2.60983	0.57889	-2.61199
C	3.99264	-1.20281	-0.93980
H	2.09836	-1.50184	0.02419
C	3.99050	0.38014	-2.76469
C	4.66835	-0.50261	-1.94534
H	4.52578	-1.89788	-0.29505
H	4.49374	0.93083	-3.55537
H	5.73664	-0.65180	-2.08869
O	2.01470	1.42121	-3.45268
H	1.05248	1.40850	-3.22142

501.3034	530.5280	537.8120
542.3992	552.0927	565.1857
570.4938	591.2502	594.7295
604.0757	616.2215	625.2705
636.8893	661.4608	673.4326
678.5127	759.9024	766.7514
769.7282	809.6433	815.9386
860.8625	865.8115	870.2572
890.2492	914.6084	953.7634
957.6520	959.1027	969.8851
974.5899	992.7029	1034.7328
1037.6404	1043.6341	1046.3163
1046.8029	1050.2470	1054.0050
1059.4635	1088.6449	1091.9352
1110.7887	1117.0030	1124.3936
1146.0564	1147.6562	1173.0205
1181.4011	1183.9265	1187.4685
1203.5325	1268.5242	1291.4342
1330.7918	1339.8891	1373.6825
1376.5523	1379.7173	1382.8779
1391.7396	1396.0773	1397.1268
1403.0353	1421.9801	1429.9115
1431.4226	1437.4607	1440.5820
1443.9209	1453.4987	1455.2958
1458.8351	1459.5076	1462.7645
1469.4966	1474.4027	1481.5964
1484.5413	1489.2536	1493.0858
1503.8956	1504.7269	1513.2758
1517.7187	1518.5421	1581.7039
1626.9899	1659.0506	1762.5962
1790.9383	1863.1594	2260.3759
3031.1707	3031.7395	3032.8199
3033.7129	3037.3725	3037.8030
3049.6242	3054.2180	3107.7720
3110.9685	3113.2549	3115.1265
3123.5992	3136.2665	3137.1023
3140.2298	3141.8310	3144.7127
3147.8082	3150.8088	3155.6842
3159.0753	3167.2476	3169.6053
3184.5315	3189.8071	3202.1352

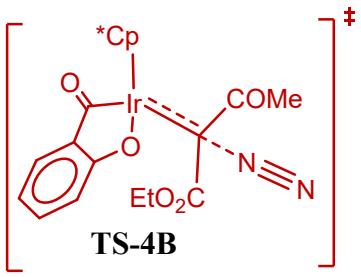
H	5.67274	-0.47492	-2.32853
C	0.63389	0.75102	-2.26539
C	2.92715	1.58077	-1.45499
C	4.85170	2.36254	-0.35019
H	4.58554	3.41370	-0.51439
H	5.46963	2.04686	-1.20246
C	5.53081	2.13074	0.97347
H	6.47248	2.68645	1.02514
H	4.88756	2.45610	1.79667
H	5.74242	1.06336	1.11047
O	3.65827	1.57347	-0.34098
O	3.14601	2.29349	-2.40703
C	0.92000	0.94807	-3.71343
H	-0.00533	0.88337	-4.29044
H	1.41585	1.91119	-3.86642
H	1.63737	0.18240	-4.03787
O	-0.52197	0.63428	-1.87363

Statistical Thermodynamic Analysis

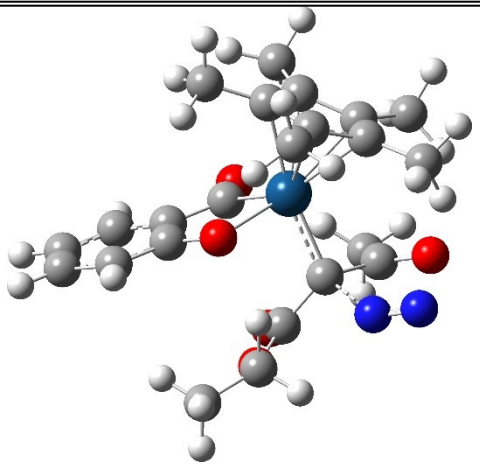
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.461471 Electronic Energy = -1482.10866577
Internal Energy (E)= -1481.61485377 Enthalpy (H)= -1481.61391077
Gibbs Free Energy (G)=-1481.70715877 Gibbs Free Energy of Solvation=-1482.91736136

St.Pt.	General Structure	Ball & Stick model

TS-4B



TS-4B



Cartesian co-ordinate

Atoms	X	Y	Z
C	1.71204	-1.20944	-1.82201
C	2.61857	-0.37695	-1.13237
C	2.65334	-0.80675	0.25969
C	1.85829	-1.99701	0.37176
C	1.20172	-2.20331	-0.88482
C	-2.31476	-0.79199	-0.50319
Ir	0.48716	-0.26415	-0.08596
O	-1.30848	-0.27507	-1.17618
C	-2.14219	-1.12546	0.85339
C	-3.19547	-1.65059	1.61115
C	-3.56990	-1.02078	-1.09994
C	-4.42587	-1.86646	1.01841
C	-4.59764	-1.55020	-0.33821
C	-0.80220	-0.88035	1.39492
O	-0.47646	-1.09230	2.54723
H	-3.70436	-0.77898	-2.15261
H	-5.56512	-1.72398	-0.80678
H	-5.25325	-2.27662	1.59131
H	-3.01335	-1.87902	2.65926
C	0.16506	1.70371	0.47428
C	1.32220	2.06735	1.42027
C	-1.22573	2.11076	0.90810
C	-2.10006	2.62662	-1.38292
H	-1.60774	3.56544	-1.67194
H	-1.54966	1.77051	-1.78467
C	-3.53380	2.60020	-1.84784
H	-3.57779	2.67098	-2.93961
H	-4.00699	1.66292	-1.53566
H	-4.09936	3.43370	-1.41960
O	-2.14399	2.55786	0.05223
O	-1.51990	2.01754	2.07640
N	0.54872	2.68002	-0.81486
N	1.48635	3.12153	-1.24947
C	3.61727	-0.32722	1.28896
H	3.25445	-0.55041	2.29860
H	4.58848	-0.82662	1.16613
H	3.78408	0.75243	1.22136
C	3.42091	0.74333	-1.68095

Frequencies

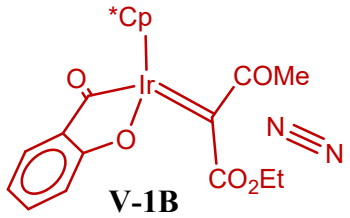
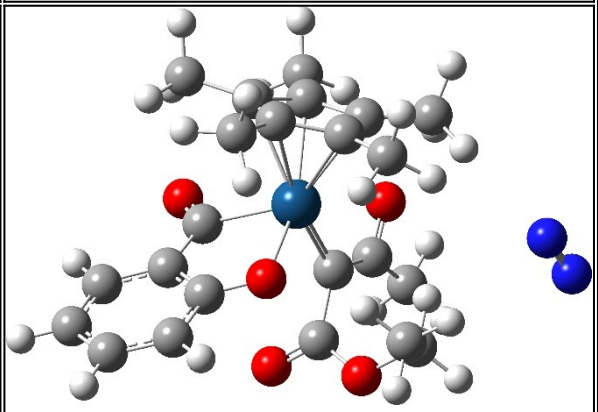
-406.4122	31.0707	44.7841
52.3251	62.2167	75.9145
93.5500	100.6851	111.2297
128.4945	133.8557	138.1901
142.5773	148.3876	156.0322
157.5878	172.9578	176.9778
180.2995	194.1270	197.4282
205.6004	214.5403	224.0500
235.0378	242.7889	246.9095
258.4799	259.4324	266.2807
277.2055	280.0401	287.1580
291.3855	298.3139	305.3536
308.7430	313.6185	327.9863
336.5771	345.4858	364.6073
395.5569	404.7527	409.4893
426.0381	433.2235	473.9496
488.4929	535.8159	536.9246
541.3501	549.3481	558.0904
570.5038	581.7421	595.0413
600.0795	608.6544	624.4499
628.9255	632.1751	645.0175
671.0989	732.5590	761.0845
765.2331	815.3830	820.8524
840.2863	844.1257	861.8269
864.0104	884.5200	907.5782
952.2940	956.9377	966.0925
977.5415	993.3549	1010.3791
1032.3259	1037.3023	1040.5148
1041.5296	1044.9865	1048.5208
1052.6164	1087.8964	1093.4615
1112.6572	1112.7886	1118.2415
1141.5313	1148.5093	1162.2550
1180.4868	1183.5069	1190.3977
1206.0904	1266.5277	1301.1855
1326.2511	1339.5913	1374.0124
1378.9212	1380.3836	1384.1805
1388.4737	1392.6437	1396.3181
1399.5629	1422.0367	1428.6711
1438.3597	1440.8754	1447.5167
1450.2853	1452.3510	1459.7136
1460.6956	1461.2260	1467.0785
1468.6036	1471.2888	1471.9889
1473.9432	1484.5403	1485.4405

H	3.31776	1.65017	-1.07061	1487.8496	1490.1867	1506.7027
H	4.48853	0.48526	-1.68160	1512.9597	1519.9044	1563.6718
H	3.13544	0.99029	-2.70855	1624.2682	1657.7258	1776.0291
C	1.27830	-1.11878	-3.24302	1776.6029	1838.7877	2212.3180
H	0.18576	-1.04344	-3.30731	3030.0425	3032.2460	3033.7606
H	1.70566	-0.24377	-3.74264	3034.3016	3034.9436	3039.2358
H	1.58356	-2.01076	-3.80554	3051.5528	3057.8412	3105.9101
C	0.26959	-3.30763	-1.24868	3111.8869	3112.2474	3116.1141
H	-0.51847	-2.94207	-1.91662	3123.5954	3123.7284	3140.3951
H	0.79538	-4.12432	-1.76071	3141.6787	3144.7898	3145.2455
H	-0.22341	-3.72108	-0.36265	3146.3656	3151.0847	3154.6058
C	1.77150	-2.84513	1.58980	3157.2099	3168.4472	3171.2958
H	2.73683	-3.33215	1.77803	3190.2900	3193.3606	3207.1997
H	1.49827	-2.24651	2.46659			
H	1.01080	-3.62494	1.48544			
C	1.13997	1.72328	2.87085			
H	0.40911	2.40330	3.31794			
H	0.73808	0.71249	3.00184			
H	2.11364	1.83534	3.35461			
O	2.36010	2.55915	1.01650			
H	-1.15188	3.66418	1.61106			
Ir	-0.62047	-0.70041	0.11904			
C	0.44977	0.11053	-1.40954			
C	1.90963	-0.11000	-1.58743			
C	2.63591	-0.98942	-0.76992			
C	2.60983	0.57889	-2.61199			
C	3.99264	-1.20281	-0.93980			
H	2.09836	-1.50184	0.02419			
C	3.99050	0.38014	-2.76469			
C	4.66835	-0.50261	-1.94534			
H	4.52578	-1.89788	-0.29505			
H	4.49374	0.93083	-3.55537			
H	5.73664	-0.65180	-2.08869			
O	2.01470	1.42121	-3.45268			
H	1.05248	1.40850	-3.22142			
H	5.67274	-0.47492	-2.32853			
C	0.63389	0.75102	-2.26539			
C	2.92715	1.58077	-1.45499			
C	4.85170	2.36254	-0.35019			
H	4.58554	3.41370	-0.51439			
H	5.46963	2.04686	-1.20246			
C	5.53081	2.13074	0.97347			
H	6.47248	2.68645	1.02514			
H	4.88756	2.45610	1.79667			
H	5.74242	1.06336	1.11047			
O	3.65827	1.57347	-0.34098			
O	3.14601	2.29349	-2.40703			
C	0.92000	0.94807	-3.71343			
H	-0.00533	0.88337	-4.29044			
H	1.41585	1.91119	-3.86642			
H	1.63737	0.18240	-4.03787			
O	-0.52197	0.63428	-1.87363			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.459023 Electronic Energy = -1482.10151968
Internal Energy (E)= -1481.61023768 Enthalpy (H)= -1481.60929368

Gibbs Free Energy (G)=-1481.70227968	Gibbs Free Energy of Solvation=-1482.91180229

St.Pt.	General Structure	Ball & Stick model
V-1B	 **V-1B**	

Cartesian co-ordinate

Atoms	X	Y	Z
C	0.47545	2.11894	-1.52651
C	-0.90653	1.71237	-1.55309
C	-1.50107	2.06699	-0.28158
C	-0.46127	2.60371	0.54960
C	0.74872	2.67338	-0.25244
C	2.20432	-1.24195	-0.77018
Ir	0.02774	0.45467	0.04265
O	0.93931	-1.06359	-1.07736
C	2.76274	-0.57778	0.33992
C	4.10228	-0.76891	0.71171
C	3.03368	-2.09386	-1.52525
C	4.90509	-1.59860	-0.04310
C	4.35583	-2.25539	-1.15838
C	1.86266	0.28194	1.09061
O	2.08398	0.87818	2.11173
H	2.60896	-2.61540	-2.37914
H	4.98865	-2.91446	-1.75039
H	5.94867	-1.74982	0.21919
H	4.47627	-0.24728	1.59000
C	-0.73191	-0.90819	1.12633
C	-1.69493	-0.68122	2.24970
C	-0.26693	-2.32472	0.98528
C	-2.07721	-2.72440	-0.57786
H	-2.88103	-3.45094	-0.40067
H	-2.42836	-1.74226	-0.22697
C	-1.69186	-2.66583	-2.03569
H	-2.55389	-2.37311	-2.64759
H	-0.87917	-1.94651	-2.18133

Frequencies

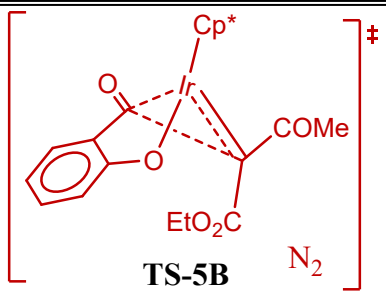
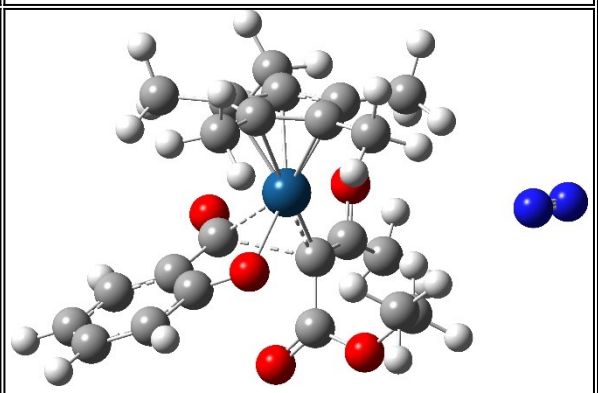
20.8074	33.2824	37.0582
41.9100	47.4103	53.6751
68.8856	74.0482	84.6281
88.4159	104.4796	111.6069
114.9893	128.7511	146.2143
150.7227	155.4222	166.1243
173.7100	187.2636	190.7329
196.9793	198.5387	202.3193
206.8231	215.3108	227.0888
235.7233	240.7459	245.4130
255.6639	262.3443	268.5484
290.8550	294.2059	309.1886
314.2195	319.7226	335.3350
361.2731	368.2457	373.2984
377.1710	412.5197	414.2411
417.8928	421.4407	442.3889
471.7675	505.6278	533.7092
538.1920	540.4489	552.7446
568.7700	580.3991	589.3912
601.1426	607.4002	624.0480
631.2509	646.8292	658.6568
693.0748	722.3591	753.1491
762.2339	812.2526	816.3708
819.9088	843.7858	857.1354
877.8722	917.4574	941.3287
950.4869	962.6049	980.7452
981.5524	1002.0784	1024.1597
1034.2272	1037.3705	1038.1098
1041.7864	1045.2174	1049.6525
1055.4514	1094.2739	1097.6718
1112.2883	1119.2358	1123.0113
1146.5136	1147.0798	1178.7615

H	-1.34462	-3.64677	-2.37633	1185.7818	1187.3763	1208.4152
O	-0.97184	-3.16912	0.21046	1230.7828	1261.2343	1282.7114
O	0.68070	-2.73654	1.61101	1341.6227	1353.2469	1374.7211
N	-5.34829	-1.56204	-1.05821	1379.3310	1383.5877	1394.4794
N	-4.83639	-0.80705	-1.68226	1398.7926	1400.4845	1402.0917
C	2.02801	3.28281	0.19878	1404.6398	1426.7661	1437.8140
H	2.00565	4.36668	0.02638	1439.9791	1447.6279	1450.0875
H	2.19450	3.11266	1.26634	1451.7122	1453.6584	1454.6891
H	2.88788	2.87305	-0.34212	1460.1937	1464.0555	1465.8458
C	1.43940	1.89493	-2.63975	1471.7804	1478.5655	1483.3135
H	1.23148	2.56362	-3.48471	1485.1834	1495.6903	1498.3282
H	2.47154	2.06667	-2.31899	1502.3810	1507.9621	1515.9808
H	1.37536	0.86256	-3.00468	1517.9314	1519.1699	1552.2476
C	-1.59831	1.13906	-2.74148	1623.1529	1660.8983	1777.7905
H	-1.89087	1.92786	-3.44805	1835.3120	1847.8454	2464.8003
H	-0.94056	0.44326	-3.27532	3017.6714	3032.2760	3036.7113
H	-2.50423	0.59057	-2.46157	3037.5473	3040.2389	3041.3469
C	-2.95045	2.00062	0.04444	3042.5045	3046.9164	3077.1247
H	-3.42924	2.96089	-0.18897	3109.8219	3114.0442	3120.9833
H	-3.45818	1.22952	-0.54561	3121.2128	3128.0203	3128.2132
H	-3.10885	1.77896	1.10301	3131.5315	3137.8911	3141.9976
C	-0.61044	3.17050	1.91696	3152.9933	3155.8097	3170.0977
H	-0.67770	4.26617	1.87847	3174.1288	3175.9400	3176.8912
H	-1.50222	2.77592	2.40913	3196.0693	3204.2831	3210.7723
H	0.25042	2.90320	2.53860			
O	-2.11875	0.43235	2.51880			
C	-2.09881	-1.87755	3.07164			
H	-1.21546	-2.30512	3.56121			
H	-2.82974	-1.57432	3.82342			
H	-2.51609	-2.67270	2.44087			
H	-1.15188	3.66418	1.61106			
Ir	-0.62047	-0.70041	0.11904			
C	0.44977	0.11053	-1.40954			
C	1.90963	-0.11000	-1.58743			
C	2.63591	-0.98942	-0.76992			
C	2.60983	0.57889	-2.61199			
C	3.99264	-1.20281	-0.93980			
H	2.09836	-1.50184	0.02419			
C	3.99050	0.38014	-2.76469			
C	4.66835	-0.50261	-1.94534			
H	4.52578	-1.89788	-0.29505			
H	4.49374	0.93083	-3.55537			
H	5.73664	-0.65180	-2.08869			
O	2.01470	1.42121	-3.45268			
H	1.05248	1.40850	-3.22142			
H	5.67274	-0.47492	-2.32853			
C	0.63389	0.75102	-2.26539			
C	2.92715	1.58077	-1.45499			
C	4.85170	2.36254	-0.35019			
H	4.58554	3.41370	-0.51439			
H	5.46963	2.04686	-1.20246			
C	5.53081	2.13074	0.97347			
H	6.47248	2.68645	1.02514			
H	4.88756	2.45610	1.79667			
H	5.74242	1.06336	1.11047			
O	3.65827	1.57347	-0.34098			
O	3.14601	2.29349	-2.40703			
C	0.92000	0.94807	-3.71343			
H	-0.00533	0.88337	-4.29044			
H	1.41585	1.91119	-3.86642			
H	1.63737	0.18240	-4.03787			

O	-0.52197	0.63428	-1.87363

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.459234 Electronic Energy = -1482.14652904
Internal Energy (E)= -1481.65317904 Enthalpy (H)= -1481.65223504
Gibbs Free Energy (G)=-1481.75243804 Gibbs Free Energy of Solvation=-1482.97001474

St.Pt.	General Structure	Ball & Stick model
TS-5B		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.04859	-2.54328	-1.04283
C	1.29695	-2.02928	-1.00942
C	1.70279	-1.89978	0.38610
C	0.57723	-2.24528	1.19111
C	-0.51131	-2.63238	0.29365
C	-2.33497	0.67975	-1.02167
Ir	0.09385	-0.48787	-0.06129
O	-1.10766	0.52613	-1.45805
C	-2.63713	0.62083	0.36199
C	-3.95548	0.76019	0.82634
C	-3.39898	0.90852	-1.91742
C	-4.98360	0.96372	-0.06948
C	-4.68829	1.04200	-1.44142
C	-1.55798	0.41026	1.30879

Frequencies

-235.1842	-17.0819	23.4387
27.0306	32.4427	35.9095
47.2275	57.5048	65.1597
88.0761	90.3639	94.5811
101.6127	104.1865	109.6818
133.4839	134.2155	144.7698
153.6594	167.9343	173.7572
176.0973	183.6277	192.2059
201.3334	204.6189	212.1934
223.9501	229.8711	235.6723
247.0556	249.2624	257.2234
275.8470	282.9552	291.7949
298.6458	306.6377	317.0160
324.0614	330.4055	349.3384
386.6048	399.6129	412.6562
416.2070	433.2779	444.5016
461.2635	499.7676	527.0492
532.5974	539.5196	546.7510

O	-1.60879	0.21412	2.49002	548.8539	560.8700	575.8531
H	-3.17146	0.96987	-2.97868	586.1216	598.1222	605.6974
H	-5.49679	1.20791	-2.15140	618.1381	638.4123	641.2960
H	-6.00788	1.06804	0.27739	687.2464	717.6288	750.7991
H	-4.13424	0.70507	1.89792	759.4963	792.1632	806.6185
C	0.25773	1.26624	0.76312	810.9546	812.9233	857.9106
C	0.98648	1.47952	2.05070	876.8786	915.5166	938.1586
C	-0.16450	2.54398	0.08779	950.4643	951.8072	958.7938
C	1.87506	2.46805	-1.26720	979.9933	1001.6198	1027.0930
H	2.64873	3.24640	-1.25280	1033.6940	1038.5884	1039.6826
H	2.18309	1.66470	-0.58383	1042.8191	1045.8309	1046.4030
C	1.65872	1.93142	-2.66089	1046.9489	1083.4096	1088.9576
H	2.58652	1.49365	-3.04838	1103.1406	1116.0682	1120.5314
H	0.87495	1.16512	-2.65285	1144.8109	1147.0492	1172.6107
H	1.34214	2.73442	-3.33425	1180.9444	1183.0744	1202.5467
O	0.68609	3.10345	-0.79552	1233.8523	1258.3591	1262.8944
O	-1.17178	3.14416	0.37724	1340.0945	1343.2043	1371.1375
N	5.63639	1.37166	-0.34068	1375.1379	1378.3787	1381.6955
N	4.91713	1.06166	-1.12062	1389.2908	1393.1299	1396.5458
C	-1.86400	-3.06074	0.74547	1398.5908	1414.7722	1431.7313
H	-1.91342	-4.15303	0.84400	1435.6880	1443.7121	1445.5778
H	-2.10677	-2.62629	1.72020	1449.3609	1450.2536	1454.8481
H	-2.64205	-2.74897	0.04050	1459.2330	1460.8426	1461.6054
C	-0.84215	-2.76505	-2.28242	1467.2392	1468.0183	1471.6795
H	-0.56504	-3.71080	-2.76521	1476.9450	1480.9180	1484.6095
H	-1.91570	-2.79558	-2.07066	1490.2222	1492.1243	1497.9690
H	-0.67594	-1.95668	-3.00384	1516.3651	1523.8035	1552.2037
C	2.15468	-1.80423	-2.20602	1610.7668	1663.3914	1778.6853
H	2.55020	-2.75527	-2.58842	1837.9132	1857.5058	2464.7591
H	1.58882	-1.32718	-3.01443	3022.7485	3032.5236	3037.6306
H	3.00961	-1.15756	-1.97651	3038.4877	3038.9749	3041.2710
C	3.05087	-1.51302	0.87712	3041.6191	3049.1408	3085.7989
H	3.64561	-2.39831	1.13717	3101.7491	3115.8031	3118.3553
H	3.60033	-0.95398	0.11275	3119.2400	3120.9619	3124.1073
H	2.95861	-0.87908	1.76412	3129.6674	3138.3858	3139.8052
C	0.51630	-2.33803	2.67539	3146.1088	3160.5401	3170.5493
H	0.30002	-3.37250	2.97364	3171.5470	3172.9914	3179.5395
H	1.45807	-2.02912	3.13286	3193.5820	3202.1694	3209.8152
H	-0.26360	-1.68553	3.08302			
O	1.37470	0.53775	2.72345			
C	1.22100	2.89827	2.49820			
H	0.25603	3.38887	2.67505			
H	1.81719	2.89857	3.41259			
H	1.72660	3.48482	1.71948			
H	-1.15188	3.66418	1.61106			
Ir	-0.62047	-0.70041	0.11904			
C	0.44977	0.11053	-1.40954			
C	1.90963	-0.11000	-1.58743			
C	2.63591	-0.98942	-0.76992			
C	2.60983	0.57889	-2.61199			
C	3.99264	-1.20281	-0.93980			
H	2.09836	-1.50184	0.02419			
C	3.99050	0.38014	-2.76469			
C	4.66835	-0.50261	-1.94534			
H	4.52578	-1.89788	-0.29505			
H	4.49374	0.93083	-3.55537			
H	5.73664	-0.65180	-2.08869			
O	2.01470	1.42121	-3.45268			
H	1.05248	1.40850	-3.22142			
H	5.67274	-0.47492	-2.32853			
C	0.63389	0.75102	-2.26539			

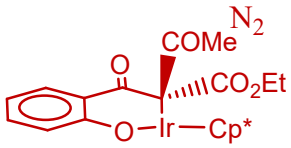
C	2.92715	1.58077	-1.45499
C	4.85170	2.36254	-0.35019
H	4.58554	3.41370	-0.51439
H	5.46963	2.04686	-1.20246
C	5.53081	2.13074	0.97347
H	6.47248	2.68645	1.02514
H	4.88756	2.45610	1.79667
H	5.74242	1.06336	1.11047
O	3.65827	1.57347	-0.34098
O	3.14601	2.29349	-2.40703
C	0.92000	0.94807	-3.71343
H	-0.00533	0.88337	-4.29044
H	1.41585	1.91119	-3.86642
H	1.63737	0.18240	-4.03787
O	-0.52197	0.63428	-1.87363

Statistical Thermodynamic Analysis

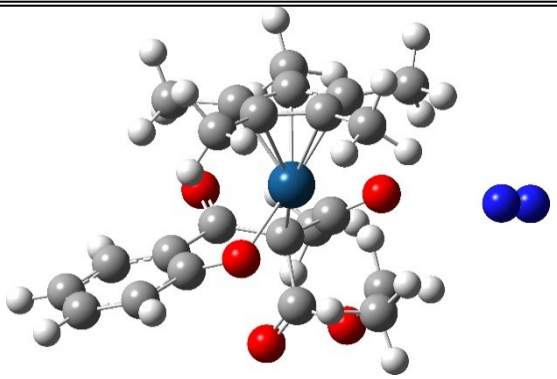
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.456202 Electronic Energy = -1482.12927983
Internal Energy (E)= -1481.63951383 Enthalpy (H)= -1481.63856983
Gibbs Free Energy (G)=-1481.73810283 Gibbs Free Energy of Solvation=-1482.95800532

St.Pt.	General Structure	Ball & Stick model

VI-1B



VI-1B



Cartesian co-ordinate

Atoms	X	Y	Z
C	0.46464	-2.67915	-0.03927
C	1.77667	-2.17846	-0.17572
C	2.07987	-1.33328	0.98484
C	0.94167	-1.31642	1.83444
C	-0.10819	-2.08313	1.16538
C	-2.36884	-0.13695	-1.13094
Ir	0.34558	-0.43424	-0.06366
O	-1.10103	-0.25855	-1.52022
C	-2.74888	0.39104	0.12631
C	-4.09400	0.38585	0.50620
C	-3.37814	-0.60673	-1.98706
C	-5.08025	-0.08253	-0.34620
C	-4.70891	-0.57159	-1.60027
C	-1.75688	0.94069	1.08210
O	-1.96645	0.91187	2.29471
H	-3.07670	-1.01062	-2.95139
H	-5.46956	-0.94632	-2.28311
H	-6.12449	-0.06614	-0.04589
H	-4.33923	0.77590	1.49188
C	-0.45433	1.43453	0.51308
C	0.44811	2.21793	1.46922
C	-0.71667	2.40267	-0.64176
C	1.36553	1.78516	-1.78282
H	2.25151	2.42038	-1.64999
H	1.48754	1.02285	-0.96583
C	1.31649	1.14940	-3.14750
H	2.20776	0.53008	-3.30721
H	0.42196	0.52615	-3.23683
H	1.28543	1.92110	-3.92307
O	0.23566	2.60095	-1.57706
O	-1.70348	3.09256	-0.67663
N	4.91376	1.85181	-0.83768
N	4.48134	1.01082	-1.40980
C	-1.45708	-2.38330	1.71361
H	-1.42227	-3.29897	2.31958
H	-1.82536	-1.56437	2.34138
H	-2.18593	-2.53445	0.90902
C	-0.30691	-3.51733	-0.99562
H	-0.63094	-4.45211	-0.52152
H	-1.20286	-2.98463	-1.33969
H	0.28576	-3.77349	-1.87820

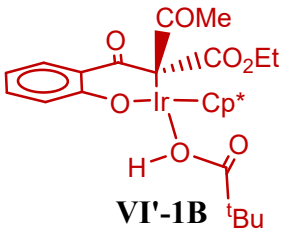
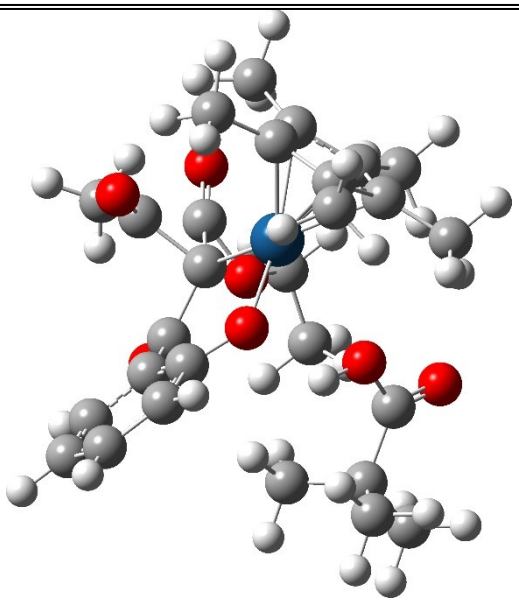
Frequencies

35.4976	40.6966	50.9289
62.4410	69.8747	73.9471
89.1487	92.7410	98.9091
100.0937	108.7539	110.4346
115.3284	126.3654	133.7208
141.7102	155.5138	158.9813
163.4935	168.9870	190.6685
196.2246	211.5746	215.1941
217.8074	221.1314	232.5653
233.7832	240.6802	258.6831
266.6086	272.5395	277.9095
279.2167	294.9694	302.7888
309.2104	319.9889	330.0036
340.8588	356.5126	375.0578
391.8967	400.7234	412.5147
433.4952	473.4456	479.7077
520.4019	529.4026	537.1452
539.4742	543.0173	550.1981
554.2398	579.6104	589.2726
595.4549	610.1223	632.8635
637.0163	668.3883	690.4314
719.1218	741.5636	762.8115
773.4666	806.6797	813.9185
847.5640	864.4532	877.5890
885.1715	912.2144	956.8862
961.4275	964.9379	968.3998
976.8773	1018.7323	1032.7070
1037.3989	1040.9117	1050.5669
1051.0354	1052.6322	1058.8136
1087.7981	1090.6507	1097.4731
1109.9626	1112.5783	1128.8426
1132.4487	1150.8720	1154.4089
1179.9881	1187.1045	1208.2781
1218.5682	1252.2845	1269.6407
1282.9875	1329.8735	1366.0182
1367.5522	1369.4308	1374.4478
1378.9979	1389.8565	1394.4037
1398.6488	1401.4430	1428.4103
1430.8601	1435.8085	1444.6149
1447.2736	1448.3938	1453.4656
1455.3746	1464.3372	1466.4235
1469.2528	1474.0319	1477.0810
1482.0912	1487.1084	1491.8585
1492.6807	1495.0332	1501.2458
1501.7131	1531.8000	1565.1837
1620.9497	1664.6673	1736.6263

C	2.70763	-2.41043	-1.31392	1803.0959	1855.4446	2464.6808
H	3.43650	-3.19590	-1.07548	2768.4586	3026.1407	3030.9367
H	2.16477	-2.71103	-2.21556	3036.5553	3036.9524	3042.0064
H	3.27045	-1.50088	-1.55637	3045.3359	3049.6601	3073.0630
C	3.39049	-0.69342	1.28814	3101.6385	3111.5877	3114.8306
H	3.84374	-1.15234	2.17607	3120.0382	3123.8567	3130.4112
H	4.09612	-0.81525	0.46114	3138.8936	3142.3143	3146.1485
H	3.26268	0.37754	1.48115	3148.1987	3149.1367	3158.3282
C	0.82786	-0.67152	3.16961	3160.5467	3170.0272	3173.6722
H	0.93506	-1.42402	3.96181	3189.1591	3194.4171	3205.6084
H	1.60638	0.08511	3.30702			
H	-0.14876	-0.18571	3.29325			
O	1.66132	2.09889	1.41761			
C	-0.20157	3.20532	2.38918			
H	-0.71422	2.65642	3.18633			
H	0.55294	3.87788	2.80319			
H	-0.98143	3.76512	1.85929			
H	-1.15188	3.66418	1.61106			
Ir	-0.62047	-0.70041	0.11904			
C	0.44977	0.11053	-1.40954			
C	1.90963	-0.11000	-1.58743			
C	2.63591	-0.98942	-0.76992			
C	2.60983	0.57889	-2.61199			
C	3.99264	-1.20281	-0.93980			
H	2.09836	-1.50184	0.02419			
C	3.99050	0.38014	-2.76469			
C	4.66835	-0.50261	-1.94534			
H	4.52578	-1.89788	-0.29505			
H	4.49374	0.93083	-3.55537			
H	5.73664	-0.65180	-2.08869			
O	2.01470	1.42121	-3.45268			
H	1.05248	1.40850	-3.22142			
H	5.67274	-0.47492	-2.32853			
C	0.63389	0.75102	-2.26539			
C	2.92715	1.58077	-1.45499			
C	4.85170	2.36254	-0.35019			
H	4.58554	3.41370	-0.51439			
H	5.46963	2.04686	-1.20246			
C	5.53081	2.13074	0.97347			
H	6.47248	2.68645	1.02514			
H	4.88756	2.45610	1.79667			
H	5.74242	1.06336	1.11047			
O	3.65827	1.57347	-0.34098			
O	3.14601	2.29349	-2.40703			
C	0.92000	0.94807	-3.71343			
H	-0.00533	0.88337	-4.29044			
H	1.41585	1.91119	-3.86642			
H	1.63737	0.18240	-4.03787			
O	-0.52197	0.63428	-1.87363			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.458819 Electronic Energy = -1482.16119943
Internal Energy (E)= -1481.66877143 Enthalpy (H)= -1481.66782843
Gibbs Free Energy (G)=-1481.76501043 Gibbs Free Energy of Solvation=-1482.98270527

St.Pt.	General Structure	Ball & Stick model
VI'-1B	 **VI'-1B**	

Cartesian co-ordinate

Atoms	X	Y	Z
C	-2.43396	-0.57391	-2.10670
C	-1.74322	-1.74611	-1.72247
C	-2.01745	-2.00896	-0.30577
C	-2.92571	-1.01173	0.16446
C	-3.11679	-0.06595	-0.92601
O	1.43007	-1.06824	-1.35264
C	2.54875	-1.72149	-0.99905
O	2.46024	-2.89153	-0.70520
C	3.84421	-0.91807	-1.03108
C	0.70688	2.37587	-0.86781
H	1.50690	-0.10676	-1.50641
C	-0.88165	-2.60686	-2.57249
H	0.00547	-2.94531	-2.02810
H	-1.44813	-3.49118	-2.89410
H	-0.53807	-2.07701	-3.46597
C	-1.49583	-3.18976	0.43371
H	-2.06719	-4.09056	0.17272
H	-0.44423	-3.37222	0.17491
H	-1.55668	-3.03928	1.51590
C	-3.98184	1.13972	-0.87464
H	-3.79361	1.79765	-1.72820
H	-5.04067	0.84807	-0.89225
H	-3.78693	1.71052	0.03837
C	-2.37380	0.11955	-3.42172
H	-2.18412	1.19021	-3.28532
H	-1.56278	-0.27597	-4.04042
H	-3.31290	0.00762	-3.97780

Frequencies

31.5043	38.7628	48.8504
63.6136	68.2999	75.6113
77.1923	82.7923	85.0118
94.4967	101.4240	114.7698
117.6008	119.6885	134.2672
137.3327	141.4768	148.1925
163.0078	169.1491	176.0941
186.1667	194.8417	196.2958
199.0940	202.7968	216.7815
222.8668	229.5664	238.1154
242.7031	248.7281	254.5620
264.4836	268.9558	274.9080
280.1311	280.7424	289.2504
298.3559	308.1830	310.7201
315.2398	322.4383	324.2429
336.4824	340.8642	369.7131
375.5369	382.6916	385.5498
390.7050	394.3012	407.5360
422.1666	432.3763	438.3569
462.2172	479.9810	522.2401
532.3752	532.8127	539.6033
544.2865	551.1033	570.6105
574.0359	581.2197	585.6263
593.7536	603.5938	630.1441
657.3469	676.4481	691.3771
724.8660	761.6756	773.0967
775.5574	786.7849	793.8191
804.8362	807.1968	812.6023
861.8401	874.7168	880.0667
889.0489	904.0935	906.7710
946.4071	953.2704	955.8535

C	-3.61496	-0.94844	1.48140
H	-4.57810	-1.47237	1.42501
H	-3.01185	-1.40393	2.27204
H	-3.81445	0.09040	1.76764
Ir	-1.06066	-0.06627	-0.40660
C	4.03296	-0.31008	-2.42630
H	3.25155	0.41746	-2.68183
H	4.99039	0.22366	-2.46095
H	4.04985	-1.08360	-3.20382
C	3.76937	0.20089	0.01248
H	3.52304	-0.18364	1.00941
H	4.73888	0.71079	0.06867
H	3.02176	0.96147	-0.24625
C	5.01261	-1.84594	-0.72046
H	4.93262	-2.26418	0.28854
H	5.05634	-2.68308	-1.42536
H	5.95313	-1.28538	-0.78387
O	0.14979	1.27432	-1.36453
C	1.11332	2.53331	0.47590
C	1.81863	3.68962	0.84756
C	0.99653	3.40770	-1.78015
C	2.08949	4.69862	-0.05584
C	1.66844	4.54815	-1.38071
C	0.90958	1.51891	1.52619
O	1.63037	1.49406	2.51587
H	0.67917	3.26664	-2.81110
H	1.87303	5.33025	-2.10951
H	2.62075	5.59326	0.25776
H	2.14202	3.75902	1.88347
C	-0.30713	0.59250	1.48571
C	-1.36947	1.46445	2.17940
C	-0.03953	-0.68854	2.21454
C	1.47350	-2.44004	2.61324
H	1.15169	-2.31589	3.65263
H	0.89936	-3.27572	2.19026
C	2.95652	-2.67348	2.50692
H	3.50909	-1.79264	2.85465
H	3.24049	-3.52326	3.13691
H	3.24239	-2.90295	1.47551
O	-0.82120	-1.23881	2.97114
O	1.14224	-1.24268	1.88813
C	-1.37626	1.50124	3.68208
H	-1.89541	2.40466	4.01068
H	-1.89608	0.61569	4.06077
H	-0.35596	1.46529	4.07902
O	-2.11766	2.17890	1.53726
H	5.67274	-0.47492	-2.32853
C	0.63389	0.75102	-2.26539
C	2.92715	1.58077	-1.45499
C	4.85170	2.36254	-0.35019
H	4.58554	3.41370	-0.51439
H	5.46963	2.04686	-1.20246
C	5.53081	2.13074	0.97347
H	6.47248	2.68645	1.02514
H	4.88756	2.45610	1.79667
H	5.74242	1.06336	1.11047
O	3.65827	1.57347	-0.34098
O	3.14601	2.29349	-2.40703
C	0.92000	0.94807	-3.71343
H	-0.00533	0.88337	-4.29044
H	1.41585	1.91119	-3.86642

963.4068	972.5467	979.3693
981.1329	1001.9518	1009.9741
1032.7660	1034.4205	1036.0817
1036.9807	1039.9653	1043.3665
1046.0872	1049.5263	1062.0273
1085.9920	1088.2451	1091.6733
1098.6558	1113.1335	1115.4729
1129.1477	1140.1356	1149.6690
1174.4793	1183.3964	1187.3640
1192.4664	1212.4817	1235.3753
1240.7751	1261.8779	1272.6859
1282.7131	1296.6902	1332.0501
1347.9160	1369.5295	1375.7717
1376.8506	1382.4776	1383.4408
1387.9758	1392.7967	1394.3201
1398.6224	1409.5641	1415.5011
1421.1202	1430.1734	1433.7119
1442.4718	1443.3278	1444.9759
1449.4073	1450.9437	1454.0097
1457.7751	1459.5128	1459.7827
1462.0778	1469.8407	1470.0457
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1484.8849	1486.5879	1487.4095
1488.3554	1492.2749	1497.5798
1503.4849	1508.9598	1510.5486
1531.3038	1559.3667	1620.7580
1666.7544	1752.1564	1793.6122
1802.6704	1862.0817	3031.4812
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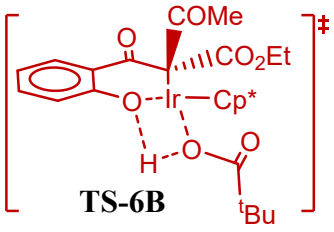
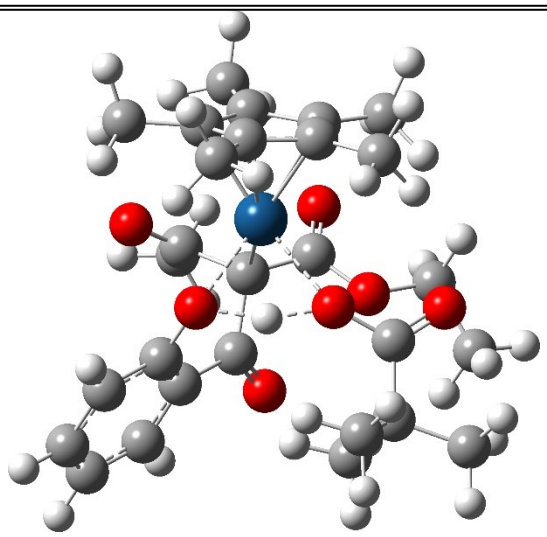
3041.7867	3042.8976	3045.5125
3048.9026	3049.3707	3055.2123
3057.8767	3112.5849	3115.0031
3119.0921	3120.4249	3124.8621
3127.9249	3128.0579	3129.1427
3130.6056	3131.3837	3132.9138
3144.8285	3146.0793	3146.8456
3148.8985	3152.1245	3161.2838
3172.7644	3172.7815	3178.4135
3193.2719	3198.0153	3201.6534
3205.2445	3209.1249	3667.9108

H	1.63737	0.18240	-4.03787
O	-0.52197	0.63428	-1.87363

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.602748 Electronic Energy = -1719.54899461
Internal Energy (E)= -1718.90715761 Enthalpy (H)= -1718.90621461
Gibbs Free Energy (G)=-1719.01333361 Gibbs Free Energy of Solvation=-1720.41701585

St.Pt.	General Structure	Ball & Stick model
TS-6B		

TS-6B

Cartesian co-ordinate

Atoms	X	Y	Z
C	-2.53848	-0.41682	-1.94745
C	-2.13050	-1.67816	-1.45000
C	-2.34383	-1.69825	-0.00357
C	-2.97742	-0.45229	0.36618
C	-3.01605	0.37630	-0.81826
O	1.00315	-0.98548	-1.30366
C	1.96541	-1.85563	-1.01507
O	1.68841	-2.93433	-0.53099
C	3.38260	-1.42730	-1.38565
C	0.93516	2.48290	-0.92052
H	0.81446	0.27448	-1.49933
C	-1.48364	-2.78526	-2.20053

Frequencies

-1640.1876	31.2332	43.2933
47.4948	58.2135	71.5914
75.0652	82.1126	87.5425
94.1025	102.4693	104.9111
111.2276	115.4342	120.2065
133.2689	137.3737	148.5347
151.2524	157.3249	163.0417
168.8998	177.2837	182.0654
192.3589	195.8082	200.0633
215.0711	218.0055	223.8164
228.6481	235.2307	241.4096
261.7717	271.2315	276.1855
294.6121	299.5262	300.8128
307.1561	315.2160	319.5326
320.1401	327.6925	331.4183
343.2593	346.5780	353.9866

H	-0.61543	-3.16682	-1.65050	367.7560	372.3143	382.8921
H	-2.19354	-3.61029	-2.34389	386.0867	387.0595	409.6541
H	-1.13431	-2.45608	-3.18353	415.1367	421.2457	435.0161
C	-2.09462	-2.87591	0.87130	445.8006	467.4536	469.8834
H	-2.89017	-3.62418	0.75757	531.3929	533.4070	537.0718
H	-1.13956	-3.34669	0.60692	548.2665	552.5929	557.0938
H	-2.03744	-2.58128	1.92389	563.5859	570.5505	592.3627
C	-3.55828	1.75532	-0.92678	594.2871	599.4780	604.6854
H	-2.99880	2.32738	-1.67501	605.5853	645.6818	689.2425
H	-4.61156	1.72768	-1.23688	717.9295	763.5002	768.6919
H	-3.47180	2.29124	0.02115	777.3339	784.7282	801.6861
C	-2.41539	0.09700	-3.33870	808.2837	811.4575	812.9790
H	-1.88377	1.05585	-3.35070	858.5741	870.7597	884.7885
H	-1.85671	-0.59762	-3.97271	896.8921	903.2865	909.8784
H	-3.40304	0.25183	-3.79133	945.0507	949.4891	956.1762
C	-3.55057	-0.12891	1.69822	962.3070	971.0944	981.0393
H	-4.54470	-0.58700	1.78373	984.3198	993.3024	1006.0032
H	-2.92216	-0.52070	2.50533	1025.5814	1033.9202	1039.3000
H	-3.65817	0.95009	1.83782	1040.3569	1041.7636	1045.9179
Ir	-0.97939	-0.11016	-0.38369	1048.8152	1058.9409	1065.1934
C	3.41883	-0.87689	-2.81286	1084.8671	1097.3304	1104.4024
H	2.80240	0.02275	-2.92208	1112.6033	1115.6528	1131.1909
H	4.45011	-0.60645	-3.07258	1135.0693	1149.5395	1180.4535
H	3.07344	-1.62170	-3.54091	1185.4454	1189.0734	1196.7898
C	3.81618	-0.33738	-0.40201	1215.0618	1237.1580	1239.3367
H	3.66773	-0.64815	0.63999	1256.4087	1264.9786	1275.2996
H	4.87956	-0.11028	-0.54983	1293.7903	1306.2335	1318.9370
H	3.25491	0.59182	-0.55952	1342.4839	1369.9288	1374.3054
C	4.31494	-2.62819	-1.27584	1375.8546	1378.5312	1380.7654
H	4.35928	-3.00817	-0.24992	1387.1396	1389.5055	1397.0793
H	3.98428	-3.45046	-1.92019	1403.0517	1407.6266	1411.2276
H	5.32884	-2.33596	-1.57664	1416.4833	1431.5115	1436.7840
O	0.20466	1.50232	-1.49062	1441.3057	1442.5453	1443.9241
C	1.53121	2.38909	0.34922	1448.4270	1450.5694	1453.5883
C	2.36243	3.43519	0.78091	1454.4595	1456.7873	1463.8425
C	1.13835	3.63252	-1.69279	1467.6006	1468.5146	1477.5855
C	2.56468	4.56686	0.01274	1478.5100	1478.7745	1480.8868
C	1.93712	4.66469	-1.22999	1483.7441	1488.3722	1490.6408
C	1.33790	1.27632	1.31374	1492.4671	1498.0406	1500.2670
O	2.20315	1.04152	2.14384	1505.1838	1514.0459	1515.2550
H	0.66468	3.67368	-2.67060	1524.7409	1557.7749	1611.5146
H	2.08127	5.54910	-1.84701	1632.4604	1667.1614	1763.2832
H	3.19887	5.37119	0.37595	1788.5846	1812.5167	1813.3275
H	2.83196	3.32652	1.75568	3029.5427	3034.3620	3034.5906
C	-0.02765	0.59665	1.42668	3035.3943	3037.8538	3038.6849
C	-0.87586	1.70416	2.07373	3039.9110	3040.3505	3041.3055
C	0.04902	-0.63877	2.27115	3045.2244	3055.8444	3110.6482
C	1.26072	-2.63114	2.67023	3114.9602	3116.6445	3116.8022
H	0.92365	-2.45952	3.69820	3119.7970	3120.9458	3121.9701
H	0.63308	-3.42032	2.23460	3124.7117	3126.7411	3128.2489
C	2.72400	-2.97737	2.59040	3132.5956	3137.9210	3142.2678
H	3.32927	-2.13822	2.95183	3147.6466	3148.1748	3148.2502
H	2.94269	-3.85629	3.20591	3148.7261	3151.6577	3164.5576
H	3.00110	-3.19918	1.55464	3170.1231	3177.3681	3180.7160
O	-0.75828	-0.94425	3.13504	3193.5898	3200.5072	3208.3310
O	1.06284	-1.42990	1.91388			
C	-0.71038	1.93810	3.55117			
H	-1.01569	2.96081	3.78498			
H	-1.34542	1.23214	4.09628			
H	0.31820	1.75251	3.87867			
O	-1.59139	2.42863	1.40879			

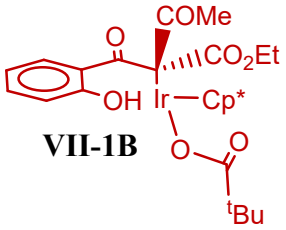
H	5.67274	-0.47492	-2.32853
C	0.63389	0.75102	-2.26539
C	2.92715	1.58077	-1.45499
C	4.85170	2.36254	-0.35019
H	4.58554	3.41370	-0.51439
H	5.46963	2.04686	-1.20246
C	5.53081	2.13074	0.97347
H	6.47248	2.68645	1.02514
H	4.88756	2.45610	1.79667
H	5.74242	1.06336	1.11047
O	3.65827	1.57347	-0.34098
O	3.14601	2.29349	-2.40703
C	0.92000	0.94807	-3.71343
H	-0.00533	0.88337	-4.29044
H	1.41585	1.91119	-3.86642
H	1.63737	0.18240	-4.03787
O	-0.52197	0.63428	-1.87363

Statistical Thermodynamic Analysis

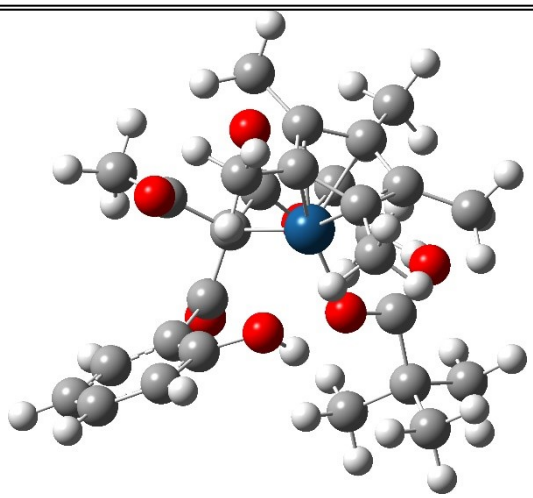
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.596957 Electronic Energy = -1719.51583524
Internal Energy (E)= -1718.88013524 Enthalpy (H)= -1718.87919124
Gibbs Free Energy (G)=-1718.98556624 Gibbs Free Energy of Solvation=-1720.38490964

St.Pt.	General Structure	Ball & Stick model

VII-1B



VII-1B



Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.28620	-2.64636	-1.62707
C	0.99836	-2.64419	-1.03561
C	0.82239	-2.62675	0.41596
C	-0.60179	-2.76060	0.69219
C	-1.28425	-2.68491	-0.56019
O	1.06493	0.73495	-0.98227
C	2.36152	0.85637	-0.87042
O	3.09470	0.05124	-0.31147
C	2.89314	2.12664	-1.55071
C	-2.21434	1.54198	-1.25211
H	-0.41992	1.05209	-1.81336
C	2.30448	-2.61852	-1.74424
H	3.02546	-1.99985	-1.20452
H	2.70339	-3.63747	-1.83638
H	2.20308	-2.20577	-2.75400
C	1.92335	-2.68961	1.41289
H	2.30177	-3.71603	1.51112
H	2.74530	-2.03839	1.09718
H	1.57941	-2.34836	2.39583
C	-2.75184	-2.72571	-0.80118
H	-3.04946	-1.92667	-1.49081
H	-3.03985	-3.68679	-1.24776
H	-3.31520	-2.57323	0.12109
C	-0.61739	-2.59476	-3.07644
H	-1.43759	-1.89376	-3.26696
H	0.24114	-2.27794	-3.67646
H	-0.93600	-3.58163	-3.43749
C	-1.20839	-2.99077	2.02990
H	-1.13971	-4.05716	2.28184
H	-0.68817	-2.42034	2.80674
H	-2.26253	-2.69932	2.04555
Ir	-0.12882	-0.87119	-0.29046
C	2.60419	2.02282	-3.05174
H	1.52858	1.96875	-3.25562
H	3.00167	2.90451	-3.57106
H	3.08117	1.13439	-3.48727
C	2.18937	3.35407	-0.97057
H	2.32720	3.42104	0.11614

Frequencies

23.1927	38.1870	59.4713
62.7886	70.2569	75.3685
79.0018	89.6360	93.0978
100.1008	108.7841	118.1650
128.0196	131.6295	134.5935
142.7793	146.2308	153.4553
159.4378	164.4357	169.8742
170.6883	176.6246	183.4169
186.9337	194.8696	199.1738
204.2837	214.8405	218.5610
225.1307	238.3549	242.2164
248.3948	256.7492	266.7605
272.8408	278.9895	284.6537
290.5650	308.4379	311.3441
314.0446	320.0397	325.1682
337.8138	365.3593	367.0008
369.5573	376.7280	392.2142
396.2780	397.6166	415.2334
428.2746	435.9772	454.4683
464.1436	468.8863	503.0778
532.3645	535.5128	544.8313
548.5661	553.7451	563.8200
575.1534	583.7965	584.4326
590.3562	601.1181	627.3658
645.4473	681.5696	711.0015
753.2809	772.1668	776.4502
789.4415	807.5005	809.3867
810.5632	824.6996	829.1934
859.9286	868.9515	880.7934
887.3270	907.5519	925.4353
941.3211	947.4639	948.1877
949.1121	971.9505	975.1472
978.6750	982.1716	1009.1643
1024.1084	1025.4266	1034.5418
1041.9295	1045.1638	1048.0434
1051.2790	1055.1254	1058.9013
1089.5683	1092.6040	1097.2703
1112.0642	1113.3186	1132.9421
1147.6160	1156.6723	1182.3581
1185.5479	1187.3114	1200.6941
1226.6711	1238.5147	1242.2141
1255.1797	1264.3784	1283.6066

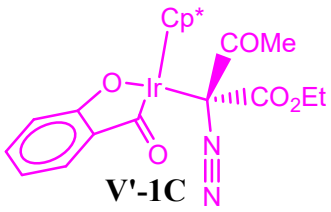
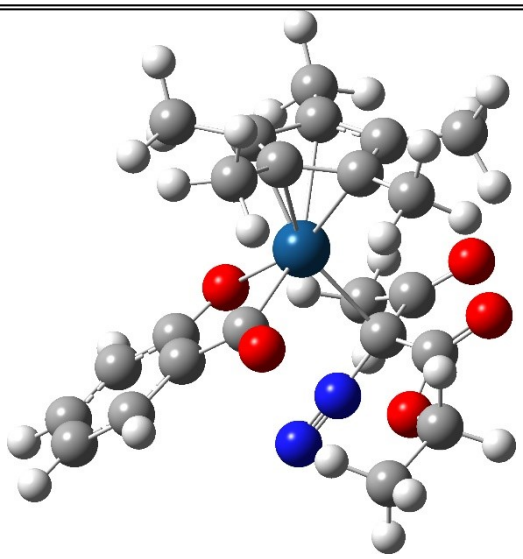
H	2.60073	4.26634	-1.42303
H	1.11028	3.33498	-1.16134
C	4.39759	2.24378	-1.33963
H	4.64206	2.38137	-0.28035
H	4.91864	1.34562	-1.68757
H	4.78396	3.11083	-1.89096
O	-1.30656	0.62248	-1.74218
C	-1.95048	2.25559	-0.08252
C	-2.85465	3.24953	0.30226
C	-3.37168	1.76024	-1.98510
C	-4.01544	3.48103	-0.42338
C	-4.28089	2.72199	-1.55979
C	-0.82266	1.96636	0.86379
O	-0.23527	2.89476	1.38552
H	-3.53050	1.18303	-2.89260
H	-5.19090	2.89168	-2.13021
H	-4.71693	4.24509	-0.09860
H	-2.63059	3.81941	1.20197
C	-0.66400	0.51868	1.30601
C	-2.04375	0.16681	1.88661
C	0.42980	0.30815	2.30634
C	2.65568	0.71500	2.91114
H	2.32955	0.91778	3.93866
H	2.92774	-0.34753	2.85725
C	3.79449	1.59958	2.48075
H	3.48375	2.65056	2.46660
H	4.63320	1.49808	3.17760
H	4.13091	1.31161	1.47927
O	0.33368	-0.44917	3.26261
O	1.55723	0.95591	2.02270
C	-2.36009	0.68610	3.26416
H	-3.44394	0.72569	3.39627
H	-1.92099	0.01076	4.00591
H	-1.91041	1.67249	3.43323
O	-2.88701	-0.42384	1.23902
H	5.67274	-0.47492	-2.32853
C	0.63389	0.75102	-2.26539
C	2.92715	1.58077	-1.45499
C	4.85170	2.36254	-0.35019
H	4.58554	3.41370	-0.51439
H	5.46963	2.04686	-1.20246
C	5.53081	2.13074	0.97347
H	6.47248	2.68645	1.02514
H	4.88756	2.45610	1.79667
H	5.74242	1.06336	1.11047
O	3.65827	1.57347	-0.34098
O	3.14601	2.29349	-2.40703
C	0.92000	0.94807	-3.71343
H	-0.00533	0.88337	-4.29044
H	1.41585	1.91119	-3.86642
H	1.63737	0.18240	-4.03787
O	-0.52197	0.63428	-1.87363

1289.4213	1317.9642	1340.8084
1357.8157	1362.2482	1370.6986
1375.1750	1376.9771	1380.8303
1387.2105	1388.8973	1391.7642
1392.6940	1399.9310	1417.7585
1424.5574	1428.3883	1433.5979
1433.9247	1435.5311	1442.4914
1443.4619	1446.9516	1453.6194
1457.8077	1459.7392	1460.2239
1461.4938	1463.0731	1468.0255
1474.5821	1475.9654	1481.7532
1486.9060	1487.9859	1490.6996
1494.8574	1497.2438	1507.7923
1516.9613	1519.9449	1527.9426
1535.8550	1560.8794	1643.4133
1674.0242	1771.6512	1774.9836
1791.0048	1820.4418	3024.0699
3029.5542	3031.2665	3036.6409
3037.9375	3039.1014	3040.4403
3041.2550	3047.0840	3049.2865
3052.7602	3100.9289	3107.2323
3112.6649	3115.5968	3116.2392
3118.4122	3118.6555	3124.4782
3127.0385	3128.1139	3128.6288
3133.9014	3137.0525	3143.8561
3144.6298	3148.2089	3169.1991
3170.6818	3177.1319	3179.6752
3182.8302	3184.9034	3192.5654
3201.7542	3209.3256	3446.5072

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.602301 Electronic Energy = -1719.55373843
Internal Energy (E)= -1718.91220643 Enthalpy (H)= -1718.91126243

Gibbs Free Energy (G)=-1719.01869443 Gibbs Free Energy of Solvation=-1720.41658241

St.Pt.	General Structure	Ball & Stick model
V'-1C	 V'-1C	

Cartesian co-ordinate

Atoms	X	Y	Z
C	1.15923	-1.12064	-2.03239
C	2.05801	-0.13702	-1.49779
C	2.71591	-0.72609	-0.33276
C	2.13621	-1.97693	-0.06977
C	1.10654	-2.20625	-1.08264
C	-1.32336	0.28982	-1.04677
C	-2.54417	-0.34151	-0.52208
C	0.26994	1.18833	1.48800
C	2.47378	1.10673	-2.20447
H	3.26023	0.90021	-2.94416
H	1.61913	1.54482	-2.73426
H	2.85487	1.85451	-1.50309
C	3.81426	-0.05092	0.40264
H	4.69606	0.02176	-0.24864
H	3.52428	0.96448	0.69609
H	4.10050	-0.59098	1.30920
C	2.43367	-2.91070	1.05227
H	3.00958	-3.78202	0.71138
H	3.01091	-2.41813	1.84182
H	1.50926	-3.29160	1.50535
C	0.28576	-3.44372	-1.19141
H	0.85409	-4.25527	-1.66499
H	-0.03319	-3.78498	-0.20083
H	-0.61947	-3.26807	-1.78266
C	0.45053	-1.02089	-3.33527
H	-0.39240	-1.71756	-3.39227
H	0.05262	-0.01146	-3.48452

Frequencies

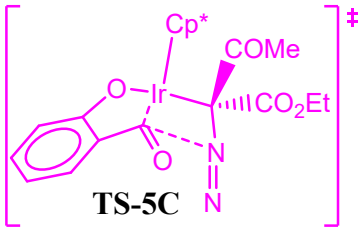
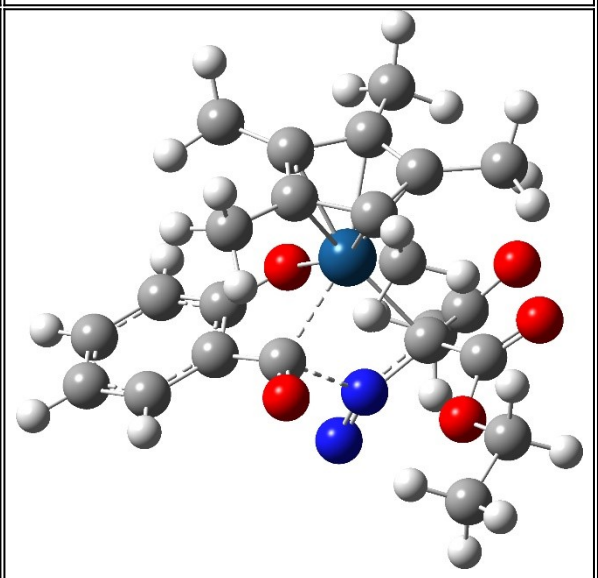
29.6845	49.8540	61.7984
72.4320	89.4290	98.0726
103.9949	109.7131	120.0544
128.3478	134.6485	137.8216
141.2319	145.8912	150.1735
167.4609	181.0049	186.8502
193.9241	200.2553	204.0528
216.1227	219.3783	226.7288
234.2142	246.9630	250.0487
260.8293	264.6605	278.5240
283.1810	289.0071	298.1245
305.2802	315.1474	319.0988
326.0543	342.5287	353.6944
355.3348	366.8513	379.7624
403.9120	414.9158	428.7746
440.5480	473.0996	504.5307
529.1990	534.6703	538.3576
542.0927	552.0823	554.8960
569.2656	592.7747	593.6634
600.5103	605.7433	608.5115
621.3121	663.2783	674.3659
749.3025	762.0630	764.8464
811.8579	815.2085	817.1398
834.3364	855.8372	865.2598
885.7272	893.0047	950.0680
953.6470	972.1295	975.1389
975.3648	1028.2311	1031.6617
1037.5567	1038.3525	1039.8291
1045.4522	1047.4913	1049.8101
1086.3913	1089.7268	1090.9138
1110.7401	1113.3851	1117.6776

H	1.14058	-1.25272	-4.15692	1141.1017	1143.7897	1177.6123
Ir	0.34022	-0.43056	-0.13334	1184.4442	1188.1440	1199.9406
O	-1.32386	1.11279	-1.95359	1223.0362	1263.3377	1281.1669
N	-1.06080	1.28241	1.80778	1300.4179	1342.5452	1373.2059
N	-2.15592	1.32234	2.04572	1380.8323	1381.3140	1383.3412
C	-2.35427	-1.19205	0.58991	1390.5848	1394.9271	1395.8013
O	-1.14201	-1.37816	1.06236	1401.1231	1421.2547	1428.7705
C	-3.82585	-0.08865	-1.02381	1434.6521	1439.8464	1443.6621
C	-3.48654	-1.77989	1.18959	1452.0766	1454.9947	1459.0990
C	-4.74369	-1.52416	0.67117	1464.2635	1467.2564	1469.0965
C	-4.92899	-0.68146	-0.43609	1471.3286	1477.7754	1483.4988
H	-3.34657	-2.42949	2.05080	1484.6756	1487.5665	1492.1195
H	-5.61104	-1.98786	1.13872	1498.4591	1508.8592	1510.9103
H	-5.92921	-0.49804	-0.82021	1513.2851	1529.1524	1574.7596
H	-3.91925	0.58044	-1.87740	1619.8260	1657.7311	1745.3496
C	0.73837	2.40868	0.73796	1831.1552	1878.0071	2293.6220
C	-0.04251	4.05893	-0.75604	3025.1417	3028.7302	3033.1091
H	0.46239	4.92289	-0.30697	3035.2316	3036.2922	3037.0606
H	0.64619	3.59847	-1.47517	3046.0966	3054.2480	3096.1900
C	-1.36433	4.40419	-1.38564	3105.7327	3110.5171	3117.3218
H	-2.05282	4.82789	-0.64691	3118.0349	3121.0539	3129.5131
H	-1.21826	5.14329	-2.17985	3136.2580	3140.8132	3140.9207
H	-1.81325	3.50316	-1.81727	3145.2159	3150.1073	3166.2605
C	1.08926	0.58483	2.62528	3170.2045	3172.0506	3175.9171
O	1.89555	2.69187	0.55639	3184.1006	3194.6765	3201.3226
O	-0.31014	3.09356	0.28139			
C	0.36930	-0.35060	3.55305			
H	-0.26049	-1.05589	2.99665			
H	1.11517	-0.87276	4.15563			
H	-0.27866	0.22082	4.23129			
O	2.25753	0.86916	2.74519			
C	0.42980	0.30815	2.30634			
C	2.65568	0.71500	2.91114			
H	2.32955	0.91778	3.93866			
H	2.92774	-0.34753	2.85725			
C	3.79449	1.59958	2.48075			
H	3.48375	2.65056	2.46660			
H	4.63320	1.49808	3.17760			
H	4.13091	1.31161	1.47927			
O	0.33368	-0.44917	3.26261			
O	1.55723	0.95591	2.02270			
C	-2.36009	0.68610	3.26416			
H	-3.44394	0.72569	3.39627			
H	-1.92099	0.01076	4.00591			
H	-1.91041	1.67249	3.43323			
O	-2.88701	-0.42384	1.23902			
H	5.67274	-0.47492	-2.32853			
C	0.63389	0.75102	-2.26539			
C	2.92715	1.58077	-1.45499			
C	4.85170	2.36254	-0.35019			
H	4.58554	3.41370	-0.51439			
H	5.46963	2.04686	-1.20246			
C	5.53081	2.13074	0.97347			
H	6.47248	2.68645	1.02514			
H	4.88756	2.45610	1.79667			
H	5.74242	1.06336	1.11047			
O	3.65827	1.57347	-0.34098			
O	3.14601	2.29349	-2.40703			
C	0.92000	0.94807	-3.71343			
H	-0.00533	0.88337	-4.29044			
H	1.41585	1.91119	-3.86642			

H	1.63737	0.18240	-4.03787
O	-0.52197	0.63428	-1.87363

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.461795 Electronic Energy = -1482.12490082
Internal Energy (E)= -1481.63084882 Enthalpy (H)= -1481.62990482
Gibbs Free Energy (G)=-1481.72260382 Gibbs Free Energy of Solvation=-1482.93419609

St.Pt.	General Structure	Ball & Stick model
TS-5C		

TS-5C

Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.28336	-1.43745	-2.04827
C	1.12731	-1.32402	-1.71784
C	1.38556	-2.19204	-0.59169
C	0.13679	-2.74741	-0.16480
C	-0.90000	-2.28510	-1.08110
C	-0.74041	1.39835	-0.61960
C	-2.17977	1.41291	-0.29219
C	1.11945	0.68164	1.30986
C	2.12254	-0.53676	-2.49843
H	2.36370	-1.02419	-3.45213
H	1.72922	0.46480	-2.71627
H	3.05303	-0.41720	-1.93335
C	2.69606	-2.49391	0.04443
H	2.96243	-3.54042	-0.15431
H	3.49435	-1.85165	-0.33131
H	2.65401	-2.34122	1.12894

Frequencies

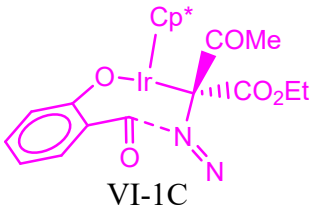
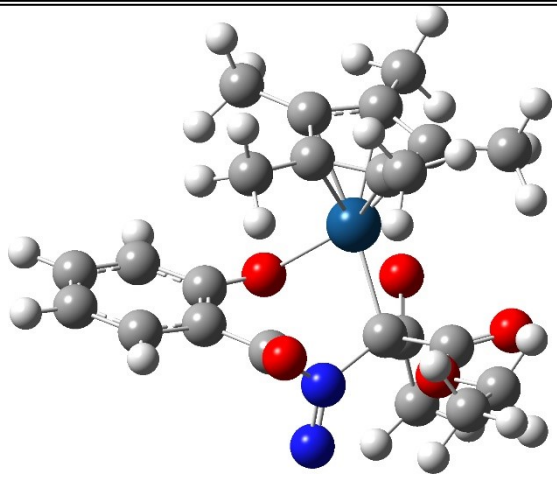
-314.1503	31.7660	43.4392
51.6962	67.4707	95.2563
100.8651	102.2048	111.0611
116.5169	119.9981	125.6149
139.3124	153.6050	167.2130
170.8463	180.5408	184.1819
192.4851	195.6807	203.0331
211.5339	213.4734	226.2604
227.1090	237.2776	242.6254
247.0071	259.0710	269.9316
279.1562	292.8043	297.7153
302.4471	308.8954	316.0171
319.9025	327.3206	336.0217
359.0121	395.8584	403.6772
408.2702	414.3012	428.3652
440.5797	461.0400	468.0349
503.3889	526.1423	537.1690
537.9706	544.2608	549.4795
560.4557	581.8208	588.0965
594.8846	599.9747	613.7653
627.8765	650.4529	667.8132

C	-0.05391	-3.65058	1.00194	758.7477	761.8881	768.4300
H	0.05117	-4.70655	0.71712	798.2510	807.5791	810.0012
H	0.68620	-3.43270	1.78053	813.3071	840.0646	857.4688
H	-1.04722	-3.51790	1.44421	872.1610	891.3881	949.0709
C	-2.34075	-2.64325	-0.98203	953.6206	958.3189	968.7553
H	-2.52383	-3.65084	-1.37658	974.9043	996.0467	1030.3429
H	-2.67176	-2.62017	0.06232	1036.6529	1042.3514	1045.2022
H	-2.96910	-1.93861	-1.53581	1046.4541	1048.0924	1056.8512
C	-0.94446	-0.74281	-3.18710	1060.5140	1091.2309	1093.6613
H	-2.02101	-0.63136	-3.02301	1108.2185	1109.6956	1111.2929
H	-0.52784	0.25985	-3.32940	1144.8581	1145.2859	1170.5298
H	-0.79976	-1.30773	-4.11709	1182.9377	1184.6872	1189.8355
Ir	-0.02643	-0.56098	-0.01456	1236.3459	1264.1169	1278.8586
O	-0.19890	2.05042	-1.48834	1299.0387	1336.6260	1366.8388
N	0.14059	1.72609	1.09463	1377.1401	1377.9851	1383.1358
N	-0.42977	2.61055	1.54917	1383.8611	1395.8752	1401.4155
C	-2.58986	0.50166	0.70874	1407.7546	1423.5633	1434.4640
O	-1.70792	-0.30158	1.27000	1440.7182	1442.9928	1447.4040
C	-3.09169	2.26484	-0.91809	1450.7622	1451.5005	1452.3368
C	-3.94686	0.49193	1.08079	1460.7058	1463.2495	1468.3532
C	-4.83948	1.33943	0.44569	1469.7127	1474.9453	1478.6345
C	-4.42861	2.22703	-0.55942	1484.5176	1485.5079	1494.2756
H	-4.26984	-0.19911	1.85635	1497.7116	1500.3153	1507.4914
H	-5.88938	1.30980	0.73275	1509.8694	1516.4445	1540.2500
H	-5.15177	2.87805	-1.04358	1617.1940	1659.1698	1760.7078
H	-2.72138	2.94597	-1.68264	1798.8971	1862.9537	2049.9443
C	2.41271	1.04637	0.64871	3028.4576	3029.4017	3036.6016
C	3.45263	2.60449	-0.77272	3038.6397	3039.3965	3040.2945
H	4.29720	2.78229	-0.09551	3048.4191	3056.8352	3098.7362
H	3.73308	1.76950	-1.42866	3101.6416	3110.1454	3119.6645
C	3.05779	3.82970	-1.55126	3120.3606	3121.7685	3127.8868
H	2.77973	4.64741	-0.87890	3136.3162	3141.7513	3144.4743
H	3.89084	4.16523	-2.17702	3145.8342	3146.2124	3155.8486
H	2.19901	3.60919	-2.19250	3167.5555	3168.0191	3175.8216
C	1.15343	0.03735	2.67194	3182.3704	3194.3852	3204.2118
O	3.41672	0.37767	0.68808			
O	2.31134	2.21535	0.00567			
C	0.16082	0.48605	3.70236			
H	-0.85377	0.30081	3.32537			
H	0.33148	-0.08572	4.61642			
H	0.25052	1.55800	3.91129			
O	1.94303	-0.86644	2.86553			
C	0.42980	0.30815	2.30634			
C	2.65568	0.71500	2.91114			
H	2.32955	0.91778	3.93866			
H	2.92774	-0.34753	2.85725			
C	3.79449	1.59958	2.48075			
H	3.48375	2.65056	2.46660			
H	4.63320	1.49808	3.17760			
H	4.13091	1.31161	1.47927			
O	0.33368	-0.44917	3.26261			
O	1.55723	0.95591	2.02270			
C	-2.36009	0.68610	3.26416			
H	-3.44394	0.72569	3.39627			
H	-1.92099	0.01076	4.00591			
H	-1.91041	1.67249	3.43323			
O	-2.88701	-0.42384	1.23902			
H	5.67274	-0.47492	-2.32853			
C	0.63389	0.75102	-2.26539			
C	2.92715	1.58077	-1.45499			
C	4.85170	2.36254	-0.35019			

H	4.58554	3.41370	-0.51439
H	5.46963	2.04686	-1.20246
C	5.53081	2.13074	0.97347
H	6.47248	2.68645	1.02514
H	4.88756	2.45610	1.79667
H	5.74242	1.06336	1.11047
O	3.65827	1.57347	-0.34098
O	3.14601	2.29349	-2.40703
C	0.92000	0.94807	-3.71343
H	-0.00533	0.88337	-4.29044
H	1.41585	1.91119	-3.86642
H	1.63737	0.18240	-4.03787
O	-0.52197	0.63428	-1.87363

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.459833 Electronic Energy = -1482.06427040
Internal Energy (E)= -1481.5725944 Enthalpy (H)= -1481.5716504
Gibbs Free Energy (G)=-1481.6636834 Gibbs Free Energy of Solvation=-1482.87820499

St.Pt.	General Structure	Ball & Stick model
VI-1C	 VI-1C	

Cartesian co-ordinate

Atoms	X	Y	Z
C	0.78513	1.09174	-1.74320
C	-0.65672	1.21649	-1.74079
C	-1.00126	2.33825	-0.91000
C	0.24515	2.96257	-0.47906
C	1.33335	2.22034	-1.00078
C	0.49791	-2.27516	-0.33305
C	1.92525	-2.04920	-0.11842
C	-1.08405	-0.75879	1.02747
C	-1.58812	0.33168	-2.49171
H	-1.52320	0.54616	-3.56608

Frequencies

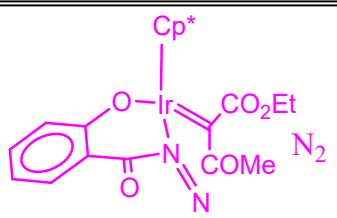
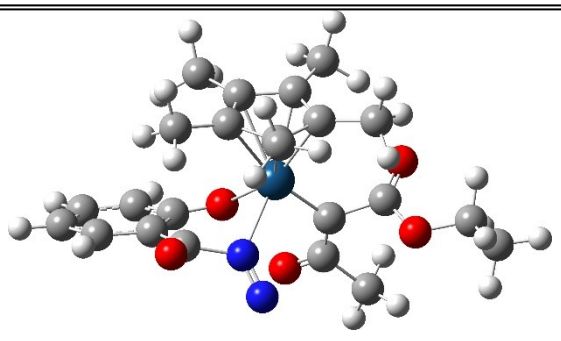
40.6926	51.8624	62.9009
80.1627	86.4024	95.6488
98.1419	105.3115	109.0234
110.7614	122.1253	127.2913
133.9257	155.6280	160.2123
171.9259	177.9432	187.8288
191.5034	195.1241	204.5812
207.3222	212.1903	225.9699
235.5253	242.9554	250.3681
261.9189	263.7920	275.6603
296.5078	302.5336	314.7827
317.9058	325.5994	326.6934
330.9942	344.5103	354.4026
384.5709	397.1192	400.4047

H	-1.34653	-0.72770	-2.33773	416.2272	441.0348	444.5788
H	-2.62507	0.49477	-2.17874	452.3034	455.1409	516.8627
C	-2.37150	2.84489	-0.62198	529.8255	535.6447	537.4729
H	-2.69796	3.56650	-1.38233	544.6576	547.9148	555.9620
H	-3.09617	2.02485	-0.58147	584.2058	597.6852	602.2785
H	-2.40749	3.34335	0.35289	605.8103	640.2894	671.4349
C	0.31158	4.13264	0.43765	677.8934	715.5705	761.9897
H	0.03240	5.05499	-0.08750	769.0711	789.8624	800.8009
H	-0.38018	4.00686	1.27873	810.1717	811.8371	829.5499
H	1.31512	4.26482	0.85182	854.9297	869.4579	877.6298
C	2.78573	2.45576	-0.78231	897.3442	940.0776	953.6942
H	3.25380	2.87292	-1.68350	956.0884	970.9430	978.7433
H	2.96201	3.15146	0.04357	998.0179	1011.4350	1033.1841
H	3.30315	1.51845	-0.54239	1039.6563	1044.2271	1045.5279
C	1.57894	0.12648	-2.55172	1050.7768	1058.4714	1060.4487
H	2.53346	-0.11015	-2.06740	1070.2798	1091.6948	1093.2588
H	1.04282	-0.81854	-2.69321	1111.9009	1119.1925	1126.2725
H	1.79514	0.55162	-3.54113	1145.2532	1149.1278	1171.1244
Ir	0.06842	0.86285	0.26158	1183.9393	1187.5479	1217.6008
O	-0.02710	-2.70531	-1.33179	1273.3030	1276.0929	1284.6642
N	-0.36431	-2.09937	0.92097	1319.0696	1337.6699	1374.1627
N	-0.41637	-3.02312	1.69460	1379.1012	1381.7443	1386.8969
C	2.37748	-1.00734	0.73294	1399.9224	1402.1446	1402.5728
O	1.56463	-0.17674	1.34468	1408.7774	1413.0087	1425.6888
C	2.83410	-2.84191	-0.83085	1433.4302	1436.6745	1441.1569
C	3.77274	-0.86389	0.88746	1441.4803	1443.4602	1447.5599
C	4.65619	-1.68196	0.20340	1453.6358	1458.0771	1467.0932
C	4.19777	-2.67287	-0.67279	1472.7332	1476.2601	1477.7615
H	4.12390	-0.07670	1.55174	1480.7594	1487.2064	1489.6587
H	5.72684	-1.53864	0.34031	1498.4360	1500.3156	1511.4247
H	4.90034	-3.30174	-1.21267	1516.9897	1520.2182	1553.1358
H	2.43301	-3.60185	-1.49916	1609.8766	1660.5287	1696.4025
C	-2.47138	-0.80323	0.49762	1723.6173	1804.7331	1829.1884
C	-3.94283	-1.90998	-0.97702	3019.2892	3030.4752	3034.3009
H	-4.65063	-2.21898	-0.19726	3036.1074	3038.5095	3039.3729
H	-4.27490	-0.92803	-1.33965	3046.3690	3055.8912	3096.0269
C	-3.82127	-2.92594	-2.08149	3099.6630	3104.4637	3114.1918
H	-3.44741	-3.87695	-1.68999	3117.3331	3119.2189	3120.5010
H	-4.79400	-3.09747	-2.55318	3139.5776	3140.9828	3142.7016
H	-3.11751	-2.58182	-2.84714	3147.5946	3148.4135	3149.3926
C	-1.06427	-0.16017	2.39871	3154.0277	3171.0636	3171.1615
O	-3.34326	-0.01704	0.82051	3186.0060	3192.7813	3209.1141
O	-2.64175	-1.78262	-0.39122			
C	-1.51601	-0.85778	3.61332			
H	-1.07695	-1.86639	3.60773			
H	-1.27052	-0.29215	4.51443			
H	-2.60171	-1.00327	3.53853			
O	-0.62984	1.00494	2.39399			
C	0.42980	0.30815	2.30634			
C	2.65568	0.71500	2.91114			
H	2.32955	0.91778	3.93866			
H	2.92774	-0.34753	2.85725			
C	3.79449	1.59958	2.48075			
H	3.48375	2.65056	2.46660			
H	4.63320	1.49808	3.17760			
H	4.13091	1.31161	1.47927			
O	0.33368	-0.44917	3.26261			
O	1.55723	0.95591	2.02270			
C	-2.36009	0.68610	3.26416			
H	-3.44394	0.72569	3.39627			
H	-1.92099	0.01076	4.00591			

H	-1.91041	1.67249	3.43323
O	-2.88701	-0.42384	1.23902
H	5.67274	-0.47492	-2.32853
C	0.63389	0.75102	-2.26539
C	2.92715	1.58077	-1.45499
C	4.85170	2.36254	-0.35019
H	4.58554	3.41370	-0.51439
H	5.46963	2.04686	-1.20246
C	5.53081	2.13074	0.97347
H	6.47248	2.68645	1.02514
H	4.88756	2.45610	1.79667
H	5.74242	1.06336	1.11047
O	3.65827	1.57347	-0.34098
O	3.14601	2.29349	-2.40703
C	0.92000	0.94807	-3.71343
H	-0.00533	0.88337	-4.29044
H	1.41585	1.91119	-3.86642
H	1.63737	0.18240	-4.03787
O	-0.52197	0.63428	-1.87363

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.461821 Electronic Energy = -1482.07454869
Internal Energy (E)= -1481.58081869 Enthalpy (H)= -1481.57987569
Gibbs Free Energy (G)=-1481.67197969 Gibbs Free Energy of Solvation=-1482.88461466

St.Pt.	General Structure	Ball & Stick model
VI'-1C	 **VI'-1C**	

Cartesian co-ordinate

Frequencies

Atoms	X	Y	Z
C	0.20936	1.89601	1.25379
C	1.30462	1.94124	0.30871
C	0.73895	2.10800	-1.01084
C	-0.68363	2.14305	-0.86682
C	-1.01801	2.05647	0.52359
C	-2.23088	-0.82950	1.58910
C	-2.99943	-0.99665	0.37931
C	-2.42547	-1.20300	-0.91218
C	1.52741	-1.19075	-0.36369
Ir	0.15070	0.09880	-0.06938
C	1.30121	-2.64460	-0.31827
H	0.36100	-2.91322	-0.81292
H	2.13658	-3.24988	-0.68891
H	1.14498	-2.87463	0.76176
C	2.95128	-0.81204	-0.52961
O	3.67117	-1.21301	0.53126
C	5.08955	-0.98176	0.46739
H	5.27205	-0.00461	0.00562
H	5.41142	-0.94853	1.51239
C	5.77127	-2.08841	-0.29902
H	6.85710	-1.94744	-0.28869
H	5.54706	-3.06265	0.14770
H	5.43741	-2.09215	-1.34134
O	3.42306	-0.23740	-1.48927
O	-2.59629	-0.47968	2.68124
O	-1.15753	-1.13129	-1.19876
C	-3.32723	-1.47138	-1.97456
C	-4.40282	-0.96649	0.53846
C	-4.69020	-1.46627	-1.78143
C	-5.24950	-1.19787	-0.51923
H	-2.89054	-1.64442	-2.95534
H	-5.34561	-1.65992	-2.62893
H	-6.32693	-1.18956	-0.38158
H	-4.78669	-0.77769	1.53913
N	-0.74347	-1.21920	1.46107
N	-0.29031	-2.08135	2.12471
C	0.34102	1.79299	2.73475
H	1.23466	1.22164	3.00833
H	0.42093	2.78702	3.19473
H	-0.52172	1.28057	3.17587
C	2.74451	2.07339	0.67055
H	2.97172	3.11424	0.93589
H	3.00226	1.44693	1.53230
H	3.39269	1.79243	-0.16526
C	1.50112	2.30480	-2.27468
H	1.81138	3.35391	-2.37598
H	2.39414	1.67483	-2.30335
H	0.89194	2.05394	-3.14874
C	-1.66562	2.22263	-1.98350
H	-1.83858	3.26363	-2.28622
H	-1.31161	1.67043	-2.86098
H	-2.63155	1.79207	-1.69731
C	-2.37348	2.28324	1.10198
H	-2.60122	3.35748	1.10937
H	-3.16074	1.78442	0.52491

30.1545	31.8831	46.5421
63.6618	64.9866	65.7289
89.8495	103.5438	114.5334
123.2468	134.7262	137.8544
148.1627	152.2200	157.3407
172.8681	179.7631	181.9114
199.5329	200.6381	213.2666
227.7540	239.0337	243.7050
249.7889	255.3479	271.3448
276.6063	289.2983	299.2683
305.7663	312.3848	315.8702
333.9259	346.9288	354.5547
366.2167	380.7145	393.6475
417.6317	421.9213	427.0324
439.5032	444.9332	451.3285
482.3277	527.5157	533.9556
536.0100	547.9774	566.5755
578.6198	586.2808	598.4349
606.3559	628.3253	650.2722
692.6984	727.1494	740.8612
765.6215	792.5237	811.7606
816.4379	820.3440	821.9991
853.6997	867.2668	877.0973
901.4309	928.0616	955.1293
961.0239	964.5190	983.6234
984.0171	1037.7294	1041.1331
1045.3763	1049.5998	1052.9639
1054.2387	1056.3110	1094.6951
1097.3525	1114.1187	1118.6375
1125.4415	1137.4756	1148.1126
1182.1833	1187.8164	1192.9889
1196.7152	1212.6941	1253.7132
1299.6147	1325.6127	1338.9083
1348.6916	1383.1873	1385.2808
1389.3165	1396.4179	1399.1190
1406.0412	1407.2877	1412.5886
1416.7224	1440.2981	1442.1798
1449.4524	1456.1401	1458.8949
1459.4577	1463.9201	1464.3460
1469.3658	1469.5038	1473.9507
1480.5748	1482.4973	1485.0913
1501.8555	1504.8376	1508.3052
1519.7958	1524.3375	1525.3734
1531.0363	1597.6402	1672.7647
1814.5178	1825.3419	1870.8524
2856.0010	3031.9671	3036.3741
3037.4151	3037.7022	3041.0652
3051.4983	3065.4216	3067.4823
3109.9496	3114.4590	3117.5677
3120.0379	3121.5033	3126.0071
3137.2086	3139.4867	3140.6485
3143.8816	3154.7866	3157.0565
3162.1958	3173.9528	3187.6354
3190.9280	3197.1782	3210.1633

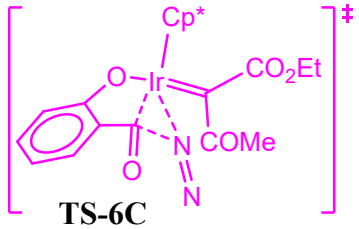
H	-2.44721	1.92005	2.13068
H	-2.60171	-1.00327	3.53853
O	-0.62984	1.00494	2.39399
C	0.42980	0.30815	2.30634
C	2.65568	0.71500	2.91114
H	2.32955	0.91778	3.93866
H	2.92774	-0.34753	2.85725
C	3.79449	1.59958	2.48075
H	3.48375	2.65056	2.46660
H	4.63320	1.49808	3.17760
H	4.13091	1.31161	1.47927
O	0.33368	-0.44917	3.26261
O	1.55723	0.95591	2.02270
C	-2.36009	0.68610	3.26416
H	-3.44394	0.72569	3.39627
H	-1.92099	0.01076	4.00591
H	-1.91041	1.67249	3.43323
O	-2.88701	-0.42384	1.23902
H	5.67274	-0.47492	-2.32853
C	0.63389	0.75102	-2.26539
C	2.92715	1.58077	-1.45499
C	4.85170	2.36254	-0.35019
H	4.58554	3.41370	-0.51439
H	5.46963	2.04686	-1.20246
C	5.53081	2.13074	0.97347
H	6.47248	2.68645	1.02514
H	4.88756	2.45610	1.79667
H	5.74242	1.06336	1.11047
O	3.65827	1.57347	-0.34098
O	3.14601	2.29349	-2.40703
C	0.92000	0.94807	-3.71343
H	-0.00533	0.88337	-4.29044
H	1.41585	1.91119	-3.86642
H	1.63737	0.18240	-4.03787
O	-0.52197	0.63428	-1.87363

Statistical Thermodynamic Analysis

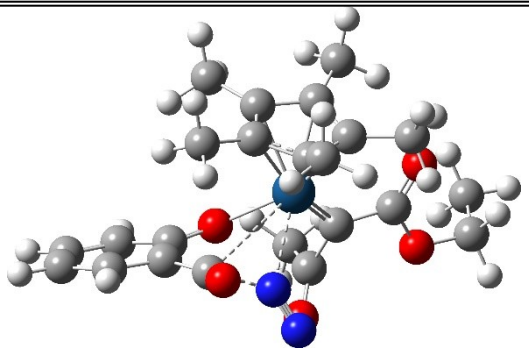
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.450883 Electronic Energy = -1368.79356929
Internal Energy (E)= -1368.31195229 Enthalpy (H)= -1368.31100829
Gibbs Free Energy (G)=-1368.40226729 Gibbs Free Energy of Solvation=-1369.53383758

St.Pt.	General Structure	Ball & Stick model

TS-6C



TS-6C



Cartesian co-ordinate

Atoms	X	Y	Z
C	0.49268	2.46700	-0.66555
C	-0.85969	2.39095	-0.13306
C	-0.74893	2.07919	1.27679
C	0.63960	1.85277	1.55446
C	1.40028	2.15980	0.37231
C	2.70249	-0.18805	-1.54784
C	3.15181	-0.92020	-0.45037
C	2.30317	-1.56911	0.52686
C	-1.63201	-0.85249	-0.19944
Ir	-0.16867	0.32752	0.04160
C	-1.41887	-2.34269	-0.21892
C	-3.05036	-0.46418	-0.22659
O	-3.81461	-1.48435	-0.69838
C	-5.22774	-1.26841	-0.72176
H	-5.43012	-0.23885	-1.03696
H	-5.60564	-1.95532	-1.48561
C	-5.83519	-1.55305	0.63217
H	-6.92467	-1.44572	0.59638
H	-5.60155	-2.57441	0.95240
H	-5.44665	-0.85155	1.37765
O	-3.54109	0.59926	0.11255
O	3.01065	0.55983	-2.39769
O	1.05704	-1.38179	0.68026
C	2.97725	-2.46784	1.41475
C	4.57593	-1.05160	-0.39418
C	4.33816	-2.59748	1.41881
C	5.16396	-1.87265	0.52193
H	2.35006	-2.99952	2.12533
H	4.80228	-3.26757	2.14020
H	6.24324	-1.98624	0.55196
H	5.16875	-0.50760	-1.12664
N	0.92156	-0.75581	-1.88847
N	0.49268	-1.24435	-2.80745
C	0.79325	2.91201	-2.05414
H	0.17434	2.37475	-2.78269
H	0.57149	3.98274	-2.16775
H	1.83914	2.75451	-2.32631
C	-2.02465	2.98991	-0.84860
H	-1.83717	4.05815	-1.02791
H	-2.18362	2.51438	-1.82380
H	-2.94771	2.88594	-0.27934
C	-1.81455	2.14290	2.31296

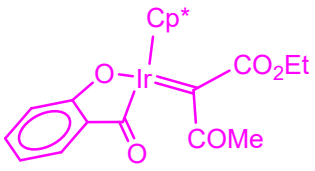
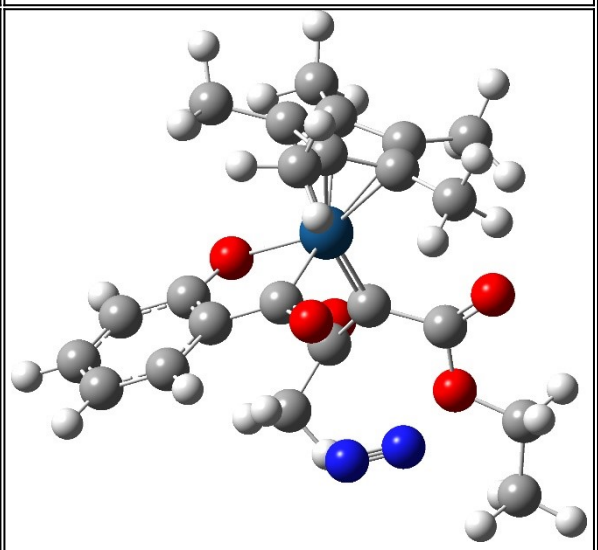
Frequencies

-326.2260	16.5648	32.4604
35.0514	50.7666	57.9876
66.1274	78.4781	79.8936
85.7895	95.1714	101.5024
109.1509	116.6216	120.3309
134.5115	139.6645	147.0527
150.0146	157.3184	158.4519
167.8460	176.2756	183.0605
186.4381	201.5837	209.1656
215.1931	228.8472	235.0818
244.3883	251.9885	253.5617
270.3489	274.5147	282.4529
298.5379	306.3770	327.4196
334.3523	347.8849	355.8141
361.9252	387.3250	395.0111
401.7976	420.6426	430.1757
461.4066	492.5731	513.9116
526.3909	530.3970	537.0688
543.7141	553.4856	573.3901
583.0718	587.9798	604.5135
607.4780	624.7757	638.5838
738.7051	752.2563	754.1336
758.6135	777.2160	802.5236
816.2225	819.4297	854.5074
881.2537	886.3870	946.2972
949.8277	950.7746	960.7844
983.4933	997.5842	1012.7005
1027.5252	1031.4031	1038.2661
1039.0895	1042.4065	1044.5996
1050.3559	1083.6102	1090.3027
1107.2635	1115.2216	1139.1690
1143.6036	1157.1091	1179.0014
1181.0865	1191.2606	1192.9620
1226.5989	1245.6490	1257.2007
1319.7023	1363.5669	1364.5512
1371.1177	1379.1019	1384.3116
1386.5509	1396.7344	1407.2545
1410.7739	1426.6985	1433.4933
1437.0993	1438.0060	1439.9272
1444.1881	1453.5422	1455.0469
1458.6166	1462.3673	1464.5030
1467.9499	1471.1692	1473.4080
1474.5708	1475.2881	1485.7744
1487.5264	1491.6800	1509.1772
1513.3851	1555.9854	1571.1107
1591.2586	1687.0305	1782.1407

H	-1.88238	3.16550	2.70984	1816.0850	2035.9879	2188.4308
H	-2.78266	1.85600	1.90133	3022.8512	3027.3034	3029.4226
H	-1.58836	1.47768	3.15320	3035.4074	3038.9561	3041.8900
C	1.22271	1.46497	2.86914	3046.5545	3068.5777	3098.4739
H	1.46370	2.34636	3.48041	3103.1170	3103.6893	3109.1950
H	0.53012	0.83898	3.44132	3113.7919	3124.4656	3131.9856
H	2.14841	0.89152	2.74063	3132.7724	3138.2721	3145.7819
C	2.88640	2.29066	0.35683	3149.8775	3159.7308	3165.5145
H	3.17226	3.22443	0.86012	3180.5332	3191.8974	3194.5296
H	3.38504	1.47669	0.89555	3204.4221	3213.7605	3217.3687
H	3.29628	2.32995	-0.65599			
C	-1.76846	-3.06353	1.05843			
H	-1.78668	-4.14339	0.88666			
H	-0.99357	-2.82499	1.79773			
H	-2.72961	-2.72460	1.46130			
O	-0.95203	-2.93160	-1.17437			
C	0.42980	0.30815	2.30634			
C	2.65568	0.71500	2.91114			
H	2.32955	0.91778	3.93866			
H	2.92774	-0.34753	2.85725			
C	3.79449	1.59958	2.48075			
H	3.48375	2.65056	2.46660			
H	4.63320	1.49808	3.17760			
H	4.13091	1.31161	1.47927			
O	0.33368	-0.44917	3.26261			
O	1.55723	0.95591	2.02270			
C	-2.36009	0.68610	3.26416			
H	-3.44394	0.72569	3.39627			
H	-1.92099	0.01076	4.00591			
H	-1.91041	1.67249	3.43323			
O	-2.88701	-0.42384	1.23902			
H	5.67274	-0.47492	-2.32853			
C	0.63389	0.75102	-2.26539			
C	2.92715	1.58077	-1.45499			
C	4.85170	2.36254	-0.35019			
H	4.58554	3.41370	-0.51439			
H	5.46963	2.04686	-1.20246			
C	5.53081	2.13074	0.97347			
H	6.47248	2.68645	1.02514			
H	4.88756	2.45610	1.79667			
H	5.74242	1.06336	1.11047			
O	3.65827	1.57347	-0.34098			
O	3.14601	2.29349	-2.40703			
C	0.92000	0.94807	-3.71343			
H	-0.00533	0.88337	-4.29044			
H	1.41585	1.91119	-3.86642			
H	1.63737	0.18240	-4.03787			
O	-0.52197	0.63428	-1.87363			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.456206 Electronic Energy = -1482.04762081
Internal Energy (E)= -1481.55701581 Enthalpy (H)= -1481.55607181
Gibbs Free Energy (G)=-1481.65701981 Gibbs Free Energy of Solvation=-1482.87802923

St.Pt.	General Structure	Ball & Stick model
VII-1C	 **VII-1C** N_2	

Cartesian co-ordinate

Atoms	X	Y	Z
C	2.11147	-1.51572	1.24468
C	0.87466	-2.27513	1.18278
C	0.72089	-2.73942	-0.16941
C	1.78980	-2.16658	-0.95482
C	2.65070	-1.42914	-0.06108
C	0.60542	1.04663	1.24993
C	1.08843	2.26539	0.61824
C	1.30652	2.19574	-0.77477
C	-1.27561	-0.12900	-0.66034
Ir	0.51619	-0.50733	-0.17033
C	-1.61131	0.89951	-1.70704
C	-2.46536	-0.87481	-0.16076
O	-3.58531	-0.16744	-0.40214
C	-4.80035	-0.68761	0.15162
H	-5.03149	-1.64120	-0.33951
H	-4.63826	-0.89787	1.21628
C	-5.86665	0.35089	-0.07393
H	-6.82628	0.00494	0.32266
H	-5.60563	1.28875	0.42981
H	-5.98865	0.55834	-1.14190
O	-2.47472	-1.92846	0.44015
O	0.30479	0.90695	2.41256
O	1.05572	1.08952	-1.42733
C	1.74877	3.36020	-1.43946
C	1.25910	3.46638	1.32769
C	1.92798	4.52645	-0.72229
C	1.68250	4.59719	0.66193
H	1.91657	3.31462	-2.51252
H	2.25957	5.42060	-1.24772
H	1.82449	5.53453	1.19302
H	1.04387	3.47076	2.39454
N	-2.86454	1.31343	2.09858

Frequencies

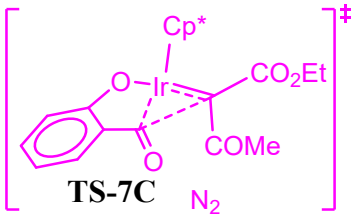
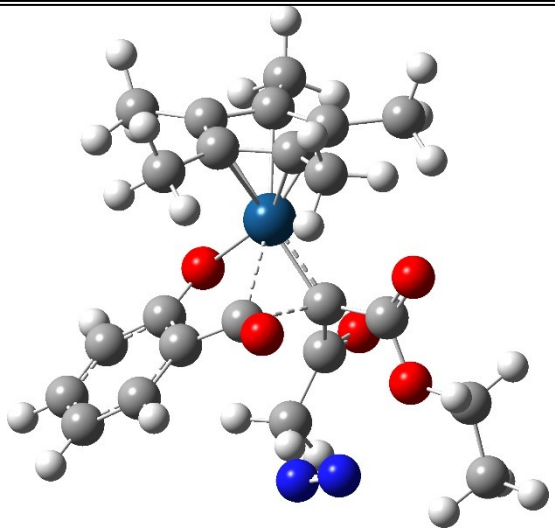
33.6961	36.4373	43.7479
56.3979	59.6844	74.5898
74.8409	84.0949	91.5606
104.5893	107.2967	112.7232
127.8548	140.4980	145.9344
151.5653	152.7770	155.4740
158.6234	162.8573	171.1977
179.2435	184.1035	189.8506
198.3320	202.7028	209.5562
216.7640	223.2911	233.8102
251.8978	258.9744	267.4436
278.4050	290.7097	295.8001
310.9632	314.1142	321.9475
336.5368	345.4501	351.6564
364.9736	373.0554	409.2442
415.6526	422.7244	426.0267
470.5271	532.6083	536.3379
539.6641	548.2768	550.7916
554.9219	570.2508	583.9226
590.0607	599.0718	605.7790
626.6313	633.0182	664.3530
754.5532	765.5769	785.7936
799.6374	805.7974	813.4583
817.1877	852.7485	858.3629
879.3742	887.1049	946.6499
953.8821	961.5914	975.3069
980.8016	1005.7266	1017.5147
1032.2626	1034.0890	1036.8650
1041.4437	1043.2772	1050.2119
1056.9409	1093.6642	1095.4420
1111.0849	1119.1987	1138.7835
1142.7258	1145.2209	1179.2434
1185.6226	1187.5202	1208.5448
1251.5332	1262.0855	1267.7755
1286.0568	1345.6861	1373.4884
1378.0577	1378.8729	1381.5095
1395.9749	1398.7889	1400.3962

N	-2.29490	2.25985	2.05592
C	-0.27553	-3.72344	-0.67121
H	0.16007	-4.73114	-0.64893
H	-1.18366	-3.71639	-0.06650
H	-0.56497	-3.50662	-1.70506
C	0.04768	-2.63876	2.36553
H	-0.96580	-2.91595	2.06490
H	0.49687	-3.47458	2.91885
H	-0.03378	-1.78380	3.04553
C	2.70028	-0.97477	2.49742
H	1.93001	-0.53857	3.14075
H	3.19147	-1.78355	3.05409
H	3.44746	-0.20009	2.29624
C	3.84764	-0.65569	-0.49383
H	3.61127	-0.04932	-1.37606
H	4.18978	0.02577	0.29147
H	4.68041	-1.32084	-0.75515
C	2.04534	-2.37266	-2.40743
H	2.42421	-1.45473	-2.87043
H	2.79097	-3.16306	-2.56946
H	1.13215	-2.65337	-2.94073
O	-1.71708	0.49565	-2.84852
C	-1.88315	2.32144	-1.31778
H	-1.71017	2.97404	-2.17839
H	-2.94103	2.38792	-1.03089
H	-1.28296	2.65032	-0.46246
C	0.42980	0.30815	2.30634
C	2.65568	0.71500	2.91114
H	2.32955	0.91778	3.93866
H	2.92774	-0.34753	2.85725
C	3.79449	1.59958	2.48075
H	3.48375	2.65056	2.46660
H	4.63320	1.49808	3.17760
H	4.13091	1.31161	1.47927
O	0.33368	-0.44917	3.26261
O	1.55723	0.95591	2.02270
C	-2.36009	0.68610	3.26416
H	-3.44394	0.72569	3.39627
H	-1.92099	0.01076	4.00591
H	-1.91041	1.67249	3.43323
O	-2.88701	-0.42384	1.23902
H	5.67274	-0.47492	-2.32853
C	0.63389	0.75102	-2.26539
C	2.92715	1.58077	-1.45499
C	4.85170	2.36254	-0.35019
H	4.58554	3.41370	-0.51439
H	5.46963	2.04686	-1.20246
C	5.53081	2.13074	0.97347
H	6.47248	2.68645	1.02514
H	4.88756	2.45610	1.79667
H	5.74242	1.06336	1.11047
O	3.65827	1.57347	-0.34098
O	3.14601	2.29349	-2.40703
C	0.92000	0.94807	-3.71343
H	-0.00533	0.88337	-4.29044
H	1.41585	1.91119	-3.86642
H	1.63737	0.18240	-4.03787
O	-0.52197	0.63428	-1.87363

1406.8548	1421.0617	1433.3830
1438.6456	1440.5122	1440.8204
1446.1334	1449.6962	1455.0851
1460.1232	1467.3367	1467.7500
1473.9646	1476.6279	1477.3274
1482.9301	1483.5837	1490.8136
1496.5953	1502.9676	1516.3048
1518.3907	1520.7216	1553.7220
1616.2099	1660.7684	1806.7045
1813.9066	1819.0060	2462.2681
3030.6833	3037.9515	3039.5331
3039.8090	3040.6346	3042.8236
3048.7840	3052.9823	3102.6145
3111.8057	3115.6855	3118.5329
3124.3820	3128.3584	3130.7585
3139.4617	3142.9371	3145.8181
3148.0889	3163.5300	3166.0785
3174.2728	3174.5347	3179.3359
3190.6769	3203.7423	3208.1208

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.458621 Electronic Energy = -1482.15556477
Internal Energy (E)= -1481.66258977 Enthalpy (H)= -1481.66164577
Gibbs Free Energy (G)=-1481.76104277 Gibbs Free Energy of Solvation=-1482.97413517

St.Pt.	General Structure	Ball & Stick model
TS-7C		

Cartesian co-ordinate

Atoms	X	Y	Z
C	2.40756	-0.20694	1.53715
C	1.76074	-1.51099	1.39627
C	2.14475	-2.05213	0.13026
C	2.97247	-1.05508	-0.53653
C	3.17539	0.04543	0.37599
C	-0.75614	0.75863	0.86716
C	-0.64179	2.15557	0.49272
C	0.14702	2.48248	-0.64303
C	-0.86746	-0.50594	-0.72391
Ir	0.98592	-0.23836	-0.22832
C	-1.53911	0.11507	-1.93927
C	-1.67229	-1.64910	-0.19096
O	-2.96799	-1.52205	-0.53035
C	-3.84877	-2.55257	-0.06366
H	-3.48960	-3.52076	-0.43387
H	-3.79851	-2.58284	1.03267
C	-5.22905	-2.22026	-0.56446
H	-5.94317	-2.98560	-0.24481
H	-5.56373	-1.25421	-0.16960
H	-5.24371	-2.16689	-1.65761
O	-1.25687	-2.57216	0.47413

Frequencies

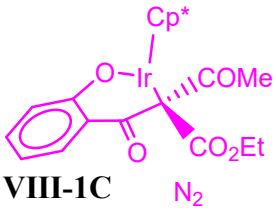
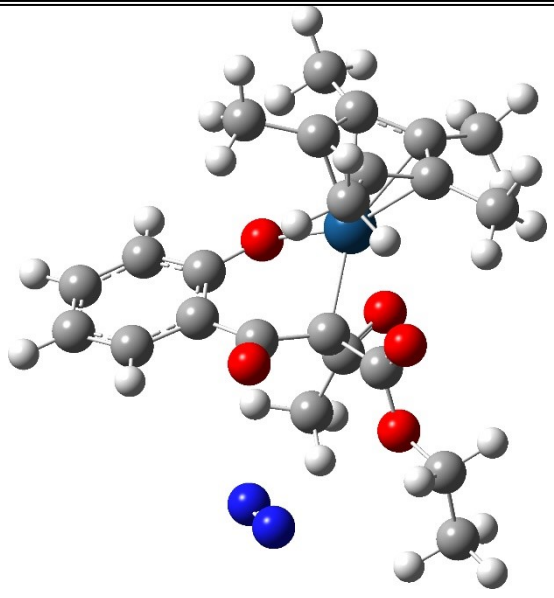
-271.6288	25.5466	40.8741
51.7439	60.5341	66.0438
72.4567	74.1025	88.7570
99.6740	117.2992	119.8424
124.6169	136.9494	142.7100
149.2009	159.7818	161.6108
167.9124	172.8375	179.0185
186.0841	197.6012	199.7822
205.1383	218.0457	223.2933
231.0950	244.8111	246.8051
249.3986	259.0060	279.3811
282.2311	295.6893	298.1382
308.0640	314.8615	322.2164
334.4213	354.2613	356.7586
373.9973	388.3238	406.3591
420.3059	431.4674	444.3770
461.1527	473.1854	536.4603
543.2364	547.1197	550.9050
556.6698	575.7890	592.3086
595.5066	599.3815	605.3793
608.0858	619.1700	647.4206
752.2777	776.7618	780.7858
799.8286	808.3835	817.4831
825.2461	832.5501	870.8717
878.2010	889.7455	957.6178
958.4858	967.6903	985.7991

O	-1.27657	0.29489	1.85407	994.9225	1010.8162	1033.7695
O	0.79737	1.56785	-1.30484	1037.7457	1043.3343	1045.9507
C	0.16592	3.83399	-1.05996	1048.5498	1051.4668	1058.3280
C	-1.35492	3.14336	1.19491	1060.1054	1090.0119	1096.5813
C	-0.55126	4.78394	-0.36185	1110.3155	1124.6275	1131.8352
C	-1.31672	4.45444	0.77278	1140.9672	1149.6457	1174.3496
H	0.75266	4.09041	-1.93857	1184.6177	1186.3744	1207.8955
H	-0.52287	5.81848	-0.70008	1236.9784	1264.7772	1274.3179
H	-1.86966	5.22549	1.30200	1295.2633	1348.7668	1376.5764
H	-1.94365	2.83648	2.05730	1378.8202	1380.7248	1387.4490
N	-4.40092	-0.09019	1.99269	1395.5132	1399.6983	1400.1489
N	-4.08688	0.82144	1.45248	1409.9290	1424.1277	1434.3421
C	1.77375	-3.38902	-0.40500	1438.5782	1441.6954	1451.9171
H	2.44640	-4.16464	-0.01623	1455.1657	1455.9032	1463.1219
H	0.74541	-3.63676	-0.12399	1463.8326	1465.2760	1471.1690
H	1.83450	-3.40641	-1.49770	1475.0744	1481.1729	1482.1666
C	0.97451	-2.18276	2.46641	1485.1464	1491.1805	1493.0703
H	0.53382	-3.11485	2.10726	1504.0767	1505.7476	1508.7899
H	1.62006	-2.39784	3.32807	1522.2535	1527.1714	1556.3601
H	0.14484	-1.55097	2.80134	1602.8561	1665.9194	1796.0379
C	2.25325	0.69227	2.71430	1818.3647	1835.9617	2462.8727
H	1.32546	0.47834	3.25397	3030.7923	3036.6121	3037.8217
H	3.08684	0.56390	3.41695	3041.5769	3047.5591	3048.5055
H	2.22502	1.74506	2.41205	3056.8053	3060.0827	3108.7844
C	3.92214	1.29305	0.05740	3113.9423	3114.9159	3118.3636
H	3.73513	1.60877	-0.97497	3125.2703	3137.7140	3140.4408
H	3.61648	2.11795	0.70953	3142.3172	3142.7699	3147.5011
H	5.00366	1.15049	0.17626	3148.4667	3150.0123	3170.0642
C	3.60728	-1.19558	-1.87547	3172.2994	3180.1347	3184.3814
H	3.72544	-0.21994	-2.35822	3185.2199	3198.3748	3205.9917
H	4.60125	-1.65668	-1.79570			
H	2.99874	-1.81571	-2.54084			
O	-1.31116	-0.43561	-2.99731			
C	-2.53650	1.23583	-1.83665			
H	-2.03163	2.20683	-1.90542			
H	-3.22787	1.14815	-2.67921			
H	-3.08553	1.21339	-0.88902			
C	0.42980	0.30815	2.30634			
C	2.65568	0.71500	2.91114			
H	2.32955	0.91778	3.93866			
H	2.92774	-0.34753	2.85725			
C	3.79449	1.59958	2.48075			
H	3.48375	2.65056	2.46660			
H	4.63320	1.49808	3.17760			
H	4.13091	1.31161	1.47927			
O	0.33368	-0.44917	3.26261			
O	1.55723	0.95591	2.02270			
C	-2.36009	0.68610	3.26416			
H	-3.44394	0.72569	3.39627			
H	-1.92099	0.01076	4.00591			
H	-1.91041	1.67249	3.43323			
O	-2.88701	-0.42384	1.23902			
H	5.67274	-0.47492	-2.32853			
C	0.63389	0.75102	-2.26539			
C	2.92715	1.58077	-1.45499			
C	4.85170	2.36254	-0.35019			
H	4.58554	3.41370	-0.51439			
H	5.46963	2.04686	-1.20246			
C	5.53081	2.13074	0.97347			
H	6.47248	2.68645	1.02514			
H	4.88756	2.45610	1.79667			

H	5.74242	1.06336	1.11047
O	3.65827	1.57347	-0.34098
O	3.14601	2.29349	-2.40703
C	0.92000	0.94807	-3.71343
H	-0.00533	0.88337	-4.29044
H	1.41585	1.91119	-3.86642
H	1.63737	0.18240	-4.03787
O	-0.52197	0.63428	-1.87363

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.459402 Electronic Energy = -1482.13708549
Internal Energy (E)= -1481.64440449 Enthalpy (H)= -1481.64346049
Gibbs Free Energy (G)=-1481.74017149 Gibbs Free Energy of Solvation=-1482.9542726

St.Pt.	General Structure	Ball & Stick model
VIII-1C	 **VIII-1C**	

Cartesian co-ordinate

Atoms	X	Y	Z
C	2.52636	0.33482	1.18229
C	1.87879	-0.87784	1.63588
C	2.12735	-1.90042	0.65237
C	2.99696	-1.32160	-0.36235
C	3.27664	0.03141	-0.02646
C	-1.51976	0.87343	0.79400
C	-1.20445	2.25086	0.37546
C	-0.15487	2.56545	-0.52845
C	-1.05648	-0.25071	-0.08224
Ir	1.07178	-0.21839	-0.25281
C	-1.16124	-0.17267	-1.57646
C	-1.61932	-1.56159	0.40069
O	-2.66503	-1.91789	-0.37422
C	-3.38394	-3.09286	0.02640
H	-2.68722	-3.93795	0.08194
H	-3.78173	-2.92810	1.03606
C	-4.47517	-3.30814	-0.98862
H	-5.06840	-4.19097	-0.73092
H	-5.14784	-2.44361	-1.02365
H	-4.05423	-3.45493	-1.98882
O	-1.25567	-2.22086	1.34307
O	-2.14134	0.63350	1.82506
O	0.68962	1.69170	-1.03217
C	-0.00395	3.91930	-0.90619
C	-2.01191	3.27493	0.89616
C	-0.82720	4.90294	-0.39354
C	-1.84174	4.59282	0.52115
H	0.79670	4.15511	-1.60414
H	-0.67590	5.93585	-0.70363
H	-2.48525	5.37207	0.92069
H	-2.79110	2.98011	1.59681
N	-5.07125	-0.20818	0.93171
N	-4.60799	0.55495	0.28019
C	1.71658	-3.32962	0.72923
H	2.45196	-3.92101	1.29105
H	0.74222	-3.43121	1.21735
H	1.63481	-3.76707	-0.27201
C	1.11505	-1.00915	2.90523
H	0.45667	-1.87936	2.88739
H	1.81030	-1.09143	3.75107
H	0.47602	-0.13481	3.07434
C	2.51423	1.64972	1.87901
H	1.58032	1.79191	2.43314
H	3.34937	1.72799	2.58742
H	2.59514	2.47168	1.15963
C	4.05615	1.03549	-0.80031
H	4.44307	0.61579	-1.73351
H	3.42288	1.89353	-1.06008
H	4.90917	1.40595	-0.21785
C	3.44044	-2.04687	-1.58376
H	3.85699	-1.36402	-2.32970
H	4.20456	-2.79506	-1.33733
H	2.59725	-2.57085	-2.04872

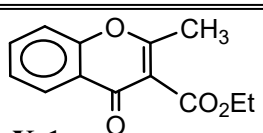
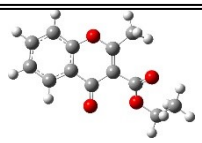
Frequencies

-3.2624	30.9011	41.1962
49.8100	54.9799	77.4854
83.7871	90.9783	101.8549
107.8573	113.4427	130.1848
131.9783	138.5674	146.2573
158.3697	162.2239	163.9124
171.6015	183.5779	187.7323
202.1928	206.5915	212.0589
216.9844	225.7381	226.8177
229.6944	234.6424	240.5773
243.8695	255.6709	266.0056
277.7679	296.1136	309.7137
314.9145	321.5602	325.5705
335.4494	349.7292	365.7430
399.6732	408.4417	416.9391
433.2802	442.6348	468.1471
496.7604	533.0851	536.1650
542.3820	545.4528	547.5893
559.3550	586.8757	595.3164
599.1127	608.7745	623.8931
645.0310	679.9037	705.9054
752.0244	764.6313	776.6093
807.0633	816.9615	819.1283
845.3744	862.0359	871.9256
895.6918	942.4393	963.1345
965.6450	977.8945	981.3919
983.3002	1028.8193	1031.8263
1036.3906	1042.7346	1048.2853
1050.5520	1053.7978	1058.1000
1089.9332	1096.9599	1099.7734
1110.0977	1119.0887	1141.4555
1142.9273	1154.8950	1180.5615
1185.4931	1190.3253	1239.3445
1264.1332	1282.5283	1284.4294
1295.9515	1346.3516	1377.8341
1379.0590	1384.4334	1386.1464
1387.2406	1399.4215	1402.9102
1412.2856	1420.2843	1428.2829
1438.3208	1441.9803	1444.1298
1444.6394	1450.6653	1456.0541
1460.4182	1461.6989	1466.3847
1471.0639	1474.3553	1480.5866
1481.3996	1490.0794	1490.4779
1498.4123	1505.0714	1511.2074
1522.1332	1524.5015	1548.5974
1607.8262	1665.3486	1686.4398
1744.8847	1862.8870	2463.9480
3030.8723	3035.8973	3038.0066
3039.1166	3042.5288	3046.3504
3047.3704	3053.6514	3103.9653
3106.1321	3115.5871	3116.4866
3118.0345	3122.4876	3134.5151
3137.2167	3139.0591	3141.5485
3144.0410	3147.7755	3167.7626
3170.8773	3177.3247	3182.6662
3189.3963	3193.3876	3205.8679

O	-0.17246	-0.67365	-2.14392
C	-2.28123	0.44282	-2.32751
H	-2.32916	1.50933	-2.07024
H	-2.13575	0.32656	-3.40355
H	-3.22788	-0.00444	-2.00392
C	0.42980	0.30815	2.30634
C	2.65568	0.71500	2.91114
H	2.32955	0.91778	3.93866
H	2.92774	-0.34753	2.85725
C	3.79449	1.59958	2.48075
H	3.48375	2.65056	2.46660
H	4.63320	1.49808	3.17760
H	4.13091	1.31161	1.47927
O	0.33368	-0.44917	3.26261
O	1.55723	0.95591	2.02270
C	-2.36009	0.68610	3.26416
H	-3.44394	0.72569	3.39627
H	-1.92099	0.01076	4.00591
H	-1.91041	1.67249	3.43323
O	-2.88701	-0.42384	1.23902
H	5.67274	-0.47492	-2.32853
C	0.63389	0.75102	-2.26539
C	2.92715	1.58077	-1.45499
C	4.85170	2.36254	-0.35019
H	4.58554	3.41370	-0.51439
H	5.46963	2.04686	-1.20246
C	5.53081	2.13074	0.97347
H	6.47248	2.68645	1.02514
H	4.88756	2.45610	1.79667
H	5.74242	1.06336	1.11047
O	3.65827	1.57347	-0.34098
O	3.14601	2.29349	-2.40703
C	0.92000	0.94807	-3.71343
H	-0.00533	0.88337	-4.29044
H	1.41585	1.91119	-3.86642
H	1.63737	0.18240	-4.03787
O	-0.52197	0.63428	-1.87363

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.460596 Electronic Energy = -1482.18200732
Internal Energy (E)= -1481.68872032 Enthalpy (H)= -1481.68777632
Gibbs Free Energy (G)=-1481.78278232 Gibbs Free Energy of Solvation=-1482.99494868

St.Pt.	General Structure	Ball & Stick model
X-1	 **X-1**	

Cartesian co-ordinate

Atoms	X	Y	Z
C	2.18086	0.65404	0.11708
C	1.73245	-0.64804	-0.07243
C	0.29976	-0.92573	-0.28908
C	-0.01102	1.51137	-0.05260
O	1.31156	1.71008	0.11127
C	2.66905	-1.68634	-0.06096
C	3.52630	0.94798	0.31835
C	4.00915	-1.41669	0.14141
C	4.43481	-0.09652	0.33025
H	2.29396	-2.69485	-0.21679
H	4.73480	-2.22540	0.15255
H	5.48931	0.11555	0.48808
H	3.82821	1.98171	0.46060
O	-0.09891	-2.05275	-0.53578
C	-0.55514	0.27030	-0.21547
C	-0.73005	2.81342	-0.02450
H	-0.91310	3.16220	-1.04649
H	-1.70870	2.72645	0.44898
H	-0.11616	3.55240	0.49615
C	-2.02783	0.16804	-0.38309
C	-3.92118	-1.17410	0.00774
H	-4.03251	-2.26097	0.05923
H	-4.23524	-0.82940	-0.98326
C	-4.69599	-0.47931	1.10071
H	-5.75940	-0.73125	1.03185
H	-4.33388	-0.78827	2.08667
H	-4.59534	0.60639	1.01083
O	-2.71596	1.01341	-0.91882
O	-2.51158	-0.95136	0.15674

Frequencies

37.9986	48.2314	75.8867
103.5721	115.0127	147.3091
150.9988	189.1005	220.8960
246.5561	279.7456	283.2309
303.0066	356.9778	372.5615
394.6257	432.9286	454.4443
473.3339	531.9558	546.5059
570.0029	587.2556	641.4769
672.6953	689.6102	755.4528
771.0897	779.5322	815.0531
832.6464	865.6759	875.8972
895.1731	920.3047	969.3136
995.4173	1013.2063	1033.6783
1046.5480	1049.8593	1110.1776
1121.0776	1130.1934	1150.0932
1169.8403	1199.1676	1237.0822
1263.2154	1287.8048	1316.4388
1342.8258	1383.3937	1389.2153
1393.7019	1410.6278	1423.5423
1453.0925	1463.5896	1469.0155
1474.4836	1490.3486	1505.6250
1510.4655	1632.5950	1670.2560
1683.7480	1804.8843	1829.0885
3048.5348	3065.0908	3072.0439
3129.7466	3140.4830	3148.1541
3153.9869	3184.5310	3188.2735
3199.8711	3209.3918	3214.6747

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.226940 Electronic Energy = -803.032983981
Internal Energy (E)= -802.791102981 Enthalpy (H)= -802.790158981
Gibbs Free Energy (G)=-802.848610981 Gibbs Free Energy of Solvation=-803.471979142

Combined PES associated to the conversion from I to VI for S2 and S3 of first part of C-H/O-H activation

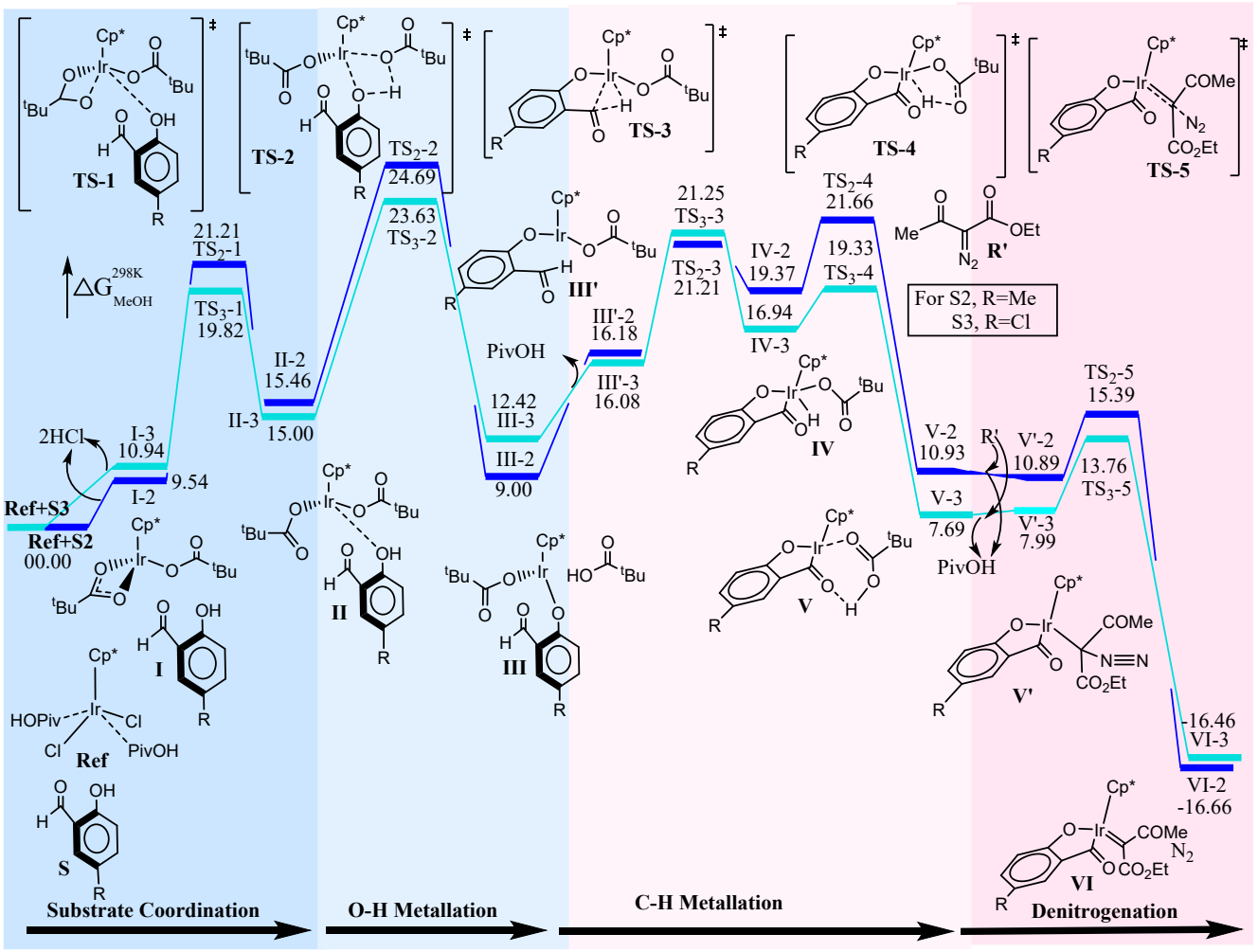


Fig-8: PES with Gibbs free energy (kcal/mol) and the structures of the stationary points of first part of path using M06L functional & 6-311++G(d,p) basis set for non-metals and triple-zeta SDD for metal (Blue colour for S2 and Cyan colour for S3)

Combined PES associated to the conversion from VI to X for S2 and S3 of second part of C-H/O-H activation

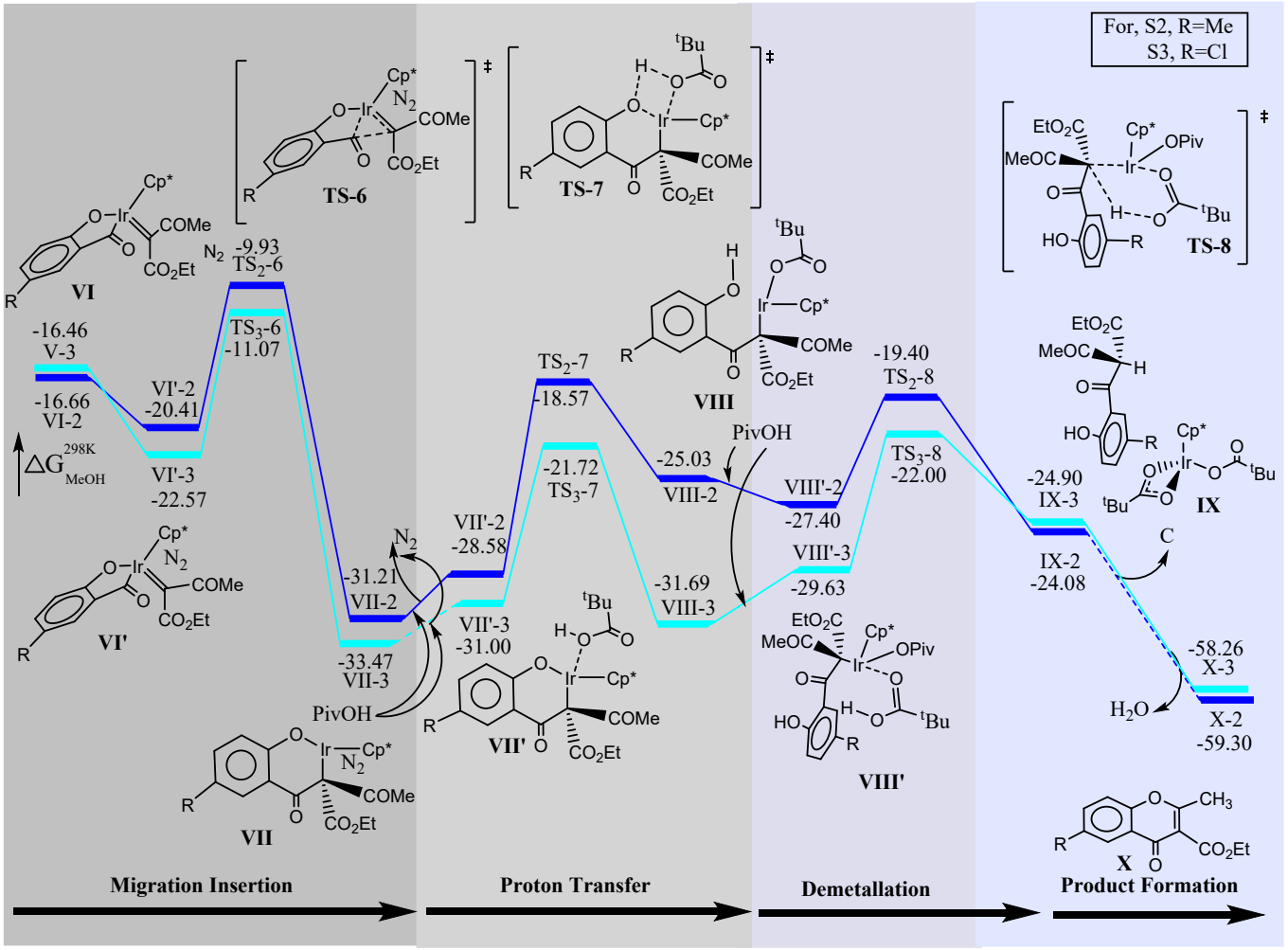
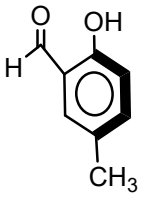
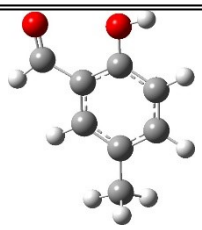


Fig-9: PES with Gibbs free energy (kcal/mol) and the structures of the stationary points of second part of path using M06L functional & 6-311++G(d,p) basis set for non-metals and triple-zeta SDD for metal (Blue colour for S2 and Cyan colour for S3)

St.Pt.	General Structure	Ball & Stick model
S2		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.74412	0.91750	0.00197
O	-1.97586	1.45792	0.00557
C	0.40559	1.70978	-0.00176
C	1.66443	1.13045	-0.00644
C	-0.60670	-0.48282	-0.00123
C	1.83244	-0.25734	-0.00620
C	0.68040	-1.03110	-0.00617
H	0.76764	-2.11933	-0.01031
H	2.54421	1.77331	-0.01143
C	-1.74270	-1.41903	-0.00240
H	-1.40587	-2.48746	-0.00793
O	-2.91893	-1.14166	0.00230
H	0.30321	2.79506	-0.00384
H	-1.89637	2.41890	0.00513
C	3.20078	-0.86978	0.00894
H	3.68644	-0.74817	0.98540
H	3.16032	-1.94259	-0.20467
H	3.85807	-0.40577	-0.73555

Frequencies

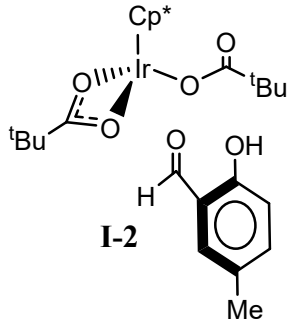
88.7026	90.7695	136.5505
178.7657	234.6471	294.2184
336.2679	404.2494	413.9829
442.1407	450.4665	483.3244
561.8327	678.6823	723.4892
773.3123	801.5432	813.2558
895.6303	948.7472	952.4873
1009.1335	1031.8652	1048.1981
1139.5954	1172.9430	1196.0046
1275.1611	1316.7237	1340.2348
1388.8169	1405.0965	1407.0189
1452.9394	1460.7630	1488.7854
1554.6250	1649.4619	1690.2023
1853.7158	2835.3976	3032.3839
3105.9166	3134.4365	3148.9724
3153.7792	3169.2156	3873.4890

Statistical Thermodynamic Analysis

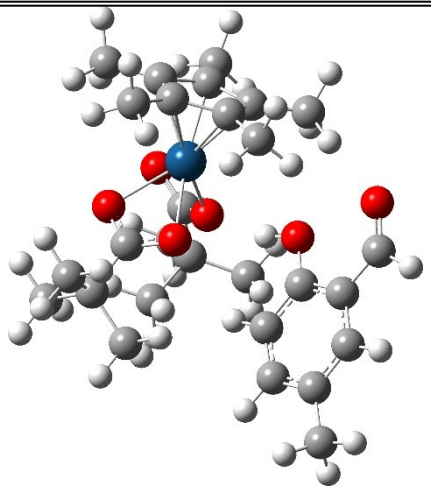
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.141333 Electronic Energy = -459.812785569
Internal Energy (E)= -459.662145569 Enthalpy (H)= -459.661201569
Gibbs Free Energy (G)=-459.705891569 Gibbs Free Energy of Solvation=-460.085238181

St.Pt.	General Structure	Ball & Stick model

I-2



I-2



Cartesian co-ordinate

Atoms	X	Y	Z
C	2.78993	-1.48190	-0.84112
C	3.22753	-1.17899	0.49700
C	2.31235	-1.80218	1.43538
C	1.30575	-2.49064	0.65586
C	1.58995	-2.29008	-0.74555
C	-2.78762	-0.74689	-0.85962
C	-0.51717	2.37097	2.65236
C	0.13013	1.37635	1.71187
O	1.32732	1.52680	1.32062
O	-0.48046	0.31575	1.36820
C	2.38622	-1.73191	2.92121
H	2.74030	-0.74865	3.25186
H	1.39768	-1.88665	3.36737
H	3.06382	-2.49205	3.33014
C	0.12218	-3.21066	1.19390
H	-0.70866	-3.18829	0.47974
H	0.37142	-4.26139	1.39014
H	-0.22207	-2.76243	2.13191
C	0.84479	-2.85933	-1.89949
H	-0.18753	-3.11720	-1.64257
H	0.80345	-2.13924	-2.72449
H	1.35518	-3.76006	-2.26607
C	3.46292	-1.09333	-2.10761
H	2.72852	-0.91202	-2.89860
H	4.03558	-0.17080	-1.99345
H	4.13296	-1.89758	-2.43952
C	4.36511	-0.28490	0.84004
H	4.24857	0.13772	1.84281
H	5.31653	-0.83023	0.80382
H	4.41423	0.55210	0.13479
C	1.08751	1.71724	-1.83381
O	0.33341	0.83298	-1.22357
O	2.30676	1.74627	-1.77105
C	0.28242	2.78878	-2.57566
O	-1.60169	-1.01421	-1.40341
C	-0.84310	2.17102	-3.40382
H	-1.58175	1.65336	-2.78229
H	-1.36945	2.95780	-3.96010

Frequencies

21.6385	30.8477	48.6523
54.7311	56.0786	59.9544
71.8112	73.4384	80.1235
84.8070	89.7075	95.2909
102.2772	109.8681	126.5978
132.5780	143.8525	147.9061
152.2547	165.7810	167.7903
170.1821	174.5319	177.4473
185.2280	194.1763	202.9649
206.5573	214.3581	218.6450
225.2284	229.5269	244.3362
246.5154	251.5875	260.3957
271.3558	276.5062	290.4330
301.3796	309.0462	311.6913
316.7921	325.2645	328.0224
330.7220	339.5528	343.9627
346.7759	349.1167	360.6119
391.1472	394.6894	413.4185
422.4044	426.7721	432.8799
440.9475	455.7081	458.8004
463.2296	469.6576	477.9977
488.6130	534.9373	538.4328
544.4367	549.7150	562.2178
568.9734	582.0352	592.4455
603.3142	624.3303	634.3960
681.4847	740.7729	781.0747
788.0254	798.8534	803.2236
809.5430	812.1313	816.1904
832.9203	858.1849	897.0051
912.5433	929.1257	937.8536
946.0105	950.3209	953.6283
954.5056	954.9745	958.7694
962.3242	974.0303	979.6817
982.3527	1011.8693	1022.0467
1034.6650	1035.6676	1038.5698
1041.8369	1043.4768	1046.1928
1046.6512	1047.6066	1050.9198
1054.9749	1091.9719	1093.1627
1105.8870	1155.5375	1180.8329
1183.7497	1189.6346	1224.1373
1235.8420	1238.6331	1242.2410
1262.2011	1263.9988	1271.3593

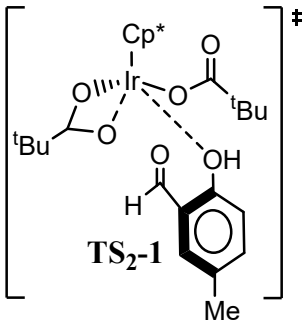
H	-0.45226	1.45148	-4.13460	1272.8883	1345.9386	1353.1954
C	1.20594	3.59385	-3.48095	1365.0756	1373.9844	1379.3843
H	0.64333	4.39580	-3.97655	1382.4121	1383.1545	1385.1466
H	2.02656	4.03796	-2.90952	1392.9893	1395.6976	1400.4180
H	1.65040	2.95744	-4.25522	1401.9777	1406.6101	1409.1098
C	-0.30222	3.70187	-1.49217	1413.7226	1416.5207	1416.6072
H	0.50258	4.17773	-0.91608	1428.1700	1437.9405	1440.4268
H	-0.91540	4.49182	-1.94534	1443.1056	1449.0251	1450.5711
H	-0.92743	3.12991	-0.79300	1453.1006	1453.8954	1456.9009
C	-2.01254	2.48164	2.37019	1459.2859	1460.5492	1462.2091
H	-2.50148	1.50198	2.39510	1465.6254	1468.2985	1469.8376
H	-2.48207	3.13148	3.11973	1472.2694	1475.2515	1477.6688
H	-2.19667	2.92591	1.38265	1481.9452	1482.7814	1483.4368
C	0.15153	3.73616	2.53909	1486.6177	1487.0077	1492.2655
H	-0.30775	4.43165	3.25305	1498.7611	1503.1384	1504.7333
H	1.22346	3.67566	2.75137	1515.1055	1520.6981	1522.7873
H	0.03373	4.15411	1.53187	1547.9508	1559.9500	1602.5991
C	-0.29547	1.79653	4.05925	1642.9835	1693.5476	1788.9519
H	0.77604	1.68204	4.26819	1823.2311	2837.0910	3018.6175
H	-0.71990	2.47445	4.81041	3024.3035	3028.7357	3029.9026
H	-0.77709	0.81700	4.16402	3031.4195	3034.4382	3035.4998
Ir	1.26280	-0.39112	0.21858	3035.8773	3037.6207	3038.3572
C	-3.15433	0.55707	-0.49929	3041.5486	3043.2628	3104.1359
C	-4.41710	0.82261	-0.00282	3107.3023	3109.1444	3110.9766
C	-5.37704	-0.18667	0.16316	3111.9574	3114.7378	3115.9817
C	-3.71937	-1.78810	-0.66416	3118.4607	3119.9206	3120.4408
C	-4.99748	-1.47462	-0.17315	3123.3980	3124.3686	3126.4606
H	-4.67473	1.84794	0.26631	3128.0350	3129.4633	3131.3804
H	-5.70901	-2.29305	-0.04450	3139.3509	3139.9739	3144.5863
H	-1.02887	-0.21344	-1.42372	3145.1406	3146.2020	3147.5168
H	-2.41389	1.34880	-0.60771	3148.2173	3151.9001	3158.9962
C	-3.43301	-3.20199	-0.90258	3174.2810	3191.9462	3511.0191
H	-4.34467	-3.84178	-0.78976			
O	-2.36478	-3.72055	-1.16542			
C	-6.74360	0.13179	0.69145			
H	-7.27159	0.84370	0.04472			
H	-7.36243	-0.76861	0.76516			
H	-6.69541	0.58343	1.69027			

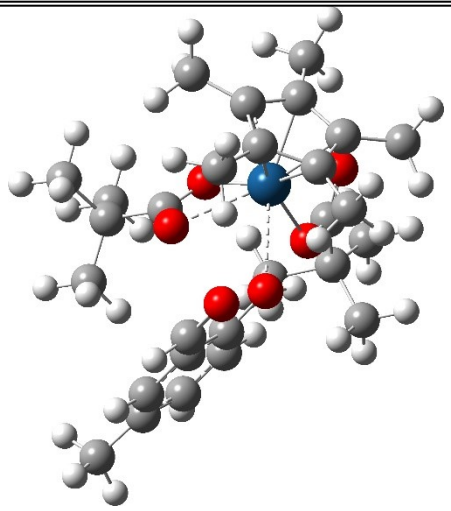
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.641097 Electronic Energy = -1646.79942349
Internal Energy (E)= -1646.11786149 Enthalpy (H)= -1646.11691749
Gibbs Free Energy (G)=-1646.22833349 Gibbs Free Energy of Solvation=-1646.28283662

St.Pt.	General Structure	Ball & Stick model

TS_2-1





Cartesian co-ordinate

Atoms	X	Y	Z
C	2.89160	-1.24275	-0.78974
C	3.00556	-1.09499	0.64867
C	2.01609	-1.97260	1.26597
C	1.29533	-2.62704	0.21943
C	1.81991	-2.16781	-1.05921
C	-2.28745	-0.50824	-1.42846
C	-1.63401	0.96852	2.90199
C	-0.73908	0.38032	1.81431
O	0.42255	0.87176	1.63876
O	-1.12724	-0.62305	1.17479
C	1.76225	-2.09463	2.72687
H	1.95131	-1.14177	3.23333
H	0.71722	-2.36198	2.91335
H	2.40315	-2.85964	3.18214
C	0.16402	-3.57296	0.38572
H	-0.60203	-3.42003	-0.38231
H	0.52695	-4.60604	0.30337
H	-0.31389	-3.45216	1.36202
C	1.39231	-2.67115	-2.39296
H	0.33703	-2.96111	-2.39004
H	1.52807	-1.90781	-3.16747
H	1.99106	-3.54555	-2.68024
C	3.75037	-0.56339	-1.79489
H	3.22999	-0.45517	-2.75215
H	4.03103	0.43619	-1.45024
H	4.66100	-1.15034	-1.97277
C	3.99015	-0.23870	1.35526
H	3.67480	-0.04041	2.38417
H	4.97066	-0.73217	1.38678
H	4.08089	0.72458	0.84401
C	1.71209	2.29392	-0.82483
O	0.86767	1.32393	-1.03574
O	2.81548	2.17705	-0.30662
C	1.16121	3.66719	-1.23292
O	-1.05658	-1.01588	-1.66258
C	0.54494	3.62591	-2.62984
H	-0.27077	2.89853	-2.69650

Frequencies

-87.2688	15.9354	36.0872
46.5896	50.8449	58.6621
64.0500	66.4370	76.2187
81.4510	90.9347	92.6116
99.6216	106.5341	123.1656
126.2964	132.8160	135.8934
158.7086	165.6118	170.5697
172.0746	181.5229	188.7584
191.5102	199.9277	204.4454
208.6368	220.0599	222.3212
226.1321	234.5918	242.8544
249.3553	254.9966	264.7709
271.2846	280.3777	292.1030
298.1059	302.3240	310.2694
315.5815	326.0869	336.3503
340.3892	345.3306	354.4270
364.1292	364.4287	368.8604
378.7010	392.6114	399.3991
417.6358	419.8241	437.6549
447.5077	452.7763	453.5050
456.9394	467.1402	489.6830
507.6093	532.5714	538.5207
546.6839	548.9943	563.9818
566.8588	582.8860	591.7016
603.2208	606.3907	620.9535
626.9464	681.7529	739.7973
782.6955	785.7635	792.0862
803.5901	808.7780	810.9929
813.3029	826.1012	853.4743
894.8771	910.4834	926.0522
945.4428	945.9933	947.7871
952.6858	954.7152	957.6171
963.5756	970.7689	978.6371
986.0544	1012.5197	1032.2721
1037.1006	1037.7673	1038.5486
1040.8243	1043.6618	1045.5381
1046.1030	1046.3564	1050.4626
1054.0052	1096.2719	1105.3318
1112.1785	1147.5195	1182.2099
1186.0197	1189.6248	1205.7503
1237.8365	1240.2493	1247.6653
1255.7658	1266.8947	1271.1345

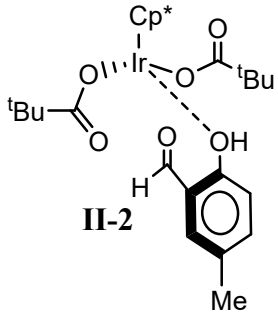
H	0.14320	4.61411	-2.89082	1275.5096	1317.7603	1327.4486
H	1.29523	3.36247	-3.38647	1365.0211	1372.3215	1376.6071
C	2.27500	4.70592	-1.19379	1379.3189	1382.9858	1384.8225
H	1.87598	5.69506	-1.45474	1388.4839	1394.9673	1398.4876
H	2.72793	4.76063	-0.19904	1404.9744	1406.7890	1409.4787
H	3.07223	4.45824	-1.90444	1415.3479	1417.3741	1418.2168
C	0.09165	4.02371	-0.19397	1425.5972	1438.5454	1442.4420
H	0.51837	4.00590	0.81754	1444.7812	1450.6338	1454.7903
H	-0.30586	5.02926	-0.38607	1455.3611	1456.2642	1457.3913
H	-0.74065	3.30819	-0.21528	1460.2669	1463.4156	1465.1912
C	-3.03767	1.18271	2.33817	1465.4695	1467.5390	1471.6981
H	-3.43926	0.25702	1.91021	1473.9548	1475.1290	1481.5489
H	-3.71152	1.52955	3.13282	1483.8235	1484.3700	1485.0237
H	-3.03075	1.94261	1.54548	1487.7615	1488.7361	1495.7854
C	-1.07608	2.27876	3.44108	1502.8437	1505.3891	1509.5947
H	-1.73386	2.66716	4.22970	1514.9088	1523.8036	1533.7987
H	-0.07325	2.14321	3.85957	1544.5298	1550.6280	1652.3246
H	-1.00542	3.03456	2.65067	1668.0773	1689.4250	1772.6976
C	-1.68640	-0.07475	4.02382	1829.7562	2854.8318	3016.6393
H	-0.68683	-0.25003	4.44407	3018.7192	3026.4149	3029.0433
H	-2.33468	0.27810	4.83628	3031.9558	3033.8334	3034.7708
H	-2.07918	-1.02792	3.65193	3035.4226	3036.3248	3037.6442
Ir	1.06899	-0.47771	0.04859	3040.7869	3042.2990	3098.5602
C	-2.48220	0.86994	-1.33087	3102.8281	3105.9411	3106.7509
C	-3.74182	1.37783	-1.06632	3112.3373	3113.7595	3117.9534
C	-4.84928	0.54083	-0.87297	3118.6686	3121.4133	3121.8292
C	-3.37999	-1.37585	-1.27406	3124.6865	3125.6551	3126.5263
C	-4.63879	-0.82394	-0.99152	3126.8394	3129.3560	3133.1786
H	-3.87032	2.45789	-0.98335	3136.9800	3139.4178	3140.0751
H	-5.47974	-1.50918	-0.86769	3142.6664	3147.8118	3153.6991
H	-0.48043	-0.28532	-1.94636	3153.8978	3155.1076	3156.8852
H	-1.61418	1.52412	-1.42334	3162.3830	3179.9197	3729.7107
C	-3.30612	-2.82897	-1.43816			
H	-4.30057	-3.32131	-1.29322			
O	-2.33327	-3.50044	-1.71775			
C	-6.18863	1.11170	-0.51721			
H	-6.45829	1.95114	-1.16887			
H	-6.97962	0.35860	-0.59538			
H	-6.19606	1.49077	0.51372			

Statistical Thermodynamic Analysis

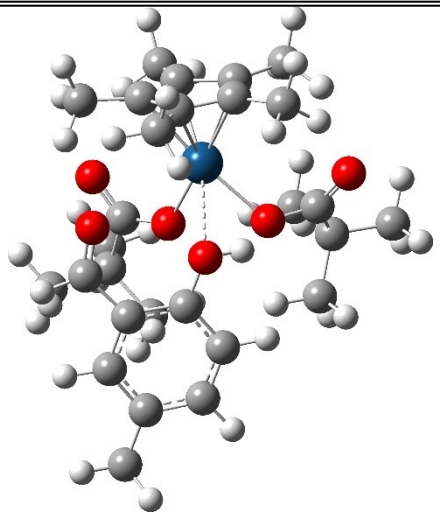
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.640796 Electronic Energy = -1646.77499852
Internal Energy (E)= -1646.09446552 Enthalpy (H)= -1646.09352252
Gibbs Free Energy (G)=-1646.20328452 Gibbs Free Energy of Solvation=-1646.2644017

St.Pt.	General Structure	Ball & Stick model

II-2



II-2



Cartesian co-ordinate

Atoms	X	Y	Z
C	2.98671	-0.63802	-1.19836
C	3.24840	-0.26473	0.16083
C	2.66524	-1.28216	1.03593
C	2.05241	-2.28117	0.20918
C	2.22717	-1.86035	-1.16616
Ir	1.12341	-0.33163	-0.10496
O	-0.63147	-0.13465	0.90242
O	0.43838	1.57086	-0.72045
O	-1.13174	-2.80757	-1.42648
C	-2.28331	-2.44773	-1.29089
H	-3.05877	-3.16944	-0.92972
C	-2.83282	-1.11075	-1.52480
C	-2.06563	-0.00134	-1.92718
C	-4.19527	-0.92573	-1.24561
C	-2.67713	1.25304	-2.00037
C	-4.81617	0.31131	-1.32438
H	-4.77453	-1.79712	-0.93205
C	-4.02184	1.40048	-1.70450
H	-2.07455	2.11296	-2.28883
H	-4.47304	2.39059	-1.76747
O	-0.76667	-0.15090	-2.24920
H	-0.31508	0.70774	-2.09776
C	-0.99223	-0.87664	1.91765
C	-2.30932	-0.44562	2.58139
C	1.16909	2.65641	-0.58569
C	0.56999	3.66216	0.40334
O	2.23776	2.85849	-1.14593
O	-0.36310	-1.82696	2.36380
C	1.73888	-2.58349	-2.36873
H	1.12909	-3.44638	-2.09727
H	1.11259	-1.93560	-2.99116
H	2.59712	-2.91628	-2.96693
C	3.38664	0.11422	-2.41816
H	3.27268	1.19181	-2.25530
H	4.42808	-0.10501	-2.68730
H	2.75434	-0.16673	-3.26755
C	4.03000	0.91782	0.59978

Frequencies

25.3785	32.0273	38.1133
47.4888	55.3686	64.7881
69.0950	80.5715	82.1650
86.1967	87.4112	94.8900
99.5393	107.8606	111.5118
124.6655	133.5167	138.4400
151.5764	160.2028	175.1514
178.6649	184.2507	185.7806
193.5266	200.4797	203.9574
210.6488	224.8725	226.3346
228.8822	235.8957	238.7847
247.4186	254.6921	272.1460
275.7225	287.5312	289.6568
297.2328	302.4112	305.9381
317.0979	320.9476	328.9493
339.4643	342.6740	348.6742
352.1779	355.7589	359.0334
377.4070	385.0558	390.2987
405.7591	416.0931	424.9249
433.0337	444.4832	454.9336
456.2786	458.0072	466.2069
487.9562	535.4806	539.9576
552.2877	558.4183	562.5969
571.3997	574.3741	579.7956
598.1245	604.2261	640.9243
677.1476	734.8129	743.0483
778.8114	792.4027	794.9888
805.5960	809.5927	813.5263
818.0171	819.4347	844.0591
905.7466	906.9226	922.4895
944.1782	945.8157	949.1518
950.7901	951.5484	955.0057
960.8446	963.7032	967.4364
986.4839	1009.1087	1030.7331
1033.8770	1039.4079	1040.3494
1041.1828	1044.2028	1046.6087
1047.7825	1048.9285	1049.9210
1052.8670	1097.0174	1105.7361
1119.3720	1153.1155	1178.6765
1190.8102	1193.1930	1226.5656
1227.9974	1235.0792	1238.7810

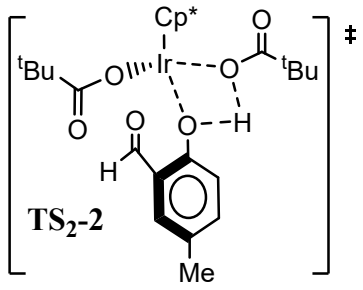
H	3.77398	1.20833	1.62398	1242.1561	1264.7258	1269.6002
H	5.10212	0.68165	0.57701	1276.2178	1324.3328	1345.3955
H	3.84747	1.77437	-0.05750	1351.5030	1361.4260	1370.9894
C	2.73336	-1.28527	2.51885	1374.3709	1377.8466	1380.9431
H	1.82500	-1.72823	2.93678	1384.1257	1389.6313	1396.3914
H	3.60894	-1.85273	2.86044	1398.4474	1399.5548	1406.8012
H	2.81868	-0.26481	2.90876	1408.5156	1410.8892	1413.7501
C	1.43358	-3.56164	0.63819	1417.2318	1427.7140	1436.8552
H	2.08801	-4.39865	0.35984	1437.8945	1443.8354	1445.7280
H	1.26536	-3.57948	1.71509	1451.7838	1453.3666	1453.8339
H	0.46415	-3.70345	0.15238	1458.5888	1460.8388	1462.0508
C	-2.96086	0.75199	1.90186	1462.3431	1462.7114	1464.9846
H	-3.18465	0.54516	0.84946	1470.8937	1473.7775	1476.9451
H	-3.90223	0.99753	2.41359	1479.5965	1480.4714	1482.5143
H	-2.31360	1.63728	1.93670	1484.4108	1487.4679	1489.1733
C	-1.97504	-0.09480	4.03347	1495.7640	1500.6850	1503.2370
H	-2.88883	0.18219	4.57554	1505.6328	1508.0468	1518.1353
H	-1.50678	-0.94396	4.54197	1540.7930	1550.1391	1646.9643
H	-1.28524	0.75925	4.08007	1686.3042	1768.1487	1775.7264
C	-3.25954	-1.64358	2.55009	1830.0935	2844.6476	3013.2855
H	-2.79363	-2.52168	3.00919	3020.1238	3022.7322	3026.6712
H	-4.18305	-1.40783	3.09514	3030.5572	3031.6215	3033.0371
H	-3.53590	-1.89807	1.51721	3033.7411	3036.5157	3040.1050
C	1.32667	4.98172	0.33687	3042.2707	3044.1563	3096.1210
H	1.24801	5.43398	-0.65873	3099.4044	3104.9924	3105.7316
H	0.91776	5.68898	1.07020	3106.9324	3108.8070	3116.9390
H	2.39172	4.83597	0.54654	3118.6841	3119.8523	3121.8374
C	-0.91402	3.88006	0.11107	3123.2498	3125.0186	3135.7715
H	-1.46659	2.93485	0.16481	3136.1836	3137.4873	3138.8262
H	-1.34016	4.57941	0.84276	3140.5910	3140.9742	3142.9067
H	-1.06296	4.31363	-0.88759	3151.1643	3154.2840	3163.6995
C	0.72268	3.04067	1.79919	3165.1895	3172.5469	3182.2244
H	1.78209	2.85573	2.03287	3185.1586	3197.5417	3551.2525
H	0.32863	3.72831	2.55952			
H	0.17740	2.09053	1.86826			
C	-6.25750	0.49842	-0.95891			
H	-6.80104	-0.45199	-0.96732			
H	-6.35700	0.92410	0.04856			
H	-6.76435	1.18249	-1.64917			

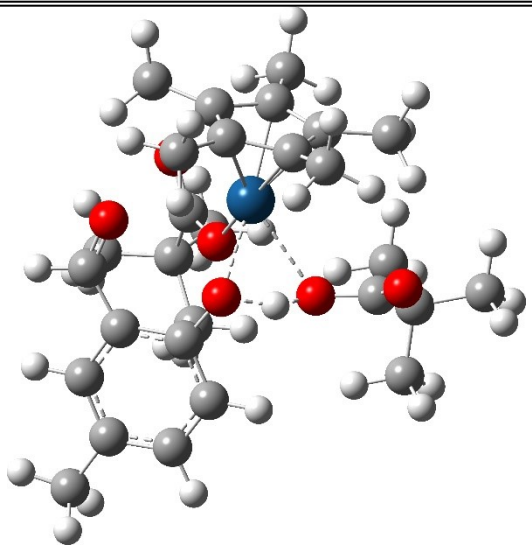
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.640374 Electronic Energy = -1646.78386422
Internal Energy (E)= -1646.10288722 Enthalpy (H)= -1646.10194322
Gibbs Free Energy (G)=-1646.21354322 Gibbs Free Energy of Solvation=-1646.27446113

St.Pt.	General Structure	Ball & Stick model

TS_2-1





Cartesian co-ordinate

Atoms	X	Y	Z
C	2.76740	-0.90965	-1.26422
C	3.05482	-0.45930	0.07341
C	2.47540	-1.39277	1.01758
C	1.82517	-2.43671	0.24870
C	2.02095	-2.12736	-1.15851
Ir	0.90951	-0.55633	-0.16407
O	-0.73977	-0.16651	0.94499
O	0.36977	1.79662	-0.62105
O	-1.11995	-2.66761	-1.14160
C	-2.26354	-2.24908	-1.11227
H	-3.09887	-2.93793	-0.83307
C	-2.72265	-0.90013	-1.40974
C	-1.86988	0.18177	-1.72564
C	-4.11101	-0.68711	-1.34633
C	-2.46153	1.43607	-1.95412
C	-4.69540	0.54430	-1.58309
H	-4.74437	-1.54069	-1.09425
C	-3.83158	1.60612	-1.88997
H	-1.81441	2.27755	-2.19326
H	-4.25392	2.59315	-2.08016
O	-0.54330	0.06438	-1.84563
H	-0.04000	1.10909	-1.49618
C	-1.08966	-0.76799	2.04840
C	-2.32198	-0.15507	2.72845
C	1.31292	2.71482	-0.69935
C	1.22171	3.72765	0.44166
O	2.14502	2.77829	-1.58993
O	-0.51927	-1.73076	2.54653
C	1.54397	-2.92445	-2.31830
H	0.91371	-3.75731	-2.00477
H	0.95199	-2.30542	-3.00056
H	2.40945	-3.31408	-2.86968
C	3.15289	-0.21725	-2.52402
H	3.03074	0.86881	-2.42908
H	4.19763	-0.43336	-2.78359
H	2.52324	-0.54943	-3.35586

Frequencies

-163.0783	34.7415	41.9272
53.3159	58.1494	59.1288
71.7238	74.2968	82.3388
88.7104	92.4689	97.3825
105.3640	108.7580	119.5344
123.1040	129.0040	133.1552
142.2263	152.8986	161.8724
169.3697	177.7008	180.8094
187.1099	203.7594	207.5890
210.7375	216.9372	225.7149
227.4026	232.6944	238.8900
244.3467	251.9749	263.9398
269.0729	281.2849	287.4947
301.4104	303.8185	308.3904
308.8359	316.0845	317.2145
320.3699	335.7832	337.5145
347.3588	359.0940	362.6023
377.6251	385.5027	392.4501
396.4196	414.3060	437.8866
444.1172	451.0881	451.9670
466.3048	469.4405	484.4702
509.2370	534.8061	539.1190
547.2717	565.4315	573.5414
577.8155	581.8837	595.8765
603.8250	624.5955	644.1333
684.4922	723.0211	746.3015
777.1433	790.9304	800.3742
808.0165	809.6639	813.6223
816.5756	825.1429	844.3274
898.0274	918.5727	924.9889
947.0964	947.8923	951.4328
956.3169	957.6666	963.1826
965.9473	966.8075	967.8575
982.8690	1009.8528	1028.1642
1033.3752	1037.6098	1041.1975
1044.2282	1044.5768	1046.6465
1048.7735	1050.9798	1052.6936
1052.8281	1099.7983	1101.9378
1112.9499	1158.6532	1187.9629
1189.0783	1192.0013	1232.6872

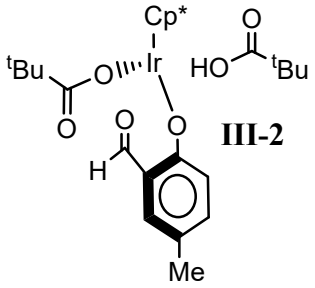
C	3.86172	0.74235	0.40323	1235.5947	1240.2951	1245.9995
H	3.67504	1.09066	1.42396	1250.2239	1266.9500	1268.3863
H	4.92792	0.48941	0.32925	1278.6055	1331.0552	1356.7277
H	3.66546	1.56536	-0.29405	1366.0481	1377.3996	1378.3573
C	2.59850	-1.33499	2.49786	1382.4214	1384.9150	1386.0189
H	1.69203	-1.72716	2.96773	1391.4770	1394.2085	1395.4041
H	3.46691	-1.91551	2.83557	1399.6012	1403.5155	1409.7260
H	2.72783	-0.30235	2.84047	1412.0221	1415.3081	1418.4615
C	1.17305	-3.65808	0.78374	1423.5037	1434.0081	1440.9141
H	1.88554	-4.49406	0.77311	1443.2866	1446.5077	1447.8074
H	0.81734	-3.49019	1.80215	1448.7684	1453.7887	1455.2435
H	0.30277	-3.92333	0.17506	1456.7017	1459.2978	1461.5312
C	-2.91763	1.00353	1.93709	1463.8029	1466.3721	1467.4394
H	-3.29522	0.66933	0.96349	1468.9508	1473.5630	1475.1050
H	-3.75492	1.44118	2.49782	1477.3946	1481.8207	1482.6875
H	-2.17637	1.79065	1.74837	1486.1148	1486.5580	1494.8241
C	-1.87103	0.32994	4.10878	1499.9935	1500.8689	1501.6944
H	-2.72822	0.72730	4.66788	1505.7642	1507.0358	1513.5761
H	-1.42697	-0.49050	4.68234	1527.3220	1543.3740	1620.6276
H	-1.12610	1.13240	4.02293	1630.8228	1691.9289	1770.1504
C	-3.36260	-1.26324	2.89474	1809.7542	1812.3755	2849.5089
H	-2.94279	-2.11088	3.44623	3022.3102	3022.8970	3025.7533
H	-4.23565	-0.88262	3.44111	3029.8837	3030.6434	3031.9490
H	-3.71165	-1.62731	1.91858	3032.1607	3035.1484	3037.2705
C	2.46265	4.60791	0.46046	3038.5644	3040.8891	3046.8970
H	2.59813	5.12010	-0.49762	3099.3868	3104.0987	3105.9362
H	2.37989	5.36100	1.25432	3106.4746	3111.2865	3112.8093
H	3.36643	4.01366	0.64592	3113.4136	3115.6665	3120.7631
C	-0.02712	4.57586	0.16632	3121.4364	3127.4498	3129.4483
H	-0.92861	3.95077	0.16215	3133.6850	3137.3794	3138.9840
H	-0.13890	5.34162	0.94472	3139.5821	3140.3192	3140.7808
H	0.04851	5.08742	-0.80200	3141.6423	3142.3017	3145.4666
C	1.04706	3.00847	1.78088	3151.1644	3158.9694	3161.6025
H	1.92595	2.39668	2.02691	3185.6654	3186.8536	3191.0724
H	0.92192	3.74588	2.58449			
H	0.17235	2.34818	1.76369			
C	-6.17795	0.75270	-1.51004			
H	-6.70151	-0.18214	-1.28457			
H	-6.44407	1.47781	-0.73082			
H	-6.57879	1.13830	-2.45572			

Statistical Thermodynamic Analysis

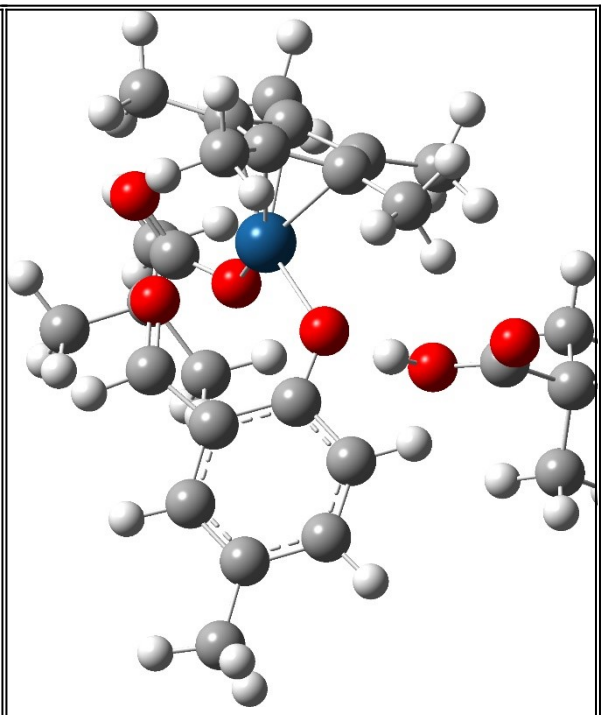
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.636466 Electronic Energy = -1646.77309506
Internal Energy (E)= -1646.09686706 Enthalpy (H)= -1646.09592306
Gibbs Free Energy (G)=-1646.20460406 Gibbs Free Energy of Solvation=-1646.26035019

St.Pt.	General Structure	Ball & Stick model

III-2



III-2



Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.30221	-2.43465	-1.29260
C	-1.02593	-2.54257	0.13105
C	-2.16098	-1.98733	0.84201
C	-3.08968	-1.47725	-0.12303
C	-2.56020	-1.77076	-1.45323
Ir	-1.20988	-0.47375	-0.36437
O	-0.37152	0.72190	1.13094
O	2.44460	-0.79772	0.50507
O	-2.00801	1.43383	-1.03316
C	-1.31648	2.42915	-1.31425
H	-1.87747	3.35962	-1.52201
C	0.09811	2.53766	-1.43156
C	0.97374	1.41072	-1.42491
C	0.61876	3.83835	-1.64471
C	2.34655	1.67009	-1.66688
C	1.95872	4.07771	-1.83265
H	-0.08325	4.67482	-1.64663
C	2.81186	2.95042	-1.84710
H	3.01752	0.81404	-1.69375
H	3.87884	3.10661	-2.01100
O	0.60698	0.17361	-1.25509
H	1.71110	-0.52128	-0.10222
C	-1.12990	1.35508	1.97135
C	-0.38088	2.38983	2.82730
C	3.13205	-1.77864	-0.07068
C	4.35767	-2.17710	0.73907
O	2.81105	-2.29129	-1.12671
O	-2.34039	1.19763	2.11548
C	-3.22820	-1.41464	-2.73425
H	-3.66746	-0.41263	-2.68105
H	-2.51895	-1.42097	-3.56738

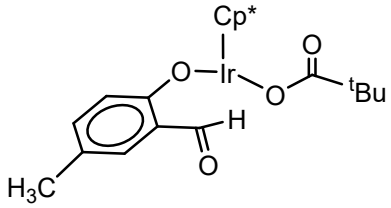
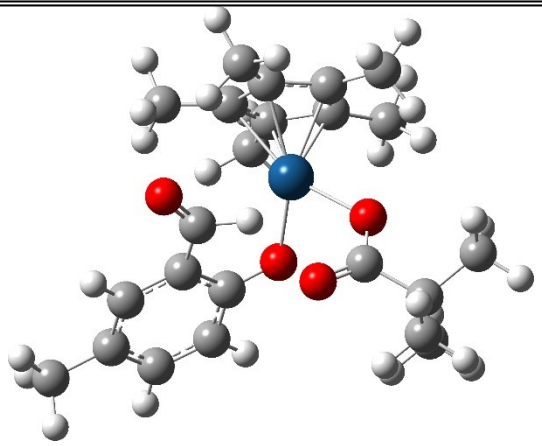
Frequencies

32.3977	35.7457	38.3135
44.4336	46.2987	49.8471
63.8559	72.5851	76.7213
78.8129	83.3145	85.8624
89.7656	107.1717	119.3618
123.5332	138.4585	144.7459
152.1685	157.4843	167.5935
169.9525	184.5394	191.9958
193.1327	201.5983	207.8168
211.6642	217.5123	225.5922
233.2647	244.2035	256.1347
260.0936	262.6081	287.4590
289.8949	301.3607	309.3623
311.8938	312.7127	322.0541
327.7619	334.5889	338.5990
340.2967	341.5251	346.2169
358.8357	368.7008	378.7205
383.7668	386.8597	388.9989
403.2539	408.2947	435.1498
442.3618	449.1111	452.1605
460.2433	467.4120	501.7206
533.5736	537.7788	542.6617
548.6527	552.2521	561.4124
570.2022	587.9456	591.4171
592.5609	606.4175	638.7674
690.9125	745.8781	765.3513
786.3348	791.7748	794.1104
807.6339	815.6693	817.0163
828.5371	840.7389	884.5765
890.8915	916.8552	947.7217
950.2233	950.4646	954.5155
955.1243	958.9456	961.8931
963.4573	966.9324	979.1886
989.5278	1011.0672	1016.5588
1041.3119	1042.6102	1043.4450

H	-4.03256	-2.12390	-2.96706	1043.7393	1046.6217	1047.0992
C	-0.36194	-2.85722	-2.36398	1047.1784	1051.0126	1052.6863
H	0.66874	-2.57495	-2.11277	1055.1422	1098.0610	1102.8527
H	-0.39545	-3.94636	-2.49472	1118.9302	1156.8498	1187.6215
H	-0.61393	-2.39251	-3.32202	1190.8588	1195.5528	1229.5751
C	0.12941	-3.23859	0.76088	1242.8499	1243.8333	1244.9584
H	0.51072	-2.66325	1.61256	1247.9481	1259.2150	1268.5873
H	-0.16999	-4.22964	1.12739	1272.0459	1315.6295	1359.6799
H	0.94869	-3.37146	0.04669	1376.1142	1378.6933	1379.6849
C	-2.30712	-1.93992	2.32033	1381.4251	1382.5464	1383.5909
H	-2.88611	-1.06604	2.62911	1386.9876	1396.9533	1398.2953
H	-2.80008	-2.85390	2.67702	1400.6483	1405.5463	1405.6676
H	-1.32796	-1.87328	2.80720	1410.6896	1419.6852	1427.2595
C	-4.35652	-0.76369	0.19157	1438.4145	1439.1525	1440.5867
H	-5.13884	-1.46546	0.50705	1442.9229	1449.2536	1451.6190
H	-4.17737	-0.03868	0.99295	1453.5580	1456.5055	1458.8674
H	-4.72539	-0.21132	-0.67814	1460.8963	1463.5224	1465.7826
C	1.09895	2.48172	2.47383	1465.9079	1466.5519	1469.1254
H	1.24284	2.77093	1.42459	1471.1223	1472.6248	1476.2607
H	1.58690	3.23441	3.10854	1478.0088	1478.3011	1487.3292
H	1.60737	1.52264	2.62056	1488.4509	1489.4869	1489.9800
C	-0.55001	1.98164	4.29098	1494.8269	1500.3913	1505.7108
H	-0.07597	2.71978	4.95162	1507.2587	1513.7788	1519.9399
H	-1.61134	1.90754	4.55069	1524.7443	1536.3977	1588.3529
H	-0.08059	1.00740	4.48320	1697.8309	1713.5478	1757.3883
C	-1.05391	3.74260	2.59117	1836.7065	2988.8884	3016.1868
H	-2.12317	3.68924	2.81982	3023.6902	3025.2923	3029.6561
H	-0.59230	4.51283	3.22345	3030.0768	3031.3257	3036.3126
H	-0.94073	4.05810	1.54405	3036.7386	3037.0120	3038.3667
C	5.06590	-3.33425	0.04913	3039.3950	3041.1549	3094.2744
H	5.37857	-3.05987	-0.96397	3101.8533	3102.5457	3104.4243
H	5.95436	-3.62414	0.62393	3107.1502	3112.8809	3117.7987
H	4.40779	-4.20623	-0.03618	3118.4517	3119.8276	3119.9890
C	5.29020	-0.96498	0.82888	3121.4461	3126.7241	3133.3825
H	4.80253	-0.12301	1.33087	3136.8383	3137.8892	3139.0453
H	6.19193	-1.23242	1.39446	3140.0150	3142.2328	3142.2988
H	5.60654	-0.63562	-0.16942	3143.5905	3145.8070	3146.4172
C	3.91526	-2.59227	2.14451	3150.7554	3154.0111	3158.1813
H	3.25423	-3.46826	2.10857	3161.5172	3197.4491	3417.0117
H	4.79406	-2.86334	2.74343			
H	3.38517	-1.77985	2.65253			
C	2.51302	5.45580	-2.02943			
H	1.71970	6.21035	-2.01414			
H	3.23282	5.71697	-1.24348			
H	3.04008	5.54693	-2.98762			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.641582 Electronic Energy = -1646.80527302
Internal Energy (E)= -1646.12340202 Enthalpy (H)= -1646.12245802
Gibbs Free Energy (G)=-1646.23400502 Gibbs Free Energy of Solvation=-1646.28521795

St.Pt.	General Structure	Ball & Stick model
III'-2		

Cartesian co-ordinate

Atoms	X	Y	Z
C	0.94547	-2.45196	-0.99208
C	2.05626	-2.05241	-0.18930
C	1.59269	-1.94406	1.18726
C	0.19643	-2.36571	1.21717
C	-0.20697	-2.66424	-0.12095
C	-2.45610	0.50672	-0.50993
Ir	0.47397	-0.57801	0.03275
C	-3.82401	0.64282	-0.82186
C	-4.71718	1.18300	0.07687
C	-1.95905	0.88682	0.76557
C	-4.20761	1.60165	1.32812
C	-2.88248	1.46690	1.67007
H	-2.50883	1.78189	2.64147
H	-4.89827	2.04102	2.04948
H	-0.43908	0.40334	-1.36662
O	1.77945	1.02348	0.04602
C	1.45764	2.15106	-0.53232
C	2.37162	3.31420	-0.13054
O	0.50104	2.31687	-1.27657
H	-4.15193	0.31877	-1.80945
C	-1.54004	0.02008	-1.51152
O	-1.78851	-0.56435	-2.54891
O	-0.72477	0.70120	1.14704
C	2.28163	4.42125	-1.17390
H	1.24516	4.74222	-1.31318
H	2.88281	5.28470	-0.85985
H	2.65554	4.08001	-2.14696
C	1.82634	3.81958	1.21009
H	1.87639	3.03512	1.97451
H	2.41062	4.68319	1.55492
H	0.77865	4.12873	1.10815
C	3.82109	2.86553	0.03504
H	4.21729	2.44781	-0.89998
H	4.44824	3.72411	0.31014
H	3.91896	2.10357	0.81561
C	3.42668	-1.68772	-0.63880
H	3.67014	-0.66499	-0.32402

Frequencies

20.8743	36.1718	44.3079
47.6848	63.9882	67.0506
79.9820	90.4817	92.2496
113.1737	125.3191	149.8214
154.8496	164.0287	164.5216
168.8445	173.1781	179.6150
184.9250	193.7839	200.3294
209.9459	216.2697	218.8683
231.9153	237.2907	242.0462
267.7984	275.1406	284.5779
300.6006	304.5714	306.5550
316.8299	319.9498	324.7481
335.2879	352.2321	374.2323
391.0362	417.5441	423.9420
428.0465	440.0530	458.9242
468.2371	489.4322	536.0787
537.7189	540.1136	546.1405
572.2011	581.5471	591.9960
598.1530	605.8361	620.0171
640.8497	652.1550	736.2677
748.5215	789.7600	804.3741
812.7607	818.4612	834.8409
854.7165	898.9977	916.6834
945.3512	947.9682	948.6062
953.8351	960.0831	961.1766
971.6386	1018.1598	1034.9495
1039.4973	1040.3402	1043.5933
1045.0682	1046.6080	1047.6081
1048.0619	1070.7354	1090.0084
1095.7679	1105.4089	1140.5566
1155.2739	1182.5137	1188.3190
1226.6426	1236.3836	1244.4448
1265.7616	1273.0211	1339.6517
1356.5476	1372.2535	1376.0558
1380.3681	1385.9043	1394.2141
1397.6893	1400.9673	1403.3976
1404.2504	1410.5079	1437.2345
1437.7636	1440.7821	1446.3584
1448.7346	1449.3656	1452.8424
1455.0735	1456.9448	1459.1743
1459.7167	1460.6334	1461.4882
1465.7028	1466.0242	1471.2348

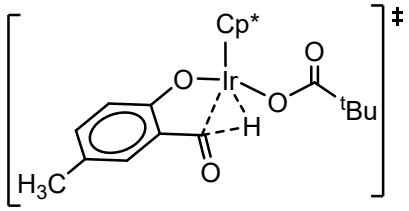
H	4.17131	-2.37004	-0.21064	1474.4522	1477.4749	1479.1846
H	3.51432	-1.72869	-1.72805	1487.3490	1490.1864	1497.0417
C	0.90847	-2.60748	-2.47069	1502.3137	1521.0106	1535.7105
H	1.81263	-2.20505	-2.93623	1543.5895	1598.0972	1690.6112
H	0.82317	-3.66654	-2.74573	1781.9205	1802.1037	2313.9836
H	0.04583	-2.07432	-2.89203	3023.4477	3025.8069	3028.6461
C	-1.53163	-3.17730	-0.56468	3034.0012	3034.3448	3036.1109
H	-1.76137	-2.85108	-1.58377	3036.7592	3042.8174	3044.5407
H	-1.54202	-4.27468	-0.54494	3097.8482	3104.0850	3113.3693
H	-2.33879	-2.81985	0.08320	3113.6802	3114.9323	3115.3702
C	-0.67490	-2.37729	2.42182	3121.2059	3125.8039	3129.2267
H	-1.72341	-2.21912	2.14898	3129.8175	3133.5272	3133.9335
H	-0.59639	-3.33307	2.95435	3145.1210	3147.6164	3147.9698
H	-0.39746	-1.57278	3.11006	3150.1098	3150.9078	3152.2181
C	2.44522	-1.56857	2.34608	3153.7427	3178.6554	3200.1775
H	1.84101	-1.25275	3.20163			
H	3.07029	-2.41382	2.66310			
H	3.10508	-0.73525	2.08106			
C	-6.17403	1.34094	-0.23960			
H	-6.48461	2.39302	-0.20383			
H	-6.40545	0.96223	-1.24058			
H	-6.80646	0.79859	0.47520			
H	-6.67522	-1.41624	-0.26110			
H	-1.64368	0.47723	0.30469			
C	-3.18164	-0.68887	-0.69599			
C	-4.16135	0.14311	-0.13037			
C	-3.58554	-1.74568	-1.53671			
C	-5.51687	-0.03227	-0.36126			
H	-3.82610	0.95771	0.51450			
C	-4.94823	-1.93085	-1.77634			
C	-5.88741	-1.09049	-1.19954			
H	-5.26915	-2.74517	-2.42591			
H	-6.94415	-1.25844	-1.40615			
O	-2.65484	-2.54543	-2.08767			
H	-3.09511	-3.22033	-2.61740			
C	-6.55053	0.85833	0.25923			
H	-6.08738	1.70031	0.78297			
H	-7.23316	1.26832	-0.49438			
H	-7.16446	0.31377	0.98712			

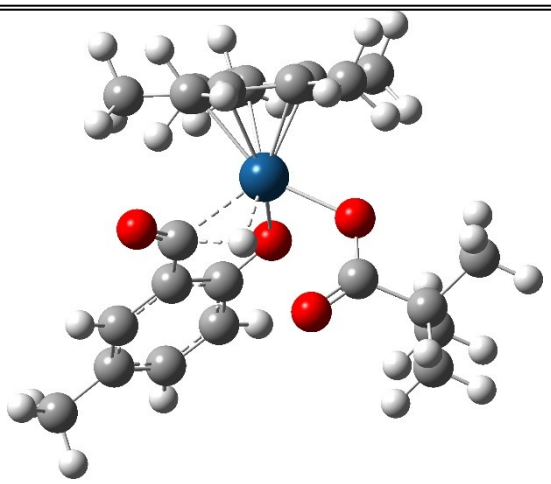
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.489734 Electronic Energy = -1299.93516804
Internal Energy (E)= -1299.41379904 Enthalpy (H)= -1299.41285504
Gibbs Free Energy (G)=-1299.50667604 Gibbs Free Energy of Solvation=-1300.60862537

St.Pt.	General Structure	Ball & Stick model

TS_2-3





Cartesian co-ordinate

Atoms	X	Y	Z
C	1.40542	-2.33034	-0.92083
C	2.40954	-1.55852	-0.26022
C	2.07481	-1.48963	1.15753
C	0.87179	-2.23790	1.35700
C	0.42557	-2.72439	0.07727
C	-2.43510	-0.03479	-0.38781
Ir	0.48988	-0.50870	-0.03325
C	-3.78367	-0.06471	-0.78677
C	-4.76278	0.50775	-0.00179
C	-2.04204	0.56052	0.82777
C	-4.35878	1.12100	1.20643
C	-3.04629	1.15721	1.62280
H	-2.75486	1.63079	2.55703
H	-5.12335	1.58254	1.83302
H	-0.25198	0.29690	-1.31922
O	1.45845	1.32684	0.02137
C	0.92529	2.34139	-0.60186
C	1.53290	3.68358	-0.18139
O	-0.00919	2.27795	-1.39168
H	-4.03116	-0.54132	-1.73464
C	-1.38887	-0.60637	-1.20943
O	-1.51608	-1.27663	-2.21074
O	-0.79464	0.54127	1.21509
C	1.25699	4.73572	-1.24817
H	0.18491	4.81866	-1.44903
H	1.63300	5.71239	-0.91616
H	1.75276	4.48196	-2.19305
C	0.81430	4.05810	1.12065
H	0.96898	3.28974	1.88754
H	1.19233	5.01706	1.49948
H	-0.26541	4.15475	0.95097
C	3.03416	3.56856	0.06741
H	3.56288	3.23820	-0.83643
H	3.44106	4.54700	0.35497
H	3.25276	2.85526	0.86914
C	3.59972	-0.90227	-0.86410
H	3.64520	0.15160	-0.56309
H	4.52340	-1.39490	-0.53472

Frequencies

-294.0967	-157.4336	-23.5044
24.3028	34.3561	37.7231
52.0164	64.7373	72.9212
83.9380	86.1907	110.2838
122.1226	132.6960	148.1008
153.7445	159.5093	165.1175
168.0953	175.3686	178.1913
186.4847	199.7208	209.4055
226.8833	233.1996	240.6859
251.9471	262.6682	275.3826
283.0458	291.0584	306.9004
316.2256	322.3645	327.4276
329.4522	344.4112	363.9224
378.4826	392.2229	406.9199
424.9169	428.3031	442.0907
468.5854	484.7403	496.2889
537.1604	538.9788	541.6607
545.9409	570.7651	586.4351
592.0648	603.5996	639.6059
644.1499	656.0810	710.0559
747.2654	776.4834	792.2833
806.3319	812.4465	821.4745
827.2856	856.8537	874.1113
898.3447	921.9208	946.4469
949.8508	951.0237	951.8244
954.1959	955.0078	962.0621
1018.6285	1019.4390	1036.6081
1037.9559	1041.6903	1042.9361
1045.4963	1048.9553	1049.2705
1083.7842	1090.2266	1104.4257
1140.0005	1152.4769	1182.7533
1184.6800	1231.0569	1236.5242
1247.0283	1266.9531	1267.9520
1349.2905	1355.6571	1370.2225
1373.8534	1377.8300	1385.8162
1388.0422	1394.6357	1395.4155
1399.5291	1412.5238	1414.5292
1421.7909	1430.7450	1435.3070
1441.8250	1442.4888	1447.0329
1448.7227	1450.8792	1455.1644
1457.9718	1459.8883	1461.3699
1461.5073	1464.4455	1466.9242

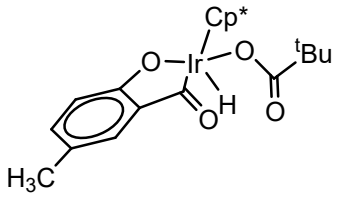
H	3.56337	-0.93536	-1.95656	1469.2491	1476.8177	1478.3286
C	1.35371	-2.70176	-2.36003	1482.8370	1483.9854	1502.6157
H	2.13542	-2.19253	-2.93097	1505.2559	1517.1431	1540.7435
H	1.49330	-3.78347	-2.48103	1545.6251	1611.2043	1685.9846
H	0.38508	-2.42772	-2.79081	1738.5370	1784.2964	1853.1230
C	-0.74163	-3.61540	-0.16840	3024.1354	3026.5837	3028.7787
H	-1.15393	-3.45391	-1.16909	3034.4759	3035.9270	3037.5681
H	-0.44582	-4.66919	-0.08336	3038.3663	3043.1388	3044.2971
H	-1.54442	-3.43130	0.55409	3098.7483	3106.7248	3112.4120
C	0.12561	-2.38256	2.63422	3115.4323	3116.9278	3117.0769
H	-0.95530	-2.34767	2.45975	3119.1089	3126.0212	3127.6274
H	0.36150	-3.33853	3.11811	3131.1084	3131.1755	3132.4582
H	0.36935	-1.57372	3.32901	3142.8337	3144.7485	3148.1751
C	2.88996	-0.78024	2.18137	3150.1392	3152.8155	3156.6724
H	2.37059	-0.72824	3.14263	3160.5396	3185.0414	3204.2085
H	3.84850	-1.29015	2.34299			
H	3.10156	0.24738	1.86353			
C	-6.20942	0.49709	-0.39684			
H	-6.60944	1.51413	-0.49788			
H	-6.35548	-0.01148	-1.35548			
H	-6.83059	-0.01641	0.34851			
H	-6.67522	-1.41624	-0.26110			
H	-1.64368	0.47723	0.30469			
C	-3.18164	-0.68887	-0.69599			
C	-4.16135	0.14311	-0.13037			
C	-3.58554	-1.74568	-1.53671			
C	-5.51687	-0.03227	-0.36126			
H	-3.82610	0.95771	0.51450			
C	-4.94823	-1.93085	-1.77634			
C	-5.88741	-1.09049	-1.19954			
H	-5.26915	-2.74517	-2.42591			
H	-6.94415	-1.25844	-1.40615			
O	-2.65484	-2.54543	-2.08767			
H	-3.09511	-3.22033	-2.61740			
C	-6.55053	0.85833	0.25923			
H	-6.08738	1.70031	0.78297			
H	-7.23316	1.26832	-0.49438			
H	-7.16446	0.31377	0.98712			

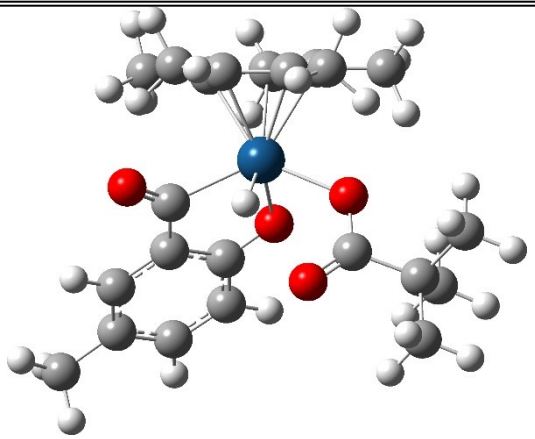
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.484330 Electronic Energy = -1299.92992170
Internal Energy (E)= -1299.4152707 Enthalpy (H)= -1299.4143267
Gibbs Free Energy (G)=-1299.5055027 Gibbs Free Energy of Solvation=-1300.60131269

St.Pt.	General Structure	Ball & Stick model

IV-2





Cartesian co-ordinate

Atoms	X	Y	Z
C	0.48616	-2.42881	-0.99962
C	1.79338	-1.94247	-0.60703
C	1.89949	-2.01764	0.84302
C	0.65288	-2.39904	1.34589
C	-0.26610	-2.58658	0.21416
C	-2.45745	0.59484	-0.41766
Ir	0.22849	-0.47609	-0.07155
C	-3.68287	1.02610	-0.94469
C	-4.69222	1.46352	-0.10541
C	-2.21848	0.58594	0.96513
C	-4.44354	1.44848	1.28241
C	-3.24525	1.02309	1.82292
H	-3.07199	1.02141	2.89621
H	-5.23266	1.78903	1.95432
H	0.86626	0.08919	-1.41969
O	1.14248	1.32227	0.42704
C	1.93258	1.89765	-0.43215
C	2.63571	3.13681	0.13612
O	2.15428	1.49702	-1.57375
H	-3.81652	1.00983	-2.02575
C	-1.36808	0.08952	-1.25688
O	-1.42102	-0.05977	-2.45566
O	-1.05716	0.16435	1.42006
C	-1.66368	-3.08617	0.35044
H	-2.22835	-2.95241	-0.57754
H	-1.67650	-4.15351	0.60725
H	-2.19669	-2.54269	1.13905
C	0.05713	-2.74098	-2.39040
H	0.63908	-3.58340	-2.78381
H	-1.00201	-3.00967	-2.42762
H	0.18286	-1.87675	-3.05152
C	2.94018	-1.68661	-1.52212
H	3.60926	-2.55712	-1.54282
H	2.59517	-1.48971	-2.54123
H	3.51838	-0.81223	-1.20515
C	3.10547	-1.58359	1.59752
H	3.98795	-2.16627	1.30530
H	3.32673	-0.52739	1.39047
H	2.96983	-1.68718	2.67748

Frequencies

21.2937	32.3270	42.8059
52.0702	55.8794	58.8492
75.8436	87.3001	107.8969
128.7963	141.7687	151.4943
153.4986	159.9386	167.7156
174.0369	176.1886	189.6062
199.2984	203.3613	204.2115
210.0928	228.8006	231.7042
240.0091	244.4557	249.4648
263.7687	283.7635	286.2598
298.4475	300.2695	307.7079
326.6997	333.0884	341.5149
355.5344	360.1810	367.2513
382.4206	393.2485	427.1399
430.3871	439.6826	447.4083
477.5140	496.7275	533.1986
535.8731	541.3435	554.2847
570.9459	594.0899	615.9479
621.2859	633.7856	646.3130
650.6313	672.0044	745.3643
758.2441	791.0474	810.6475
812.9480	814.3231	827.0599
830.7871	871.3385	907.5498
914.4166	946.7919	949.3935
952.6642	953.8713	957.0205
959.2673	959.9278	973.8831
1015.4206	1027.4851	1039.0159
1041.0564	1042.3290	1048.5976
1049.5352	1050.7182	1056.6072
1087.6972	1090.3792	1107.4411
1134.6101	1146.5920	1176.7224
1189.1535	1225.7541	1241.8206
1249.0729	1267.7240	1269.0371
1336.6147	1360.1194	1366.4375
1375.7186	1376.6937	1390.5829
1391.4998	1393.2056	1396.7510
1397.7269	1404.3158	1413.9921
1429.2545	1434.9922	1440.2814
1446.8468	1448.0842	1450.3653
1452.1310	1453.6590	1454.8332
1458.8312	1462.0642	1462.2409
1462.8044	1464.8477	1468.4468
1472.5087	1477.5783	1480.4583
1482.4321	1483.7895	1494.1479

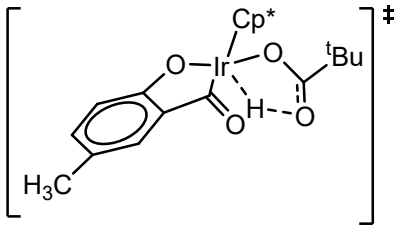
C	0.21081	-2.45458	2.76128	1508.0149	1515.7238	1536.0043
H	1.04851	-2.36001	3.45759	1585.7302	1620.6152	1678.6810
H	-0.49127	-1.62933	2.95268	1734.2117	1812.1487	2093.1198
H	-0.31238	-3.39475	2.97339	3015.7552	3017.7990	3028.2759
C	3.65048	2.64021	1.17058	3030.5118	3031.4228	3033.5069
H	4.21755	3.48665	1.57906	3037.8796	3038.9617	3045.7738
H	3.14783	2.12900	1.99968	3098.7720	3099.2211	3099.7374
H	4.36956	1.94593	0.71258	3101.3360	3111.9271	3112.7188
C	3.35796	3.87848	-0.98043	3124.1798	3125.1415	3127.6601
H	2.65317	4.22535	-1.74426	3131.8393	3132.4270	3139.1964
H	3.88064	4.75188	-0.56921	3145.2899	3145.8349	3146.1915
H	4.08835	3.23142	-1.47659	3147.4913	3151.4681	3154.1066
C	1.62030	4.05685	0.81215	3155.1775	3184.1250	3200.8701
H	2.13435	4.93043	1.23447			
H	0.87648	4.42116	0.09279			
H	1.08854	3.53882	1.61579			
C	-6.00916	1.95042	-0.63394			
H	-6.15968	3.01811	-0.42796			
H	-6.07726	1.81290	-1.71810			
H	-6.85220	1.41659	-0.17717			
H	-6.67522	-1.41624	-0.26110			
H	-1.64368	0.47723	0.30469			
C	-3.18164	-0.68887	-0.69599			
C	-4.16135	0.14311	-0.13037			
C	-3.58554	-1.74568	-1.53671			
C	-5.51687	-0.03227	-0.36126			
H	-3.82610	0.95771	0.51450			
C	-4.94823	-1.93085	-1.77634			
C	-5.88741	-1.09049	-1.19954			
H	-5.26915	-2.74517	-2.42591			
H	-6.94415	-1.25844	-1.40615			
O	-2.65484	-2.54543	-2.08767			
H	-3.09511	-3.22033	-2.61740			
C	-6.55053	0.85833	0.25923			
H	-6.08738	1.70031	0.78297			
H	-7.23316	1.26832	-0.49438			
H	-7.16446	0.31377	0.98712			

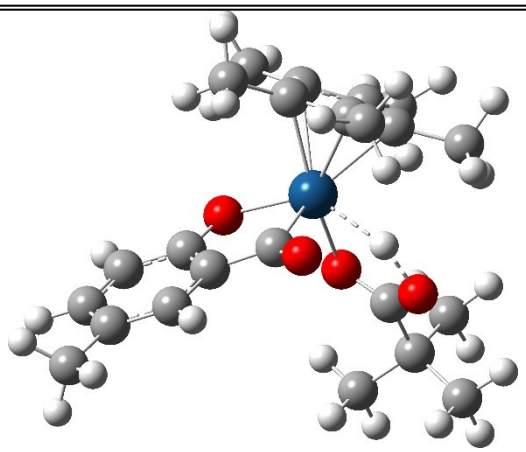
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.488106 Electronic Energy = -1299.93739201
Internal Energy (E)= -1299.41788701 Enthalpy (H)= -1299.41694301
Gibbs Free Energy (G)=-1299.51024201 Gibbs Free Energy of Solvation=-1300.60621706

St.Pt.	General Structure	Ball & Stick model

TS_2-4





Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.82203	-2.25367	1.17835
C	-2.03739	-1.66676	0.66225
C	-2.10257	-1.92135	-0.77380
C	-0.90055	-2.51805	-1.15959
C	-0.05094	-2.65968	0.03192
C	2.45257	0.42494	0.38689
Ir	-0.28364	-0.50207	0.01124
C	3.67301	0.85298	0.92715
C	4.74275	1.14780	0.10016
C	2.27931	0.27438	-0.99838
C	4.55928	0.99265	-1.28939
C	3.36700	0.56752	-1.84292
H	3.24418	0.45709	-2.91758
H	5.39572	1.22165	-1.95142
H	-0.92204	0.37479	1.26754
O	-0.98206	1.38452	-0.62556
C	-1.55701	2.09337	0.28155
C	-2.18015	3.39810	-0.20492
O	-1.66371	1.73754	1.47022
H	3.75443	0.95138	2.00918
C	1.28998	0.08345	1.21228
O	1.27460	0.07445	2.42328
O	1.12087	-0.13799	-1.46572
C	1.28107	-3.32909	0.03386
H	1.83842	-3.10034	0.94806
H	1.18033	-4.41968	-0.04265
H	1.88790	-2.98414	-0.81111
C	-0.47935	-2.42191	2.61645
H	-1.14342	-3.16264	3.07894
H	0.55297	-2.75920	2.74198
H	-0.56376	-1.47453	3.15931
C	-3.17662	-1.15773	1.47702
H	-3.92718	-1.94648	1.62060
H	-2.84061	-0.81645	2.46040
H	-3.66790	-0.30773	0.99007
C	-3.21523	-1.44448	-1.63961
H	-4.17751	-1.86095	-1.31638
H	-3.29818	-0.34962	-1.59198
H	-3.06128	-1.71768	-2.68721

Frequencies

-286.2848	22.8946	33.6469
45.2210	54.1231	71.0819
96.8001	107.0709	114.3423
120.0723	135.7310	145.1398
157.5666	160.9874	169.3231
173.9368	189.1233	190.3318
198.0535	205.5368	212.6701
216.3820	220.8383	234.5289
241.3982	249.3995	255.5347
262.1645	271.3004	291.4492
300.7974	305.4355	309.8148
327.1066	332.3746	334.7854
341.9990	353.3892	359.7255
374.6267	396.2503	422.0473
432.0107	436.1140	451.1000
475.7047	496.8319	517.0569
536.3678	540.2870	544.7216
553.7712	596.2792	620.1672
621.9811	633.1494	640.8683
648.0917	662.3009	679.8945
758.5226	762.9859	793.3192
809.5275	817.2648	835.4512
841.1120	864.9017	906.9014
915.1537	950.0328	953.5060
957.2442	958.4058	961.3119
962.7027	963.7674	967.5116
1015.5497	1032.0073	1041.0287
1042.3176	1043.7240	1045.0417
1050.0455	1052.6980	1058.6100
1088.6184	1089.6914	1108.0723
1134.5914	1149.8906	1177.8945
1186.8279	1230.5963	1241.4920
1255.2166	1268.1258	1270.7666
1340.3684	1370.9108	1374.1190
1380.0940	1384.6172	1392.9981
1394.2705	1399.4600	1402.3184
1403.0940	1404.2304	1427.9071
1429.1168	1434.3248	1439.0863
1448.8316	1449.8006	1450.7087
1452.7566	1456.3335	1459.0632
1459.6466	1461.3494	1463.5204
1465.1688	1466.3192	1468.0602
1476.9079	1478.7996	1480.5882

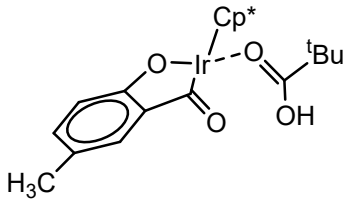
C	-0.41731	-2.80664	-2.53390	1482.3467	1482.5969	1500.3130
H	-1.20867	-2.69107	-3.27969	1505.7172	1510.0885	1538.0587
H	0.39529	-2.11047	-2.78820	1585.1993	1590.2858	1622.8217
H	-0.01940	-3.82597	-2.60654	1680.4184	1770.7450	1819.0895
C	-3.43752	3.00524	-0.98952	3018.0136	3028.2407	3030.0201
H	-3.96276	3.90682	-1.32950	3030.4735	3033.9687	3034.7377
H	-3.18033	2.40368	-1.86923	3034.7907	3039.9510	3044.7753
H	-4.13040	2.43006	-0.35951	3097.0692	3099.2416	3103.6236
C	-2.56233	4.27621	0.97979	3106.2705	3113.9219	3115.2103
H	-1.68267	4.53901	1.57801	3118.2740	3125.4762	3127.9718
H	-3.02276	5.20460	0.61842	3131.2948	3131.8552	3136.7811
H	-3.27111	3.76698	1.64052	3144.7805	3145.5331	3147.6598
C	-1.20796	4.13666	-1.12258	3150.2458	3150.9566	3151.9209
H	-1.67610	5.05848	-1.49116	3154.9454	3178.1238	3196.0261
H	-0.29282	4.41513	-0.58619			
H	-0.92289	3.51908	-1.97938			
C	6.05737	1.62633	0.64221			
H	6.29651	2.63895	0.29228			
H	6.04946	1.65046	1.73691			
H	6.88677	0.97849	0.33053			
H	-6.67522	-1.41624	-0.26110			
H	-1.64368	0.47723	0.30469			
C	-3.18164	-0.68887	-0.69599			
C	-4.16135	0.14311	-0.13037			
C	-3.58554	-1.74568	-1.53671			
C	-5.51687	-0.03227	-0.36126			
H	-3.82610	0.95771	0.51450			
C	-4.94823	-1.93085	-1.77634			
C	-5.88741	-1.09049	-1.19954			
H	-5.26915	-2.74517	-2.42591			
H	-6.94415	-1.25844	-1.40615			
O	-2.65484	-2.54543	-2.08767			
H	-3.09511	-3.22033	-2.61740			
C	-6.55053	0.85833	0.25923			
H	-6.08738	1.70031	0.78297			
H	-7.23316	1.26832	-0.49438			
H	-7.16446	0.31377	0.98712			

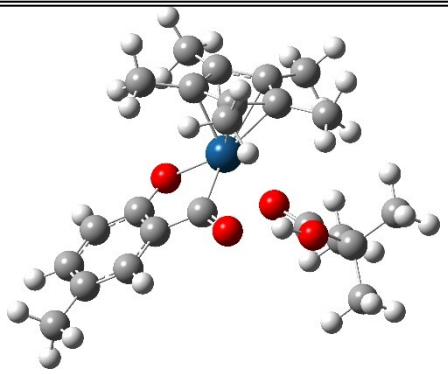
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.487024 Electronic Energy = -1299.93645448
Internal Energy (E)= -1299.41890548 Enthalpy (H)= -1299.41796148
Gibbs Free Energy (G)=-1299.50836548 Gibbs Free Energy of Solvation=-1300.60246986

St.Pt.	General Structure	Ball & Stick model

V-2





Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.41680	-2.07332	1.44534
C	-1.70479	-1.64607	0.98678
C	-1.88728	-2.14407	-0.38436
C	-0.70193	-2.75624	-0.79495
C	0.27426	-2.63763	0.29977
C	2.38970	0.79055	0.27887
Ir	-0.11990	-0.59894	-0.10213
C	3.49377	1.45162	0.83856
C	4.64191	1.65628	0.09637
C	2.39916	0.34586	-1.06312
C	4.64820	1.19939	-1.24060
C	3.56795	0.56965	-1.82387
H	3.59121	0.23987	-2.85994
H	5.54817	1.36150	-1.83638
H	-0.75992	1.55950	1.65632
O	-1.18002	1.25120	-0.72028
C	-1.78588	1.99465	0.06169
C	-2.89901	2.90237	-0.42974
O	-1.58665	2.05042	1.35033
H	3.42343	1.79422	1.87106
C	1.11624	0.58245	0.94688
O	0.79392	1.12181	2.01958
O	1.33528	-0.22802	-1.56393
C	1.63958	-3.23454	0.28025
H	2.27798	-2.77743	1.04400
H	1.61330	-4.31825	0.45633
H	2.12127	-3.05685	-0.68805
C	0.10994	-1.91806	2.82880
H	-0.33224	-2.66594	3.49901
H	1.19764	-2.03867	2.85678
H	-0.10927	-0.91888	3.22148
C	-2.78029	-1.04222	1.82443
H	-3.46503	-1.80933	2.21189
H	-2.35966	-0.50317	2.68043
H	-3.38102	-0.32355	1.25303
C	-3.11171	-1.87783	-1.18849
H	-3.99492	-2.34737	-0.73550
H	-3.31151	-0.79845	-1.24971
H	-3.01723	-2.25148	-2.21228
C	-0.35047	-3.28771	-2.13938
H	-1.18496	-3.20413	-2.84179

Frequencies

25.9116	39.5514	64.2013
69.2993	79.7181	88.1598
107.7791	112.1727	125.1286
135.5280	142.6626	149.2133
154.8861	166.3952	167.0315
171.8833	178.3326	202.8175
205.3514	208.3898	219.9779
226.1348	235.0720	246.5402
247.3348	250.9407	277.6542
288.7071	290.6307	310.4867
315.1442	323.7936	325.5580
332.9416	336.2659	343.0851
358.9915	363.7408	372.5847
397.2479	401.3672	413.1860
422.1601	430.8617	468.2082
488.4976	495.2262	534.1903
539.1268	541.3405	548.4742
554.6308	594.5528	604.1891
611.6433	628.6041	641.8325
669.3130	690.7893	760.8204
770.2793	776.3774	787.6238
806.4411	808.3029	832.4099
873.5144	898.0157	900.2471
946.6262	950.0495	953.2728
957.2989	957.7673	960.8132
964.6949	967.1371	1018.6744
1036.0284	1042.1606	1044.5977
1047.8312	1048.8758	1049.7079
1052.2525	1056.3910	1084.8544
1091.7179	1103.5576	1137.5939
1156.2270	1180.6644	1183.0039
1223.3635	1234.8532	1249.5203
1263.7316	1272.3005	1341.0302
1347.7313	1369.2264	1376.0969
1379.9235	1389.0045	1393.7308
1396.9400	1401.6980	1403.6626
1405.7713	1417.2902	1427.0066
1434.3563	1444.1450	1447.7290
1452.3222	1454.5397	1456.0530
1457.9288	1459.1757	1461.1498
1462.5365	1464.1666	1465.9180
1471.2949	1472.5970	1476.0111
1480.4883	1484.3805	1485.9507
1486.9583	1495.4858	1503.4832
1512.5154	1520.7677	1539.8870
1591.3275	1606.7005	1656.2141

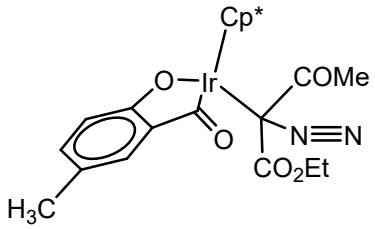
H	0.49607	-2.72790	-2.55805	1683.5875	1742.8442	3022.6575
H	-0.05850	-4.34437	-2.08374	3023.1066	3025.6825	3030.2201
C	-4.21058	2.34681	0.14197	3031.7819	3032.2416	3039.4730
H	-5.04688	2.97718	-0.18399	3039.8801	3046.6243	3053.5223
H	-4.40226	1.32761	-0.22265	3090.3121	3091.2512	3101.5354
H	-4.19613	2.33001	1.23723	3106.0966	3112.6787	3114.4029
C	-2.67037	4.32403	0.08746	3124.0009	3124.2541	3127.0205
H	-1.72500	4.73491	-0.28671	3132.7200	3134.1730	3138.0093
H	-3.48132	4.97318	-0.26455	3140.3660	3141.1818	3142.4059
H	-2.64940	4.35696	1.18076	3143.5604	3148.7437	3148.9673
C	-2.95407	2.89580	-1.95211	3152.1251	3172.1200	3193.2503
H	-3.77328	3.54231	-2.28905			
H	-2.02006	3.26707	-2.38744			
H	-3.12415	1.88769	-2.34527			
C	5.84825	2.34256	0.66607			
H	6.11855	3.23699	0.08950			
H	5.67251	2.65783	1.70018			
H	6.72994	1.68804	0.66613			
H	-6.67522	-1.41624	-0.26110			
H	-1.64368	0.47723	0.30469			
C	-3.18164	-0.68887	-0.69599			
C	-4.16135	0.14311	-0.13037			
C	-3.58554	-1.74568	-1.53671			
C	-5.51687	-0.03227	-0.36126			
H	-3.82610	0.95771	0.51450			
C	-4.94823	-1.93085	-1.77634			
C	-5.88741	-1.09049	-1.19954			
H	-5.26915	-2.74517	-2.42591			
H	-6.94415	-1.25844	-1.40615			
O	-2.65484	-2.54543	-2.08767			
H	-3.09511	-3.22033	-2.61740			
C	-6.55053	0.85833	0.25923			
H	-6.08738	1.70031	0.78297			
H	-7.23316	1.26832	-0.49438			
H	-7.16446	0.31377	0.98712			

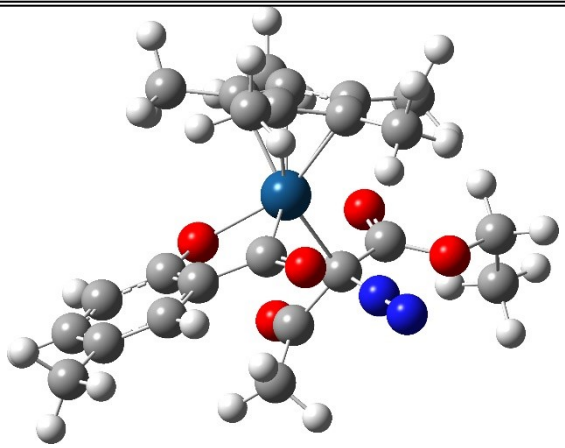
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.492606 Electronic Energy = -1299.97034305
Internal Energy (E)= -1299.44713005 Enthalpy (H)= -1299.44618505
Gibbs Free Energy (G)=-1299.53608705 Gibbs Free Energy of Solvation=-1300.61901874

St.Pt.	General Structure	Ball & Stick model

V'-2





Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.37434	2.62858	0.46876
C	0.87861	2.24986	1.06981
C	1.82768	2.04277	-0.01165
C	1.16971	2.19786	-1.25529
C	-0.22140	2.49750	-0.95773
C	-2.62906	-0.49024	0.39953
Ir	0.05918	0.52556	-0.04202
C	-2.37509	-0.68040	-0.97544
C	-3.43446	-1.14286	-1.78534
C	-3.88965	-0.75413	0.95338
C	-4.67221	-1.37690	-1.21874
C	-4.93355	-1.18943	0.15557
H	-4.02402	-0.60529	2.02515
H	-5.48589	-1.72649	-1.85640
H	-3.25146	-1.30692	-2.84476
C	1.16274	-1.36762	0.13897
C	2.61578	-1.22429	-0.25245
C	0.45685	-2.50001	-0.65095
O	0.85774	-2.77316	-1.75106
N	1.03353	-1.52721	1.51739
N	0.85811	-1.61370	2.62530
C	3.27710	1.78159	0.19818
H	3.75079	1.38333	-0.70392
H	3.78706	2.71365	0.47392
H	3.44083	1.06903	1.01647
C	1.16366	2.22387	2.53311
H	2.10952	1.71007	2.74159
H	1.23397	3.23347	2.95969
H	0.37110	1.67625	3.05993
C	-1.58738	3.08505	1.20232
H	-1.64123	2.63040	2.19644
H	-1.56985	4.17562	1.32739
H	-2.50778	2.82287	0.66898
C	-1.28364	2.71598	-1.97793
H	-2.28160	2.60080	-1.54225
H	-1.21025	3.71970	-2.41550
H	-1.19856	1.97984	-2.78408
C	1.75554	2.02068	-2.61445
H	2.15819	2.96106	-3.01536

Frequencies

23.1859	28.9335	34.8334
50.9235	68.5001	80.2592
86.7880	100.6912	104.9129
114.3659	122.0237	132.7133
133.9148	138.6172	142.6237
151.5691	161.6004	166.6094
174.1549	182.8222	187.9704
192.6409	197.4148	200.8907
214.4230	215.6132	222.3383
231.5623	236.0736	248.5784
264.5014	271.3069	289.1528
295.5295	305.9399	315.4215
320.7998	332.7284	335.4860
339.5901	356.5432	360.4731
362.3259	371.2441	380.4800
409.0497	430.6609	433.6131
452.8337	479.5466	491.3871
493.3410	502.5926	532.5733
536.2309	537.6698	545.0141
546.9431	585.2015	590.2382
597.8240	605.0970	622.9936
637.3312	670.7804	678.4723
752.5728	756.4445	764.0650
774.4632	811.6708	813.5534
822.8318	833.4210	867.7127
878.5815	903.2455	953.6914
953.8730	957.6755	958.8159
966.8288	971.0491	1018.2264
1032.3209	1033.5799	1038.0182
1044.9407	1049.6841	1049.7708
1052.0629	1059.6630	1090.3299
1093.8029	1095.3645	1110.9490
1123.5842	1134.5613	1145.3759
1176.3893	1180.5175	1187.6185
1194.1575	1228.2322	1262.9320
1270.0064	1319.5309	1343.0117
1377.1921	1381.2375	1384.7102
1385.4085	1389.4668	1396.0443
1396.7745	1402.2439	1405.3994
1416.4485	1439.3860	1439.5278
1446.4177	1450.0268	1450.9622
1452.9394	1454.8522	1459.8685
1463.1930	1464.1144	1465.5600

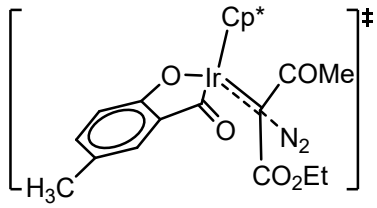
H	2.55694	1.27327	-2.60592	1468.9434	1470.7390	1472.1193
H	0.99773	1.65751	-3.31718	1480.5047	1483.0062	1487.2100
C	-1.45724	-0.07642	1.17832	1492.8827	1493.3273	1500.4122
O	-1.17072	-0.47351	-1.45106	1508.1538	1512.3264	1536.2001
O	-1.42040	-0.03375	2.40222	1546.9506	1608.6289	1679.0631
O	2.98028	-0.90249	-1.35158	1734.5227	1853.0524	1894.6027
C	4.84496	-1.51289	0.48566	2255.9220	3023.9459	3025.6480
H	5.31934	-1.34507	1.45715	3029.3218	3036.6064	3036.9842
H	5.06981	-0.66750	-0.17313	3039.3756	3043.2004	3053.0303
O	3.43150	-1.51913	0.77392	3073.9131	3094.5665	3102.8452
C	5.26508	-2.82154	-0.13506	3107.5817	3112.7484	3116.7999
H	4.78348	-2.95664	-1.10838	3123.3360	3124.8507	3128.8292
H	6.34939	-2.83555	-0.28550	3131.2393	3136.5183	3139.9389
H	4.99792	-3.66313	0.51197	3141.5001	3146.7896	3148.3014
C	-0.63522	-3.25411	0.04714	3151.0309	3157.0949	3158.2410
H	-1.19496	-3.81388	-0.70529	3170.3482	3180.0224	3197.3953
H	-0.18579	-3.96570	0.75262			
H	-1.32110	-2.60799	0.60387			
C	-6.30206	-1.45375	0.71113			
H	-6.31408	-1.34781	1.80116			
H	-7.04882	-0.75838	0.30539			
H	-6.65018	-2.46691	0.47231			
C	-3.18164	-0.68887	-0.69599			
C	-4.16135	0.14311	-0.13037			
C	-3.58554	-1.74568	-1.53671			
C	-5.51687	-0.03227	-0.36126			
H	-3.82610	0.95771	0.51450			
C	-4.94823	-1.93085	-1.77634			
C	-5.88741	-1.09049	-1.19954			
H	-5.26915	-2.74517	-2.42591			
H	-6.94415	-1.25844	-1.40615			
O	-2.65484	-2.54543	-2.08767			
H	-3.09511	-3.22033	-2.61740			
C	-6.55053	0.85833	0.25923			
H	-6.08738	1.70031	0.78297			
H	-7.23316	1.26832	-0.49438			
H	-7.16446	0.31377	0.98712			

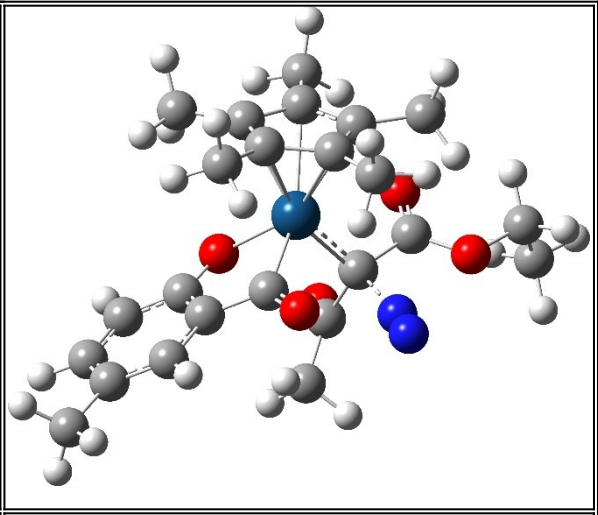
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.488065 Electronic Energy = -1521.39530407
Internal Energy (E)= -1520.87269207 Enthalpy (H)= -1520.87174707
Gibbs Free Energy (G)=-1520.97103207 Gibbs Free Energy of Solvation=-1522.22368415

St.Pt.	General Structure	Ball & Stick model

TS_2-5





Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.54074	2.61503	0.44148
C	0.65889	2.26199	1.16021
C	1.70861	2.07318	0.18038
C	1.16799	2.27183	-1.12661
C	-0.23638	2.55723	-0.95908
C	-2.59394	-0.57486	0.37921
Ir	0.07197	0.50610	-0.06166
C	-2.36054	-0.69406	-1.00636
C	-3.42851	-1.12494	-1.82247
C	-3.84427	-0.87437	0.93984
C	-4.65522	-1.39493	-1.24902
C	-4.89691	-1.27598	0.13703
H	-3.96483	-0.77781	2.01905
H	-5.47673	-1.71808	-1.89048
H	-3.26113	-1.23426	-2.89130
C	1.17232	-1.22834	0.03319
C	2.64947	-1.12099	-0.27021
C	0.57733	-2.43293	-0.71906
O	0.98984	-2.67579	-1.82703
N	1.13576	-1.64674	1.61784
N	0.82037	-1.56126	2.68823
C	3.14350	1.85232	0.51488
H	3.70828	1.51002	-0.35703
H	3.59547	2.78840	0.86764
H	3.26456	1.11028	1.31427
C	0.80674	2.24024	2.64347
H	1.81147	1.91682	2.93673
H	0.64073	3.23640	3.07400
H	0.08572	1.54511	3.09328
C	-1.84034	2.99078	1.06682
H	-1.98632	2.46620	2.01728
H	-1.87736	4.06962	1.26808
H	-2.68947	2.74114	0.42177
C	-1.19829	2.76587	-2.07621
H	-2.23359	2.75112	-1.72094
H	-1.02191	3.73034	-2.56908
H	-1.09732	1.97314	-2.82614
C	1.89819	2.20554	-2.42374

Frequencies

-398.7991	18.7427	29.6523
37.6777	55.1765	80.4389
83.3278	88.7999	99.3782
113.4440	118.6139	131.3231
134.1087	141.3897	145.2391
148.8037	151.1019	153.2944
159.4593	177.0891	177.8540
179.7661	189.7045	195.4706
199.8725	202.5916	210.8424
220.9348	222.0505	226.7936
243.2733	254.6937	255.9997
259.3353	278.6770	284.2337
294.7951	302.2289	328.0682
330.0899	340.0232	348.1666
357.1596	362.4299	369.2292
403.4853	414.7666	415.7838
428.7281	438.9544	452.7501
483.2691	492.6636	508.0266
535.7163	539.1561	545.2813
546.5462	570.6367	589.4068
591.2307	601.6170	610.9918
640.5859	666.3912	676.8341
709.0065	755.1565	760.0006
763.9776	809.7865	812.3796
814.4225	834.9164	868.3171
885.2207	896.6842	904.1042
945.9868	953.5321	955.8133
961.5728	964.1830	1018.0045
1018.4589	1032.2796	1036.3414
1039.1587	1043.5266	1048.5289
1049.7809	1054.4772	1083.0495
1087.7463	1091.5573	1110.4945
1124.2184	1136.3134	1147.5498
1178.2676	1185.3033	1191.0317
1208.2127	1228.2781	1269.9330
1276.1107	1332.5988	1344.7376
1377.3449	1379.0636	1383.9179
1387.9805	1389.9131	1393.6015
1396.6055	1400.8542	1402.5352
1419.6082	1436.7231	1439.6898
1444.5232	1448.0867	1450.1600
1451.0435	1453.4916	1455.1769

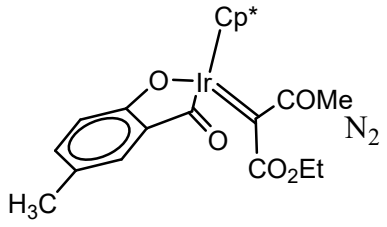
H	2.40014	3.15571	-2.65362	1458.0368	1462.6222	1463.6241
H	2.64779	1.40796	-2.41781	1470.5070	1471.0686	1475.3779
H	1.20827	1.98892	-3.24584	1476.6681	1479.4139	1482.2908
C	-1.41604	-0.18407	1.15540	1490.2832	1491.6078	1493.9378
O	-1.16800	-0.44508	-1.48878	1502.0462	1519.4117	1535.4139
O	-1.36071	-0.20001	2.37883	1537.8038	1610.7241	1678.7987
O	3.06017	-0.71221	-1.32608	1728.3989	1837.8768	1877.3698
C	4.85025	-1.54195	0.47708	2259.4247	3025.5569	3026.0058
H	5.31040	-1.46290	1.46652	3033.0123	3033.5896	3035.9095
H	5.10420	-0.65131	-0.10808	3039.0049	3046.3167	3051.6567
O	3.43234	-1.53971	0.73758	3072.9990	3094.8806	3104.9117
C	5.25109	-2.80655	-0.24030	3106.2562	3113.0155	3118.5700
H	4.76616	-2.86036	-1.21990	3120.5333	3126.7430	3128.9618
H	6.33509	-2.82771	-0.39234	3130.1293	3135.6402	3136.7753
H	4.96911	-3.68978	0.34185	3144.0824	3145.6814	3150.0931
C	-0.46509	-3.27385	-0.03913	3155.1812	3157.6621	3169.6589
H	-1.00741	-3.82661	-0.80985	3170.7821	3177.0064	3199.3909
H	0.03193	-3.99726	0.62056			
H	-1.17195	-2.69573	0.56324			
C	-6.25604	-1.57531	0.69754			
H	-6.26175	-1.49055	1.78940			
H	-7.01745	-0.88568	0.30990			
H	-6.58811	-2.58979	0.44191			
C	-3.18164	-0.68887	-0.69599			
C	-4.16135	0.14311	-0.13037			
C	-3.58554	-1.74568	-1.53671			
C	-5.51687	-0.03227	-0.36126			
H	-3.82610	0.95771	0.51450			
C	-4.94823	-1.93085	-1.77634			
C	-5.88741	-1.09049	-1.19954			
H	-5.26915	-2.74517	-2.42591			
H	-6.94415	-1.25844	-1.40615			
O	-2.65484	-2.54543	-2.08767			
H	-3.09511	-3.22033	-2.61740			
C	-6.55053	0.85833	0.25923			
H	-6.08738	1.70031	0.78297			
H	-7.23316	1.26832	-0.49438			
H	-7.16446	0.31377	0.98712			

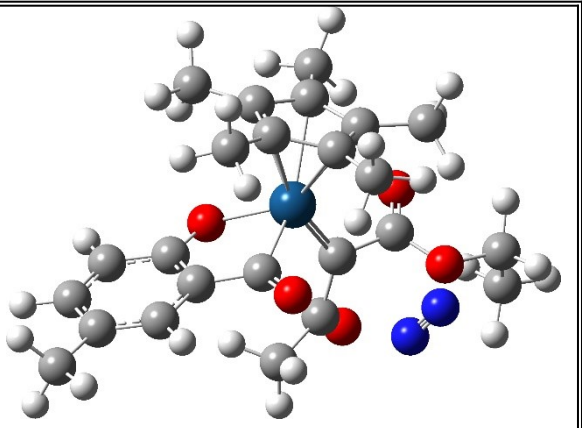
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.485815 Electronic Energy = -1521.39030742
Internal Energy (E)= -1520.86986142 Enthalpy (H)= -1520.86891742
Gibbs Free Energy (G)=-1520.96833042 Gibbs Free Energy of Solvation=-1522.21696003

St.Pt.	General Structure	Ball & Stick model

VI-2





Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.82669	2.36847	0.79742
C	0.40808	1.97724	1.43669
C	1.47029	2.10343	0.46218
C	0.88696	2.55138	-0.77126
C	-0.52444	2.70012	-0.55580
C	-2.55270	-0.80922	0.26665
Ir	0.05002	0.44094	-0.14371
C	-2.47536	-0.49598	-1.10010
C	-3.62924	-0.66323	-1.89065
C	-3.73474	-1.30001	0.83913
C	-4.78583	-1.13946	-1.30417
C	-4.86950	-1.46836	0.06541
H	-3.73895	-1.53481	1.90314
H	-5.67475	-1.26904	-1.92293
H	-3.58152	-0.42454	-2.95031
C	1.23553	-0.99774	-0.50441
C	2.70554	-0.73798	-0.63720
C	0.97238	-2.41260	-0.94352
O	1.82015	-2.94237	-1.64626
N	1.47555	-2.15893	2.43041
N	1.89690	-1.41826	3.13391
C	2.92405	2.00603	0.77328
H	3.52196	1.89192	-0.13521
H	3.25718	2.91182	1.29619
H	3.13453	1.14933	1.42483
C	0.57765	1.70209	2.89081
H	1.62340	1.49426	3.13782
H	0.25919	2.57169	3.47989
H	-0.01837	0.83670	3.20207
C	-2.15338	2.45781	1.47336
H	-2.20402	1.76994	2.32424
H	-2.33369	3.47284	1.85074
H	-2.97491	2.19736	0.79663
C	-1.50718	3.05506	-1.61570
H	-2.53204	3.04601	-1.23263
H	-1.30436	4.05337	-2.02165
H	-1.45715	2.33094	-2.43876
C	1.61473	2.83722	-2.03831
H	2.09172	3.82621	-2.00285
H	2.38961	2.08549	-2.21996

Frequencies

19.3135	36.1646	38.5375
49.3872	51.1225	56.9392
71.0017	75.7407	82.3814
95.2624	99.9230	102.7187
121.6400	125.0358	131.7800
136.8615	143.0307	149.5574
153.7448	157.3902	164.0298
166.9960	177.6573	181.0976
192.2479	198.4098	205.4996
214.9386	221.3827	225.0190
237.4803	247.6573	257.8252
259.4998	274.9544	291.8917
297.8118	304.3834	322.5066
332.5411	340.0434	352.7117
360.6394	369.6659	375.1183
392.7580	397.2211	411.8886
434.0407	435.9949	449.3468
479.0199	488.6671	491.8323
531.8156	539.9260	542.8327
551.2806	572.4265	587.6303
597.4803	602.8977	636.2330
651.4476	669.3695	672.8464
734.1887	750.6416	756.5981
757.6105	809.8409	814.0046
818.1442	830.3355	862.7782
886.0635	904.6074	950.1844
950.4619	952.7751	959.3061
966.3610	1004.8782	1010.5921
1014.9878	1024.1727	1037.6962
1041.2867	1045.1114	1045.7390
1049.8887	1050.8355	1085.7021
1092.9257	1110.2428	1117.2393
1128.3998	1134.4911	1148.3911
1177.9608	1186.4305	1189.0141
1232.8637	1242.6055	1268.4030
1288.0811	1313.0612	1335.4963
1366.2708	1372.4298	1380.6668
1381.3395	1388.0208	1390.9521
1393.1674	1399.2258	1402.3181
1415.3582	1419.6723	1435.8927
1439.2480	1444.1165	1447.2268
1448.2356	1455.6644	1460.1230
1461.9780	1463.4222	1471.4652
1474.2879	1474.7992	1478.8307

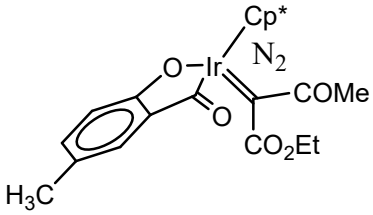
H	0.93140	2.82749	-2.89338	1481.3348	1482.4217	1488.5706
C	-1.32302	-0.58308	1.02897	1494.9329	1508.8041	1516.6893
O	-1.33636	-0.07818	-1.60864	1523.3111	1528.2088	1532.5864
O	-1.17840	-0.83832	2.20464	1541.2063	1618.8680	1675.4109
O	3.20307	-0.05428	-1.50538	1777.7221	1795.4474	1821.4563
C	4.83284	-1.32622	0.20159	2460.5419	3029.8635	3031.6476
H	5.20152	-1.51182	1.21507	3032.5401	3036.2526	3038.3706
H	5.14808	-0.32479	-0.11373	3040.3084	3055.5422	3060.1579
O	3.39938	-1.35005	0.32956	3069.0174	3100.2867	3110.5741
C	5.28826	-2.38476	-0.77243	3112.9787	3113.9839	3116.7112
H	4.92372	-2.16086	-1.77921	3123.7104	3128.9373	3132.6316
H	6.38211	-2.43076	-0.79973	3134.0858	3142.7831	3145.4728
H	4.90332	-3.36671	-0.47937	3145.9732	3150.2842	3156.8762
C	-0.27342	-3.13261	-0.53950	3157.4987	3166.2361	3171.4302
H	-1.14019	-2.70011	-1.05101	3174.3448	3180.0037	3199.4407
H	-0.17578	-4.18279	-0.82317			
H	-0.44895	-3.04635	0.53894			
C	-6.15874	-1.97315	0.64284			
H	-6.05676	-2.19305	1.71056			
H	-6.96779	-1.23988	0.53120			
H	-6.49213	-2.89256	0.14515			
C	-3.18164	-0.68887	-0.69599			
C	-4.16135	0.14311	-0.13037			
C	-3.58554	-1.74568	-1.53671			
C	-5.51687	-0.03227	-0.36126			
H	-3.82610	0.95771	0.51450			
C	-4.94823	-1.93085	-1.77634			
C	-5.88741	-1.09049	-1.19954			
H	-5.26915	-2.74517	-2.42591			
H	-6.94415	-1.25844	-1.40615			
O	-2.65484	-2.54543	-2.08767			
H	-3.09511	-3.22033	-2.61740			
C	-6.55053	0.85833	0.25923			
H	-6.08738	1.70031	0.78297			
H	-7.23316	1.26832	-0.49438			
H	-7.16446	0.31377	0.98712			

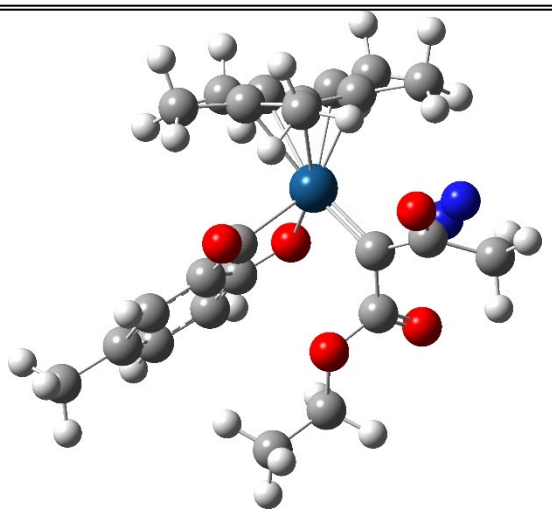
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.486291 Electronic Energy = -1521.44111907
Internal Energy (E)= -1520.91884007 Enthalpy (H)= -1520.91789607
Gibbs Free Energy (G)=-1521.02177207 Gibbs Free Energy of Solvation=-1522.26923556

St.Pt.	General Structure	Ball & Stick model

VI'-2





Cartesian co-ordinate

Atoms	X	Y	Z
C	1.20257	-2.54295	-0.29216
C	2.12196	-1.68935	-1.02379
C	2.84297	-0.90285	-0.05896
C	2.31471	-1.22355	1.25149
C	1.31648	-2.24227	1.09000
C	-2.18581	-0.77160	-0.29265
Ir	0.69326	-0.28048	-0.02545
C	-1.99515	-0.20296	0.97920
C	-3.11751	-0.09358	1.82808
C	-3.44772	-1.21179	-0.71935
C	-4.34861	-0.54317	1.39254
C	-4.54625	-1.11430	0.11662
H	-3.53917	-1.62875	-1.72213
H	-5.20766	-0.45449	2.05912
H	-2.98744	0.35149	2.81198
C	0.65889	1.49859	-0.68500
C	1.77503	2.08111	-1.48433
C	-0.41149	2.44480	-0.26188
C	-2.70020	2.94872	-0.30222
H	-2.83297	2.73013	0.76650
H	-2.43703	4.00916	-0.39333
C	-3.91057	2.57640	-1.11437
H	-4.78003	3.15131	-0.77967
H	-3.74526	2.78748	-2.17598
H	-4.13613	1.50965	-1.00658
O	-1.60152	2.15355	-0.78172
O	-0.19683	3.38327	0.47756
C	4.01276	-0.02315	-0.33007
H	4.08197	0.79020	0.40226
H	4.94226	-0.60394	-0.27342
H	3.95276	0.43020	-1.32441
C	2.35740	-1.76398	-2.49184
H	2.94982	-0.91602	-2.84167
H	2.87316	-2.69709	-2.75514
H	1.40271	-1.73009	-3.02774
C	0.35685	-3.60248	-0.90603
H	0.04530	-3.32748	-1.91762

Frequencies

33.9384	42.0257	52.9466
55.5591	66.8233	70.3071
84.3384	88.2315	94.3234
103.6148	109.8362	117.9250
118.8646	125.2613	134.2879
143.7589	150.9629	155.6322
159.5211	164.5676	172.9606
179.3725	182.9351	188.2618
197.5554	203.1521	214.8953
222.2744	227.5215	232.4556
244.0821	249.7876	257.8778
263.3284	276.0259	289.0119
290.4176	296.4220	315.2428
320.8336	333.4298	336.5605
346.5479	356.3718	360.3926
363.7638	371.6431	399.4504
407.2729	418.4788	433.7293
478.6065	499.8417	526.5059
532.5197	543.8619	545.1448
557.0501	577.9403	586.9297
596.3846	606.9948	631.9190
648.4819	657.2074	668.3560
740.9753	755.2659	758.4439
801.0637	806.7538	815.7078
823.8589	838.9901	860.6429
887.8984	911.0419	939.8279
953.4351	964.1810	966.0647
972.9586	1016.7959	1021.2842
1022.3547	1034.8039	1037.7033
1039.7805	1046.5936	1049.9148
1054.4406	1070.1607	1093.8525
1097.8989	1110.5998	1115.3824
1136.4262	1142.3952	1149.6979
1173.4159	1184.6000	1188.0621
1229.7745	1243.2511	1267.2066
1268.0861	1312.0159	1342.7424
1376.6458	1381.3463	1383.4329
1387.5730	1394.4563	1398.4827
1403.0041	1405.4945	1408.4265
1416.8915	1435.4871	1440.1059
1445.2057	1446.6344	1449.7618
1450.6731	1457.6131	1459.1717

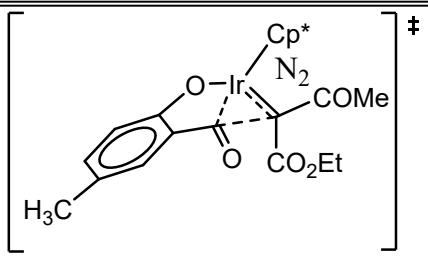
H	0.92385	-4.54065	-0.96816	1459.9139	1462.0140	1462.7070
H	-0.54814	-3.79602	-0.31990	1462.9921	1472.2432	1474.5909
C	0.49343	-2.79162	2.20285	1481.0642	1482.9631	1484.7168
H	-0.32248	-3.41693	1.82842	1487.8892	1499.1178	1504.2690
H	1.10261	-3.39784	2.88520	1511.0089	1518.1248	1536.6257
H	0.04538	-1.97579	2.78356	1548.9861	1615.4081	1678.2573
C	2.77700	-0.70915	2.57029	1775.3708	1815.4955	1828.0133
H	3.36788	-1.46887	3.09982	2464.4824	3026.1717	3026.8903
H	3.39842	0.18505	2.46452	3037.2250	3039.3075	3039.7689
H	1.92347	-0.44706	3.20740	3044.3638	3046.2193	3050.1616
C	-1.00770	-0.81001	-1.15354	3062.3686	3096.5773	3098.4668
O	-0.81156	0.23133	1.34167	3103.3192	3114.2202	3117.3721
O	-0.96523	-1.16276	-2.30524	3117.6035	3126.2015	3128.9574
N	1.96863	2.43209	2.39146	3142.9586	3145.7328	3147.4555
N	1.23473	2.49913	3.21484	3147.9225	3151.5213	3155.2200
C	2.30351	3.43584	-1.09718	3157.6305	3170.1563	3174.3284
H	2.60752	3.44296	-0.04422	3174.8686	3178.8995	3192.0365
H	3.15141	3.67804	-1.74242			
H	1.52667	4.20231	-1.18474			
O	2.26460	1.45174	-2.40940			
C	-5.90624	-1.59342	-0.29735			
H	-6.66542	-0.81070	-0.17420			
H	-5.91547	-1.90163	-1.34803			
H	-6.23605	-2.45277	0.30102			
C	-3.18164	-0.68887	-0.69599			
C	-4.16135	0.14311	-0.13037			
C	-3.58554	-1.74568	-1.53671			
C	-5.51687	-0.03227	-0.36126			
H	-3.82610	0.95771	0.51450			
C	-4.94823	-1.93085	-1.77634			
C	-5.88741	-1.09049	-1.19954			
H	-5.26915	-2.74517	-2.42591			
H	-6.94415	-1.25844	-1.40615			
O	-2.65484	-2.54543	-2.08767			
H	-3.09511	-3.22033	-2.61740			
C	-6.55053	0.85833	0.25923			
H	-6.08738	1.70031	0.78297			
H	-7.23316	1.26832	-0.49438			
H	-7.16446	0.31377	0.98712			

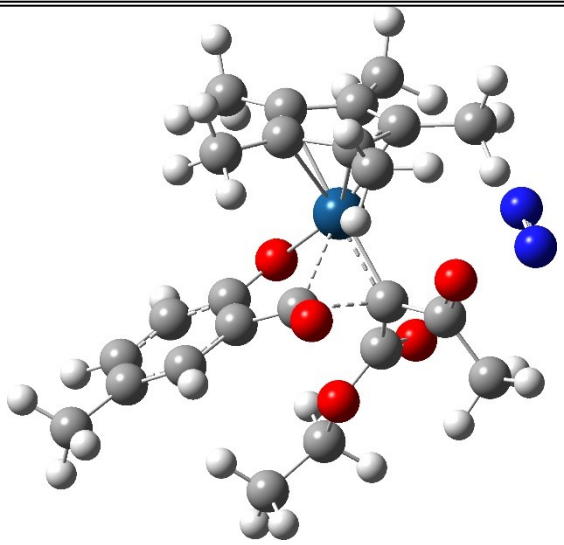
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.486866 Electronic Energy = -1521.44808054
Internal Energy (E)= -1520.92554054 Enthalpy (H)= -1520.92459654
Gibbs Free Energy (G)=-1521.02592654 Gibbs Free Energy of Solvation=-1522.27523009

St.Pt.	General Structure	Ball & Stick model

TS_2-6





Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.29777	-2.45411	0.41342
C	-2.12115	-1.50727	1.16268
C	-2.90934	-0.77704	0.22583
C	-2.54205	-1.24166	-1.10804
C	-1.59625	-2.31898	-0.96626
C	2.08964	-0.59086	0.47499
Ir	-0.79817	-0.33641	-0.17377
C	1.95107	-0.54966	-0.93404
C	3.07940	-0.90395	-1.70623
C	3.28732	-1.00610	1.07974
C	4.24516	-1.30806	-1.08702
C	4.37924	-1.37590	0.31668
H	3.33675	-1.02233	2.16807
H	5.09977	-1.59059	-1.70374
H	2.99437	-0.85903	-2.78947
C	-0.16052	1.38129	0.49483
C	-0.79964	2.06276	1.65381
C	0.70467	2.24812	-0.37090
C	2.88480	2.88556	-0.97233
H	2.66258	2.52298	-1.98484
H	2.67167	3.96167	-0.95566
C	4.29222	2.56125	-0.54774
H	5.01165	3.05462	-1.20924
H	4.47789	2.89874	0.47728
H	4.46487	1.47908	-0.59093
O	2.00450	2.21984	-0.05451
O	0.24408	2.96539	-1.23158
C	-3.94267	0.23667	0.56679
H	-4.23337	0.82063	-0.31160
H	-4.84615	-0.24788	0.95925
H	-3.55976	0.92466	1.33030
C	-2.20096	-1.44575	2.64754
H	-2.95752	-0.72793	2.97093
H	-2.45989	-2.43590	3.04507
H	-1.25064	-1.12562	3.08776
C	-0.33531	-3.40477	1.03620

Frequencies

-259.2547	29.5639	35.2321
45.3142	55.2507	69.7943
81.1726	84.1605	89.4766
94.8835	109.6390	113.2516
120.7556	123.1292	132.0593
133.6388	138.6469	144.6666
160.3912	165.9206	177.0548
180.2678	184.2831	194.1045
196.3483	204.8201	207.8484
211.2126	222.3948	223.3518
233.1632	236.4697	242.1033
251.3887	267.9775	280.6628
284.9590	304.0503	314.3164
318.3396	321.6598	332.0222
334.2492	342.6884	358.8648
363.9056	385.1766	398.7537
407.1270	422.1577	443.8157
462.3082	472.8265	487.3202
527.2152	538.6145	543.3152
554.3002	560.5089	577.4830
591.7703	601.9163	609.8501
628.4020	641.1751	681.3437
724.4969	736.7605	753.7617
793.7150	811.7839	814.3082
820.7728	839.5459	844.1653
892.3013	903.8133	927.9895
945.2675	961.0875	970.9151
971.1673	1014.3241	1019.2680
1031.4236	1033.9402	1037.9172
1044.7113	1047.5135	1048.7435
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1097.0023	1109.6883	1113.1418
1135.0377	1137.2335	1143.1133
1174.4594	1184.6867	1190.3298
1227.4628	1244.0497	1264.5738
1289.1598	1313.6126	1341.1601
1374.4808	1379.2462	1381.5142
1387.6661	1395.0504	1399.0597
1399.7414	1404.0670	1405.1612
1420.1956	1434.5051	1441.6392

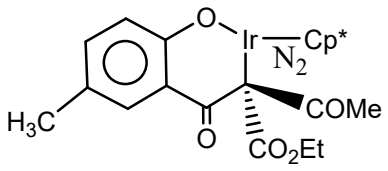
H	0.04441	-3.01279	1.98543	1442.1529	1443.3911	1445.0629
H	-0.82083	-4.36778	1.24293	1447.6071	1451.5034	1456.1451
H	0.52603	-3.59423	0.38675	1458.0640	1462.0344	1469.9785
C	-0.92563	-3.02466	-2.09242	1471.7863	1472.4957	1473.3188
H	-0.00397	-3.51392	-1.76081	1477.2115	1480.3318	1484.3680
H	-1.57955	-3.79078	-2.52745	1488.9336	1498.2400	1507.3492
H	-0.65189	-2.32107	-2.88636	1517.3589	1524.2415	1535.7829
C	-3.13201	-0.77638	-2.39232	1555.4411	1601.9526	1678.9479
H	-4.02289	-1.36485	-2.65119	1775.8311	1829.4191	1842.3278
H	-3.42769	0.27601	-2.34054	2468.9242	3026.7690	3036.0205
H	-2.41437	-0.87302	-3.21341	3036.4633	3038.9241	3040.2278
C	0.97115	-0.15444	1.29622	3044.4301	3046.8202	3047.7781
O	0.83341	-0.17715	-1.50268	3051.4562	3096.2713	3097.7100
O	0.85653	-0.21218	2.49022	3116.0333	3117.9134	3120.2680
N	-2.72202	3.32242	-0.73974	3121.1751	3131.4605	3140.6127
N	-3.00861	2.91948	-1.72779	3142.4049	3142.6660	3142.8727
C	-0.47946	3.51739	1.87926	3144.1749	3144.8829	3149.2190
H	-0.79007	4.11249	1.01246	3156.5555	3159.8373	3173.0718
H	-0.99795	3.86709	2.77408	3180.4919	3180.7825	3196.9151
H	0.60269	3.65576	1.99718			
O	-1.56047	1.46159	2.39643			
C	5.66480	-1.83601	0.93736			
H	6.51717	-1.23195	0.60141			
H	5.62297	-1.76987	2.02950			
H	5.89241	-2.87833	0.67846			
C	-3.18164	-0.68887	-0.69599			
C	-4.16135	0.14311	-0.13037			
C	-3.58554	-1.74568	-1.53671			
C	-5.51687	-0.03227	-0.36126			
H	-3.82610	0.95771	0.51450			
C	-4.94823	-1.93085	-1.77634			
C	-5.88741	-1.09049	-1.19954			
H	-5.26915	-2.74517	-2.42591			
H	-6.94415	-1.25844	-1.40615			
O	-2.65484	-2.54543	-2.08767			
H	-3.09511	-3.22033	-2.61740			
C	-6.55053	0.85833	0.25923			
H	-6.08738	1.70031	0.78297			
H	-7.23316	1.26832	-0.49438			
H	-7.16446	0.31377	0.98712			

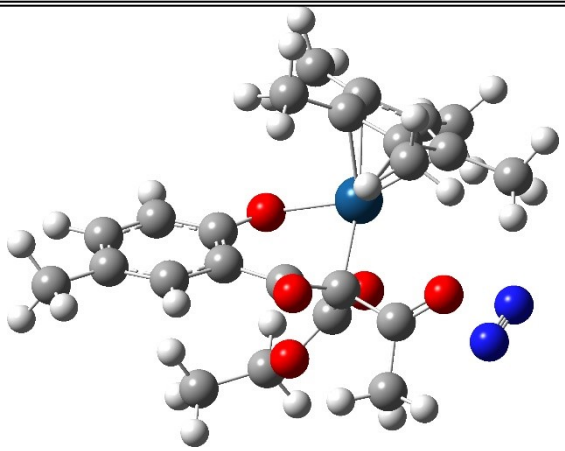
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.485726 Electronic Energy = -1521.42825650
Internal Energy (E)= -1520.9072145 Enthalpy (H)= -1520.9062695
Gibbs Free Energy (G)=-1521.0070655 Gibbs Free Energy of Solvation=-1522.25840704

St.Pt.	General Structure	Ball & Stick model

VII-2





Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.16042	-2.30792	0.56907
C	-1.95378	-1.37970	1.35126
C	-2.91322	-0.77824	0.46972
C	-2.76099	-1.40499	-0.83930
C	-1.72376	-2.36827	-0.77587
C	2.40841	-0.20196	0.66137
Ir	-0.86397	-0.38471	-0.22304
C	2.13622	-0.74674	-0.61765
C	3.20065	-1.38075	-1.29492
C	3.68367	-0.35082	1.22567
C	4.45365	-1.48396	-0.72149
C	4.72523	-0.97385	0.55884
H	3.83595	0.06394	2.22193
H	5.25155	-1.98589	-1.27110
H	2.99091	-1.79872	-2.27791
C	0.24522	1.16589	0.72532
C	-0.51647	2.11144	1.66102
C	0.43609	1.76239	-0.62112
C	1.92008	2.53802	-2.29519
H	1.42168	1.75322	-2.87444
H	1.52865	3.50911	-2.62030
C	3.42065	2.45196	-2.37658
H	3.74962	2.57198	-3.41368
H	3.89340	3.23172	-1.77125
H	3.76155	1.47531	-2.01220
O	1.57202	2.35588	-0.90209
O	-0.48856	1.60226	-1.43751
C	-3.99512	0.16223	0.86727
H	-4.39632	0.70017	0.00186
H	-4.82784	-0.38103	1.33405
H	-3.61156	0.89823	1.57936
C	-1.78282	-1.13609	2.80959
H	-2.34119	-0.25538	3.13289
H	-2.12811	-2.01040	3.37691
H	-0.73059	-0.96066	3.06425
C	-0.04960	-3.15706	1.07901
H	0.45210	-2.67688	1.92639
H	-0.42405	-4.13457	1.41111
H	0.70612	-3.32382	0.30301

Frequencies

27.0374	38.0242	45.3514
56.0190	62.4824	73.3168
77.6217	83.7397	85.8105
93.1465	99.4151	104.6044
111.0311	120.3129	126.9880
127.2452	149.0391	155.2796
164.4961	166.8989	169.9657
175.0339	178.5033	182.4628
187.4830	202.6102	207.8628
216.3317	221.9281	224.2971
238.2032	242.4485	255.2940
264.8283	268.3674	275.8335
282.0753	286.0490	301.0501
306.0386	322.0609	341.7033
355.0522	366.3891	368.2684
392.7874	401.8132	420.4833
422.4638	451.6623	473.7694
492.4650	503.1157	525.8364
536.5224	540.3312	548.2169
553.9186	563.6388	587.0410
598.3832	608.5899	637.2789
657.9873	673.7416	728.8159
741.3105	778.8378	800.3510
806.9108	813.4168	824.0670
833.7274	843.3975	864.3317
894.3725	924.1010	939.8879
955.2932	962.1385	970.9599
996.8634	1002.3543	1022.0531
1035.3642	1039.0454	1042.5985
1044.1345	1046.3444	1049.1245
1059.6760	1084.1646	1091.0992
1095.2066	1111.0199	1126.6551
1137.7976	1146.9939	1174.8059
1181.4574	1187.5396	1205.4045
1231.6208	1250.7742	1274.3857
1286.8767	1337.8037	1343.2343
1367.4080	1376.5016	1383.3219
1384.5775	1394.2917	1396.6446
1397.3547	1400.7598	1404.4098
1427.5444	1436.6941	1439.3905
1443.6034	1444.6050	1446.1633
1452.6721	1454.5604	1456.5426
1458.2719	1459.0212	1459.2038

C	-1.14182	-3.17607	-1.88206	1462.3455	1468.8299	1471.5616
H	-0.09642	-2.88063	-2.05080	1472.5130	1479.3900	1485.0932
H	-1.16143	-4.24662	-1.64282	1486.1723	1487.7009	1505.7402
H	-1.68640	-3.03034	-2.81963	1512.3302	1519.4863	1529.1626
C	-3.54718	-1.01006	-2.03960	1554.1698	1609.3607	1673.6999
H	-4.57012	-1.40414	-1.98388	1686.4142	1735.7713	1848.7216
H	-3.61501	0.08181	-2.11282	2461.5187	3022.3279	3026.1040
H	-3.08852	-1.37725	-2.96227	3030.0800	3036.3246	3037.8102
C	1.40820	0.55570	1.43728	3040.2359	3041.6788	3046.2118
O	0.96101	-0.71020	-1.21492	3059.2618	3094.1644	3099.2551
O	1.48282	0.67092	2.66051	3111.4683	3113.2453	3117.3595
N	-2.49982	3.43152	-0.41414	3118.2692	3125.3325	3129.9608
N	-3.32581	2.93483	-0.95432	3131.3988	3133.0213	3141.4628
C	0.18364	3.41028	1.95168	3142.2107	3145.7040	3147.9008
H	0.15774	4.04040	1.05208	3149.8029	3165.3143	3170.0410
H	-0.32655	3.93335	2.76356	3174.6031	3175.7327	3186.1035
H	1.23341	3.23685	2.20685			
O	-1.60976	1.86423	2.11949			
C	6.09141	-1.10416	1.16467			
H	6.85357	-0.58368	0.57004			
H	6.11824	-0.68290	2.17513			
H	6.40669	-2.15327	1.23535			
C	-3.18164	-0.68887	-0.69599			
C	-4.16135	0.14311	-0.13037			
C	-3.58554	-1.74568	-1.53671			
C	-5.51687	-0.03227	-0.36126			
H	-3.82610	0.95771	0.51450			
C	-4.94823	-1.93085	-1.77634			
C	-5.88741	-1.09049	-1.19954			
H	-5.26915	-2.74517	-2.42591			
H	-6.94415	-1.25844	-1.40615			
O	-2.65484	-2.54543	-2.08767			
H	-3.09511	-3.22033	-2.61740			
C	-6.55053	0.85833	0.25923			
H	-6.08738	1.70031	0.78297			
H	-7.23316	1.26832	-0.49438			
H	-7.16446	0.31377	0.98712			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm

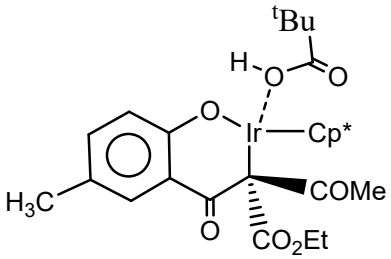
Zero-point correction= 0.486913 Electronic Energy = -1521.46594684

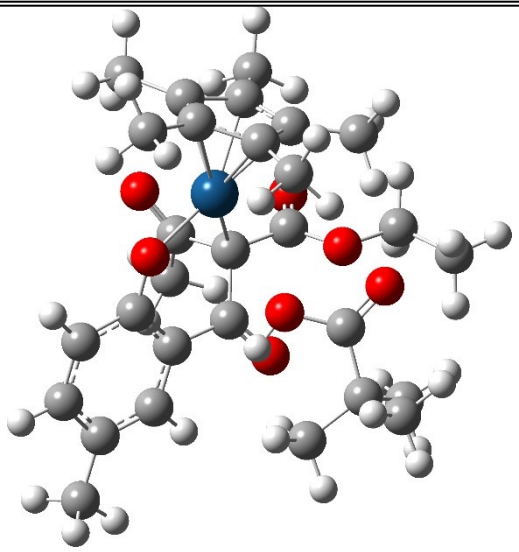
Internal Energy (E)= -1520.94323484 Enthalpy (H)= -1520.94229084

Gibbs Free Energy (G)=-1521.04488184 Gibbs Free Energy of Solvation=-1522.29013594

St.Pt.	General Structure	Ball & Stick model

VII'-2





Cartesian co-ordinate

Atoms	X	Y	Z
C	2.81326	-0.62524	-1.89362
C	2.29675	0.70690	-1.83911
C	2.57491	1.26786	-0.51931
C	3.20004	0.25332	0.26409
C	3.30090	-0.93785	-0.57451
O	-1.34180	0.97713	-1.53414
C	-1.74357	2.24082	-1.31113
O	-0.91822	3.12629	-1.30405
C	-3.23779	2.51059	-1.13472
C	-1.16936	-2.26953	-0.63266
H	-2.06786	0.34276	-1.43233
C	1.61673	1.45368	-2.92696
H	0.87678	2.14661	-2.51054
H	2.35071	2.03179	-3.50479
H	1.09510	0.77676	-3.61064
C	2.31523	2.68288	-0.14899
H	2.95070	3.34825	-0.74826
H	1.26728	2.95169	-0.33071
H	2.54116	2.86218	0.90618
C	3.86574	-2.23940	-0.13370
H	3.71024	-3.01419	-0.89031
H	4.94430	-2.14491	0.04970
H	3.38483	-2.56735	0.79438
C	2.70052	-1.58981	-3.02267
H	2.18747	-1.13645	-3.87589
H	3.68785	-1.92407	-3.36364
H	2.12015	-2.47124	-2.72280
C	3.73144	0.36579	1.64821
H	4.81843	0.51986	1.62630
H	3.27152	1.19301	2.19682
H	3.52146	-0.54202	2.22233
Ir	1.23567	-0.44988	-0.33683
C	-3.65964	3.39153	-2.31545
H	-3.57018	2.85588	-3.26943
H	-4.70768	3.69207	-2.19430
H	-3.03999	4.29254	-2.36657

Frequencies

28.0081	38.8480	44.4947
57.0181	60.5211	67.8646
76.3602	78.5430	91.3699
96.5762	97.9606	99.9269
104.2754	110.0525	113.0671
123.4579	132.9219	133.9397
142.4114	146.3367	150.0442
151.5461	158.4699	161.0820
167.4570	177.1434	181.1870
187.6267	195.4322	199.7159
202.1296	218.1391	227.4732
243.3413	244.9557	251.9508
255.3678	263.9309	277.3727
285.5518	288.6292	294.9940
297.3137	304.9096	309.0043
322.6322	334.2567	341.9017
363.4994	364.9953	370.5794
372.6987	391.1825	397.0401
398.6695	407.2150	422.1411
425.1035	442.1200	444.7566
454.9700	489.0453	513.7018
521.8276	532.2608	533.4803
540.8585	548.4036	549.2607
552.5155	576.2030	584.7761
588.7045	604.4592	642.1674
649.5177	690.4450	712.9099
738.1201	752.6448	770.4208
782.1454	799.3474	805.8715
811.8591	814.3259	822.4829
836.6902	873.2556	885.0110
890.1125	899.9253	917.0604
948.5143	956.2870	957.5308
960.6384	964.7134	968.7209
969.7033	993.4932	1003.7965
1012.0664	1025.6560	1030.0659
1037.6244	1041.5172	1044.3048
1049.1828	1050.0286	1052.4167
1052.9623	1092.0931	1096.1435
1101.0400	1112.0863	1118.5315
1140.6374	1145.6957	1170.0113

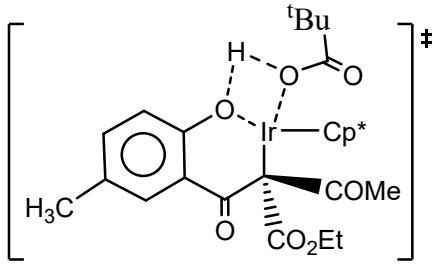
C	-4.09257	1.24714	-1.09756	1179.3036	1185.2926	1189.7475
H	-3.84682	0.62316	-0.22878	1194.4679	1213.7645	1232.4104
H	-5.14805	1.52942	-1.00667	1242.8830	1255.7780	1273.0333
H	-4.00817	0.65648	-2.02161	1276.0894	1291.2874	1304.2200
C	-3.40376	3.28188	0.17593	1332.8598	1368.9915	1372.3023
H	-3.01248	2.70020	1.02121	1374.0665	1380.2033	1382.6428
H	-2.86806	4.23542	0.12342	1386.2074	1387.5710	1389.3462
H	-4.46724	3.48753	0.35055	1391.9380	1396.5995	1401.5185
O	-0.00298	-1.85129	-1.08523	1406.8085	1417.8882	1423.1116
C	-1.95245	-1.60337	0.33787	1429.5856	1435.5971	1436.2617
C	-3.23391	-2.09647	0.64970	1441.0169	1447.5434	1448.0831
C	-1.71137	-3.42978	-1.22833	1450.6194	1452.1479	1455.5812
C	-3.75755	-3.23783	0.07062	1455.9604	1456.5388	1462.6732
C	-2.96086	-3.89749	-0.88182	1464.6752	1468.2260	1468.8701
C	-1.49300	-0.41301	1.09291	1469.9633	1471.4117	1476.1911
O	-2.31590	0.37982	1.54074	1479.6138	1482.6440	1483.9517
H	-1.10654	-3.93249	-1.97938	1492.1703	1497.0509	1497.9230
H	-3.34438	-4.80047	-1.35841	1501.8399	1516.3159	1518.3574
H	-3.80661	-1.54922	1.39922	1520.4456	1527.2851	1547.4111
C	-0.02093	-0.31859	1.40430	1607.2168	1680.3182	1743.6719
C	0.35228	-1.52939	2.29840	1789.8994	1819.5792	1859.8981
C	0.35404	0.89355	2.19249	3018.9509	3028.8775	3030.8416
C	0.22263	3.20789	2.47744	3031.6258	3031.8414	3036.1587
H	1.31475	3.30553	2.54889	3040.1692	3041.3847	3041.6445
H	-0.14144	3.04787	3.49959	3046.9291	3049.0721	3056.2307
C	-0.40848	4.40882	1.82622	3095.4069	3097.9311	3106.0487
H	-0.06825	5.32492	2.32036	3113.6294	3114.8631	3116.5583
H	-0.15062	4.46051	0.76220	3119.4018	3129.6340	3130.2019
H	-1.49887	4.36438	1.90146	3130.5284	3133.7354	3134.2387
O	-0.09273	2.05322	1.68702	3139.1955	3142.0526	3143.5052
O	1.04688	0.84580	3.19502	3144.6264	3145.0441	3146.7846
O	1.32558	-2.22668	2.09444	3149.0380	3156.1700	3156.5996
C	-0.57190	-1.80193	3.45489	3160.6974	3164.8120	3172.3886
H	-0.07226	-2.44714	4.18051	3181.0301	3201.8792	3800.4504
H	-0.90265	-0.87257	3.92794			
H	-1.46569	-2.31774	3.07897			
C	-5.10882	-3.76948	0.44413			
H	-5.76859	-3.85089	-0.42906			
H	-5.04141	-4.77214	0.88549			
H	-5.60300	-3.12006	1.17419			

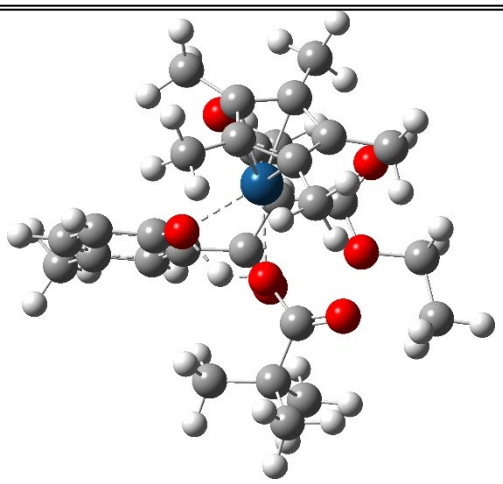
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.629696 Electronic Energy = -1758.83708295
Internal Energy (E)= -1758.16590795 Enthalpy (H)= -1758.16496295
Gibbs Free Energy (G)=-1758.27801795 Gibbs Free Energy of Solvation=-1759.7160187

St.Pt.	General Structure	Ball & Stick model

TS_2-7





Cartesian co-ordinate

Atoms	X	Y	Z
C	1.67468	-2.00349	-1.94067
C	2.63544	-1.13147	-1.37597
C	2.68538	-1.36819	0.06466
C	1.79892	-2.46674	0.36307
C	1.10265	-2.79926	-0.85775
O	0.34172	1.39349	-0.89520
C	0.92300	2.59081	-0.98344
O	2.09625	2.73533	-0.71741
C	-0.00868	3.74307	-1.34831
C	-2.34862	-0.30953	-1.06754
H	-0.52747	0.96061	-1.39702
C	3.42196	-0.07332	-2.06384
H	3.27932	0.89703	-1.57259
H	4.49218	-0.31559	-2.03104
H	3.13056	0.03011	-3.11335
C	3.62642	-0.69572	1.00042
H	4.62945	-1.13884	0.93804
H	3.70684	0.37043	0.75296
H	3.27512	-0.77862	2.03442
C	0.07882	-3.85902	-1.05294
H	-0.64672	-3.55208	-1.81565
H	0.55070	-4.79178	-1.39028
H	-0.47643	-4.04528	-0.13204
C	1.21717	-2.06715	-3.35492
H	1.65933	-1.26738	-3.95635
H	1.48805	-3.02715	-3.81248
H	0.12720	-1.96091	-3.41222
C	1.69104	-3.16023	1.67338
H	2.55754	-3.82224	1.80171
H	1.68081	-2.44423	2.50305
H	0.78201	-3.76337	1.73354
Ir	0.67716	-0.76568	-0.37612
C	0.75045	4.71540	-2.24735
H	0.97738	4.26499	-3.22206
H	0.14333	5.61198	-2.42261
H	1.69485	5.01496	-1.78326
C	-1.29211	3.28036	-2.03327
H	-1.92242	2.67819	-1.36556

Frequencies

-892.2231	-116.0005	-83.2172
-47.1077	-38.6385	31.4624
46.8324	59.6524	66.1514
69.1895	80.6594	86.8099
93.8134	105.0165	109.1578
115.5822	120.6053	122.4015
127.3210	132.4672	136.1519
141.9003	153.5861	159.5331
160.9744	168.3657	172.6953
184.1679	192.2777	201.7683
210.5753	215.6963	219.3265
225.2251	232.9466	256.5025
258.7861	266.5017	274.8005
276.1285	279.2473	288.8830
294.4038	298.1027	305.1043
315.2676	317.7048	325.2554
326.0116	348.3050	361.0656
366.6535	376.7370	385.1344
387.9299	401.9515	408.3520
414.8627	431.8559	434.2876
446.4299	457.7480	488.9051
501.5116	533.5489	535.0620
538.9496	546.0393	557.5277
560.5730	582.0235	587.8719
588.4344	602.4504	609.2257
635.3446	656.8817	689.8195
727.2756	744.7278	771.8782
783.1009	798.3953	803.9665
810.6440	812.2494	834.5457
837.0976	873.9787	882.8331
893.3533	908.4467	937.3052
945.5791	947.1461	951.2571
953.5845	956.8164	963.3446
971.0747	990.7583	1013.4066
1021.8799	1027.7199	1029.9047
1036.0609	1037.6715	1040.1982
1044.0186	1045.7995	1048.8850
1051.0911	1089.0014	1089.8520
1096.6696	1108.3926	1120.9471
1134.2720	1145.8085	1171.1954
1179.9501	1183.4479	1185.5238
1200.6856	1211.9901	1223.8895

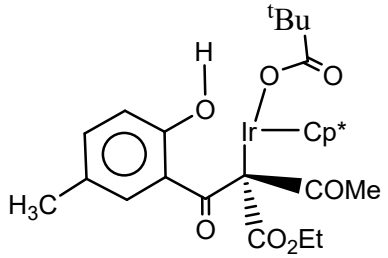
H	-1.88142	4.15726	-2.32694	1235.4861	1251.3195	1264.0903
H	-1.08981	2.70068	-2.94399	1281.5064	1288.2229	1308.8650
C	-0.36020	4.42323	-0.01761	1317.4142	1344.9942	1366.0598
H	-0.82770	3.71761	0.68255	1371.3876	1371.5113	1374.3135
H	0.53884	4.83664	0.45392	1379.4388	1380.0169	1384.5892
H	-1.06349	5.24477	-0.20450	1385.4582	1394.4209	1397.9713
O	-1.10190	-0.25176	-1.57553	1402.9393	1415.8969	1418.8414
C	-2.65489	0.24299	0.18610	1427.0652	1435.9256	1438.5660
C	-3.98821	0.30625	0.60566	1441.8972	1442.5331	1445.3080
C	-3.38259	-0.83936	-1.84481	1445.6415	1445.9713	1453.6343
C	-5.02241	-0.21709	-0.16003	1453.9411	1455.5307	1456.2598
C	-4.69068	-0.80094	-1.38949	1460.9280	1463.5607	1464.5487
C	-1.61231	0.71639	1.13472	1465.6564	1467.8715	1471.6833
O	-1.78312	1.73685	1.78259	1475.5203	1477.4663	1480.0512
H	-3.13020	-1.26194	-2.81527	1483.0819	1483.8459	1486.3717
H	-5.48449	-1.22470	-2.00514	1496.6439	1503.0693	1506.9049
H	-4.19701	0.76231	1.57382	1511.0148	1530.0538	1558.2843
C	-0.46098	-0.24689	1.40183	1628.4435	1675.7250	1771.2772
C	-1.15515	-1.47532	2.02017	1781.2211	1826.6945	1831.4997
C	0.58641	0.29029	2.32475	2070.6286	3024.0207	3027.0684
C	1.97409	2.09503	2.89919	3031.1496	3031.2595	3031.7498
H	2.91714	1.55785	2.73070	3035.1985	3035.8339	3037.0382
H	1.68815	1.92471	3.94399	3037.6523	3049.0018	3050.9509
C	2.09733	3.55826	2.56989	3051.8281	3101.1154	3103.2338
H	2.85285	4.02477	3.21082	3107.4196	3108.3593	3111.6395
H	2.39135	3.69298	1.52338	3112.8119	3115.8171	3116.0585
H	1.14167	4.06822	2.73447	3117.7603	3119.2308	3122.9524
O	0.96442	1.54113	2.04622	3133.3769	3136.0416	3137.0264
O	1.11271	-0.36384	3.21376	3138.5938	3139.6998	3144.0435
O	-1.34259	-2.50497	1.40430	3144.6648	3150.3015	3161.1196
C	-1.67899	-1.31562	3.42397	3164.2404	3164.2621	3167.2724
H	-2.47210	-2.04597	3.60050	3173.2433	3191.5842	3211.0222
H	-0.85436	-1.49608	4.12178			
H	-2.03677	-0.29696	3.61382			
C	-6.44825	-0.16184	0.30199			
H	-7.04779	0.51633	-0.31877			
H	-6.92655	-1.14766	0.25166			
H	-6.51928	0.19064	1.33611			

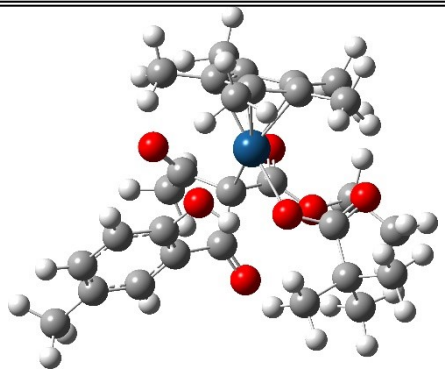
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.622812 Electronic Energy = -1758.82699130
Internal Energy (E)= -1758.1659303 Enthalpy (H)= -1758.1649863
Gibbs Free Energy (G)=-1758.2699963 Gibbs Free Energy of Solvation=-1759.69950904

St.Pt.	General Structure	Ball & Stick model

VIII-2





Cartesian co-ordinate

Atoms	X	Y	Z
C	1.13549	-2.56228	-1.57369
C	2.26642	-1.93985	-0.99353
C	2.09886	-1.97065	0.45739
C	0.90326	-2.74909	0.75230
C	0.26966	-3.03656	-0.49522
O	0.73811	1.03970	-1.10637
C	1.79365	1.79622	-0.98433
O	2.81583	1.48210	-0.38573
C	1.64698	3.17421	-1.64616
C	-2.53304	0.20373	-1.25852
H	-0.74690	0.55856	-1.93821
C	3.40835	-1.31380	-1.70903
H	3.73809	-0.40820	-1.19322
H	4.24741	-2.01972	-1.76728
H	3.13359	-1.03223	-2.73118
C	3.10003	-1.47600	1.43803
H	3.93694	-2.18133	1.53016
H	3.49017	-0.50549	1.10863
H	2.64378	-1.34766	2.42546
C	-1.00657	-3.76490	-0.72329
H	-1.57795	-3.28776	-1.52851
H	-0.80721	-4.80331	-1.02050
H	-1.63863	-3.75883	0.16643
C	0.81802	-2.69238	-3.02146
H	1.47836	-2.07117	-3.63410
H	0.92583	-3.73272	-3.35502
H	-0.21362	-2.38240	-3.22224
C	0.47555	-3.19787	2.10312
H	1.06909	-4.07252	2.40061
H	0.62509	-2.40957	2.84861
H	-0.58146	-3.47536	2.11502
Ir	0.44172	-0.88575	-0.29230
C	2.88698	3.43423	-2.49950
H	2.94489	2.73687	-3.34626
H	2.85850	4.45358	-2.90629
H	3.79635	3.32045	-1.90101
C	0.38996	3.28001	-2.50306
H	-0.51557	3.15088	-1.89764
H	0.34245	4.27250	-2.97000
H	0.38349	2.53213	-3.30692
C	1.57028	4.20364	-0.51474

Frequencies

35.1438	54.9639	62.3042
64.0574	68.4333	78.1437
82.2259	91.2906	94.5255
101.4387	103.4915	110.5772
116.4562	118.0715	126.3978
132.0394	138.1678	140.2117
143.5743	147.9218	153.4864
154.4846	167.8784	176.3248
188.0045	191.6878	198.0812
206.9178	210.2304	217.8573
220.4319	228.1678	240.6564
249.8217	253.5542	256.8415
268.9509	281.4357	288.4418
290.4920	296.6641	313.3992
323.2311	329.9390	333.6835
334.0758	343.9135	347.6790
361.3141	362.9038	373.2353
382.5421	387.1841	394.7455
404.5032	405.9866	408.8683
426.6249	433.4941	442.8987
468.1451	477.2769	482.1312
518.3172	533.4434	539.2370
544.4883	553.0329	563.8677
576.7262	585.4469	595.2534
596.9753	605.2358	631.5624
651.4780	683.5213	718.3181
734.7126	776.1087	786.7900
802.4643	808.1202	810.5087
813.4238	814.9915	828.0386
834.3563	871.9261	882.4334
895.6899	916.3418	922.6396
948.5377	949.3228	954.3049
954.7711	960.1832	970.1466
986.5939	991.0563	1014.2486
1020.5822	1021.6384	1034.2622
1037.0506	1038.0188	1039.5391
1048.0663	1048.1809	1054.5669
1058.2637	1092.7959	1099.2537
1106.0788	1119.5297	1119.9837
1137.4751	1149.5297	1182.8426
1188.2052	1190.1377	1190.3613
1211.9434	1237.3424	1244.0695
1247.4222	1260.7989	1268.9485
1286.6907	1293.3711	1319.8608
1345.6681	1365.2300	1365.8329
1376.6947	1377.7978	1378.4297

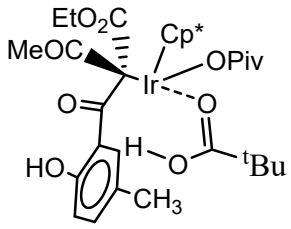
H	0.76432	3.95482	0.18817	1381.2457	1382.0370	1382.8250
H	2.51338	4.24126	0.04044	1396.0644	1400.6302	1402.5866
H	1.37769	5.20051	-0.93305	1404.5194	1416.4727	1419.5462
O	-1.31963	-0.22599	-1.77056	1431.1451	1432.2067	1440.1834
C	-2.57953	1.04544	-0.15008	1440.7069	1443.5112	1447.6371
C	-3.82318	1.52051	0.27103	1450.1711	1451.3205	1452.4916
C	-3.69587	-0.20641	-1.89306	1454.8259	1459.3091	1463.0280
C	-5.00773	1.12578	-0.34640	1463.7891	1468.2142	1469.4317
C	-4.92413	0.24140	-1.42512	1472.2864	1474.1532	1479.8153
C	-1.38506	1.39136	0.69524	1483.7691	1485.6348	1490.2404
O	-1.17536	2.55329	0.98657	1492.8240	1496.7942	1499.8715
H	-3.61924	-0.86430	-2.75529	1510.7249	1523.6576	1530.3985
H	-5.83885	-0.08848	-1.91636	1532.3549	1538.3383	1559.6099
H	-3.84990	2.19574	1.12642	1651.8322	1680.1466	1764.0861
C	-0.65277	0.19664	1.27095	1768.6223	1796.1435	1829.1818
C	-1.74416	-0.69784	1.88733	3023.8936	3027.7114	3036.2331
C	0.38995	0.49739	2.30150	3036.8991	3038.0941	3038.3591
C	2.19463	1.80073	3.00974	3038.6620	3041.2024	3044.5336
H	2.83245	0.90860	3.04312	3047.0004	3048.2784	3056.1348
H	1.75926	1.92224	4.00982	3104.2967	3107.8406	3111.0416
C	2.96268	3.01281	2.56120	3117.0202	3117.0651	3120.9465
H	3.77937	3.21538	3.26235	3122.6487	3124.3562	3128.9216
H	3.38044	2.84026	1.56332	3130.1793	3137.4138	3138.4942
H	2.31292	3.89362	2.52385	3138.9908	3140.8164	3143.5874
O	1.13184	1.57750	2.07147	3148.3739	3152.3630	3157.7383
O	0.58765	-0.23417	3.26376	3159.6963	3164.5575	3164.6876
O	-2.16357	-1.70088	1.34571	3171.8997	3172.9622	3175.7981
C	-2.34746	-0.22554	3.18706	3188.9344	3200.6236	3499.1747
H	-3.36614	-0.61210	3.27472			
H	-1.74083	-0.61596	4.01083			
H	-2.33889	0.86757	3.27377			
C	-6.33674	1.63540	0.12540			
H	-6.75411	2.37041	-0.57426			
H	-7.06843	0.82400	0.21337			
H	-6.25437	2.12232	1.10230			

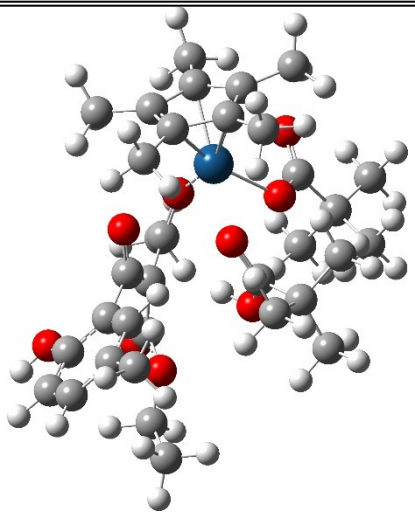
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.631281 Electronic Energy = -1758.84125177
Internal Energy (E)= -1758.16938677 Enthalpy (H)= -1758.16844277
Gibbs Free Energy (G)=-1758.27797777 Gibbs Free Energy of Solvation=-1759.70971427

St.Pt.	General Structure	Ball & Stick model

VIII'-2





Cartesian co-ordinate

Atoms	X	Y	Z
H	0.97884	1.32646	0.35925
C	-1.98705	-2.44583	-1.56000
C	-1.59155	-2.90684	-0.27039
C	-2.53737	-2.38836	0.71144
C	-3.53465	-1.62359	0.01002
C	-3.16692	-1.60167	-1.39689
C	-2.76088	1.97487	0.12516
O	-1.88122	1.15034	0.61207
O	-3.63216	1.69256	-0.69190
C	-2.56915	3.42370	0.60124
O	0.06935	-0.57709	1.36139
C	0.52059	0.40975	1.94600
O	0.98695	1.46997	1.33997
C	0.60159	0.44380	3.45989
C	-4.71581	-0.95434	0.61268
H	-5.59994	-1.59846	0.52047
H	-4.55467	-0.75002	1.67629
H	-4.90691	0.00018	0.11536
C	-3.91130	-0.93686	-2.49695
H	-4.62060	-1.63455	-2.96152
H	-4.44521	-0.05882	-2.12603
H	-3.21585	-0.58696	-3.26630
C	-2.50212	-2.69226	2.16580
H	-1.48107	-2.60598	2.55269
H	-3.13325	-2.00072	2.73284
H	-2.85454	-3.71331	2.36163
C	-0.40480	-3.73986	0.05870
H	-0.01529	-3.48248	1.05003
H	-0.67413	-4.80414	0.06467
H	0.40562	-3.56892	-0.65374
C	-1.30992	-2.72373	-2.85272
H	-0.26124	-2.98790	-2.70132
H	-1.81603	-3.54684	-3.37385
H	-1.33320	-1.84436	-3.50378
C	-0.83140	0.31019	3.98318
H	-0.82656	0.30903	5.08002
H	-1.45406	1.14356	3.63529

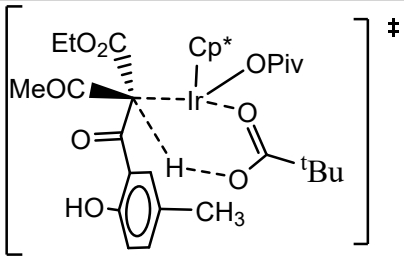
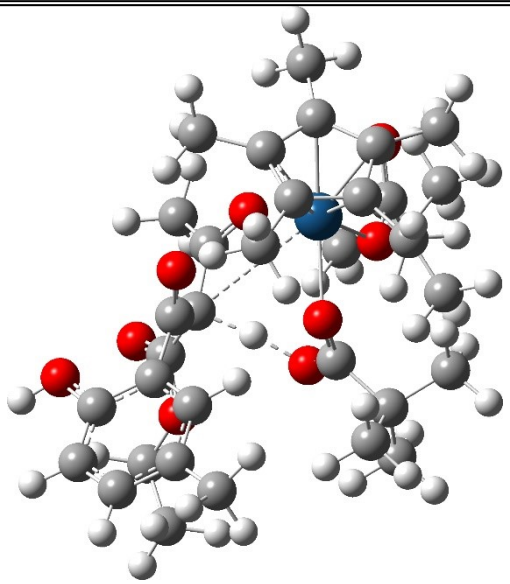
Frequencies

-26.0554	-10.4801	31.7417
40.0619	45.2716	56.5993
64.7154	67.4413	76.4374
78.4569	83.9817	87.3911
92.1241	96.7850	98.3300
104.9099	112.1095	120.1644
120.8557	125.7439	129.8184
135.8738	140.6916	145.5828
149.8269	158.7139	163.3851
167.6110	177.8825	181.1554
183.0823	190.7116	191.9295
195.8416	203.1842	207.0396
213.3808	218.9292	221.9433
224.0592	233.4488	238.0107
246.2097	248.6390	249.9629
253.9603	266.0060	273.6761
286.7023	299.8459	304.9784
309.3162	310.5881	317.3231
318.5061	319.7177	320.3180
321.6071	328.9227	332.4507
338.2895	340.1862	341.9541
351.1595	356.0243	374.9176
393.4142	395.0072	399.1456
401.7959	406.5081	420.2154
427.1699	433.5910	442.2124
448.8826	459.9567	473.0403
475.3021	504.3397	535.0865
536.5423	540.1851	543.4631
546.4498	569.9466	584.6361
586.8183	591.0729	593.6780
601.7770	621.8789	628.9774
633.2279	674.1292	686.7254
719.5650	752.7730	767.2754
781.3353	792.8306	798.2469
805.7943	807.2204	807.7719
811.5869	818.0707	819.4221
832.3243	865.7984	899.5489
906.1731	914.0707	916.5177
938.2126	948.7576	953.4661
956.6529	957.2979	962.8339
965.9464	973.6535	974.0432

H	-1.28935	-0.62010	3.63092	984.3218	996.8644	1020.3466
C	1.23176	1.73113	3.97811	1032.4145	1032.5815	1036.2505
H	1.27048	1.70026	5.07395	1038.8396	1042.8864	1045.2632
H	2.25185	1.86078	3.60094	1045.9022	1046.6854	1048.0500
H	0.64933	2.61063	3.68140	1053.5737	1056.1133	1059.4703
C	1.44203	-0.76190	3.89259	1094.7609	1100.6118	1107.9354
H	1.00325	-1.70161	3.53582	1108.3067	1139.5348	1146.8034
H	2.46370	-0.69142	3.49442	1162.9014	1179.8293	1185.4439
H	1.50282	-0.79835	4.98704	1189.0587	1191.3619	1234.8760
C	-3.87437	4.19466	0.44634	1237.1779	1239.6669	1243.3690
H	-4.64945	3.79647	1.11321	1249.8229	1269.6097	1271.3457
H	-3.72221	5.25316	0.69546	1279.5397	1282.7310	1291.2346
H	-4.25004	4.12021	-0.57835	1306.5621	1315.3823	1323.4474
C	-1.50290	4.01999	-0.32409	1364.5701	1371.2875	1372.0319
H	-1.30012	5.06467	-0.05327	1374.1779	1377.5474	1379.6025
H	-0.56185	3.45734	-0.24889	1381.2456	1383.8363	1386.9681
H	-1.83878	3.99394	-1.36835	1389.2328	1391.4958	1393.4970
C	-2.08438	3.49928	2.04569	1395.2224	1401.2364	1411.6910
H	-1.99051	4.54980	2.35233	1416.1966	1417.2321	1424.5430
H	-2.79235	3.01427	2.73131	1428.2838	1430.7600	1437.0362
H	-1.10522	3.02063	2.16118	1437.6945	1441.0973	1444.4273
Ir	-1.60858	-0.73555	-0.28125	1448.5531	1449.4067	1450.0668
C	1.50056	0.89079	-1.55437	1451.2391	1455.4582	1455.8692
C	1.81797	-0.48281	-1.19973	1458.3959	1460.1828	1460.8015
O	0.99656	-1.40436	-1.26932	1463.7517	1467.4235	1469.4788
C	3.18974	-0.88319	-0.72184	1469.9855	1472.5008	1475.6086
C	4.35931	-0.70025	-1.46487	1477.9492	1479.4508	1479.7007
C	3.26818	-1.57352	0.48499	1482.3057	1482.6168	1483.9473
C	5.57406	-1.17646	-0.98163	1487.5890	1488.6406	1493.7315
C	4.47831	-2.03817	1.00201	1502.5042	1512.4467	1513.4451
H	2.33810	-1.74654	1.03084	1515.5683	1517.0490	1539.9297
C	5.63076	-1.83156	0.24456	1552.9664	1579.9754	1661.0117
H	6.47954	-1.03768	-1.57356	1678.3960	1706.7468	1759.3303
H	6.58879	-2.19897	0.61146	1766.6549	1832.0011	3018.5153
O	4.25573	-0.05033	-2.65532	3020.2281	3023.9499	3028.7006
H	5.12507	0.01739	-3.06359	3032.0365	3037.1065	3037.8376
C	0.21835	1.18753	-2.11655	3039.3753	3039.6641	3040.4764
C	2.55756	1.91815	-1.63112	3041.2124	3043.8719	3044.6488
C	4.56443	2.61041	-0.59712	3046.3903	3054.5404	3088.5025
H	4.30980	3.67549	-0.66644	3098.8549	3102.0298	3106.5117
H	5.11842	2.35153	-1.51174	3111.5784	3113.1677	3114.8025
C	5.34561	2.28152	0.64928	3120.4414	3124.4684	3124.8540
H	6.29675	2.82384	0.66440	3125.4694	3127.0959	3127.7982
H	4.77758	2.55699	1.54408	3128.6285	3129.4319	3130.4160
H	5.55328	1.20544	0.69502	3135.9094	3136.8635	3138.7666
O	3.37126	1.83398	-0.55110	3141.0943	3146.6514	3148.7779
O	2.70423	2.77923	-2.47372	3149.5975	3153.3702	3154.1347
C	0.03234	2.32769	-3.07869	3154.6103	3163.0449	3164.7984
H	-1.02828	2.39194	-3.33497	3168.5406	3170.8096	3171.7306
H	0.38042	3.27357	-2.65298	3176.8331	3381.8933	3897.7677
H	0.64301	2.17344	-3.97399			
O	-0.83930	0.54566	-1.86585			
C	4.53895	-2.73472	2.32991			
H	5.26491	-3.55605	2.32172			
H	4.83981	-2.05140	3.13576			
H	3.56391	-3.15269	2.60580			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.777792 Electronic Energy = -2105.66317227
Internal Energy (E)= -2104.83645427 Enthalpy (H)= -2104.83551027
Gibbs Free Energy (G)=-2104.96181227 Gibbs Free Energy of Solvation=-2106.69002326

St.Pt.	General Structure	Ball & Stick model
TS_2-8		

Cartesian co-ordinate

Atoms	X	Y	Z
H	1.14898	1.16800	-0.06184
C	-1.99547	-2.27966	-1.69224
C	-1.55097	-2.86434	-0.47043
C	-2.48685	-2.47070	0.57790
C	-3.52758	-1.66932	-0.02988
C	-3.19957	-1.50265	-1.42699
C	-2.84393	1.95072	0.23709
O	-2.01027	1.09791	0.75372
O	-3.70917	1.69421	-0.59518
C	-2.58280	3.39628	0.68739
O	0.02375	-0.64460	1.22409
C	0.49892	0.38207	1.80239
O	0.93056	1.40570	1.21186
C	0.59115	0.32313	3.32605
C	-4.68704	-1.06352	0.67558
H	-5.56384	-1.71928	0.60032
H	-4.46318	-0.91198	1.73686
H	-4.92184	-0.08520	0.24606
C	-3.98239	-0.77586	-2.46153
H	-4.54815	-1.48152	-3.08471
H	-4.66546	-0.05708	-2.00550

Frequencies

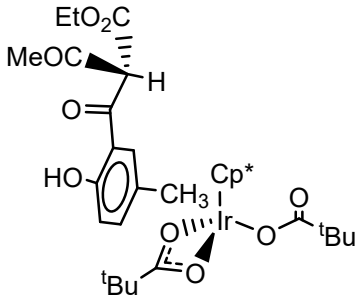
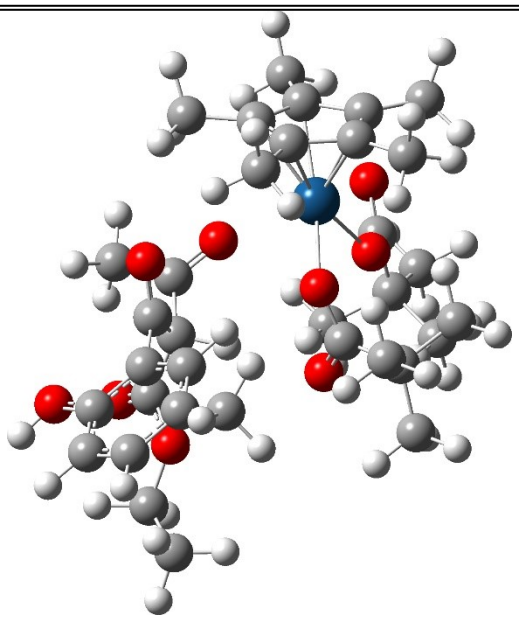
-1460.5629	-85.0322	29.4182
32.7415	38.0021	44.1669
52.9975	59.7711	67.2918
74.0594	76.6495	79.9012
83.5646	92.4229	95.6480
104.1104	108.4854	111.5102
114.3929	116.3070	120.3718
126.4208	132.6780	139.3049
141.4048	146.4381	153.2072
158.4680	164.6894	171.8692
180.5918	193.5591	196.6040
201.4680	204.4035	210.1287
216.0357	218.3752	224.6195
228.0019	230.8523	233.5380
237.3333	248.4446	251.2287
253.9035	262.8106	272.7194
279.1581	286.1258	300.3066
304.8660	305.9301	310.4398
318.6329	323.4546	324.3647
327.7090	330.7103	336.9560
341.5723	344.5034	346.6667
349.3246	358.2168	372.5515
387.2421	393.5282	397.8626
404.2500	407.4511	413.2196
421.8572	433.1174	441.8789
446.6683	458.3330	463.2696

H	-3.31331	-0.20230	-3.11245	468.4766	471.1499	519.8935
C	-2.40146	-2.91290	1.99498	536.7641	538.7233	540.5044
H	-1.38488	-2.76969	2.37867	548.2193	567.5238	572.1974
H	-3.08196	-2.34252	2.63453	587.6507	591.5429	595.7860
H	-2.65664	-3.97638	2.08905	605.3477	614.7276	623.0608
C	-0.33590	-3.69479	-0.25431	634.9473	677.6173	692.1958
H	0.06118	-3.53577	0.75565	712.9266	750.0867	779.2624
H	-0.56767	-4.76247	-0.36095	789.6959	801.5417	804.0612
H	0.45516	-3.42454	-0.95974	805.4656	807.7001	813.7524
C	-1.37650	-2.40968	-3.03649	814.1049	817.5157	822.7114
H	-0.36402	-2.81163	-2.98179	854.9180	872.2660	907.0385
H	-1.99329	-3.07239	-3.65811	911.6078	916.4916	920.9324
H	-1.32284	-1.43755	-3.53731	931.2620	945.1560	947.4302
C	-0.83110	0.20353	3.87870	948.5103	952.6498	958.1701
H	-0.79825	0.08929	4.97009	962.6456	962.9565	972.2108
H	-1.42423	1.09496	3.64210	974.6861	995.1744	1013.9505
H	-1.34526	-0.66281	3.44758	1029.5558	1032.1088	1036.4055
C	1.26851	1.56756	3.88496	1037.9099	1041.1425	1041.4452
H	1.33408	1.49513	4.97837	1042.6168	1048.0489	1048.8318
H	2.28052	1.68316	3.48152	1050.1743	1051.5731	1055.9491
H	0.70637	2.47337	3.63217	1090.9562	1096.0842	1097.9240
C	1.40240	-0.91990	3.70169	1109.5058	1138.6268	1143.4030
H	0.92889	-1.83396	3.32262	1154.1423	1173.6972	1176.3607
H	2.41880	-0.86397	3.28701	1186.2959	1189.3450	1216.5441
H	1.48466	-0.99761	4.79338	1235.0614	1240.6852	1250.1240
C	-3.84557	4.23037	0.51373	1251.9497	1268.1059	1270.4789
H	-4.64288	3.88222	1.18250	1273.4730	1281.5284	1291.8366
H	-3.64073	5.28334	0.74841	1296.2743	1311.6340	1326.0593
H	-4.22010	4.16047	-0.51190	1357.2065	1368.6977	1370.7660
C	-1.48201	3.91149	-0.24899	1372.4071	1374.2365	1375.1190
H	-1.25021	4.96084	-0.02287	1377.9047	1379.0552	1381.3295
H	-0.56402	3.32073	-0.11917	1385.9688	1386.9689	1393.8409
H	-1.80195	3.84547	-1.29734	1397.6764	1400.5026	1403.0143
C	-2.08519	3.47541	2.12688	1403.5878	1404.2399	1413.1069
H	-1.93944	4.52594	2.41281	1417.2033	1429.2696	1431.7813
H	-2.80723	3.03457	2.82723	1435.9229	1439.6260	1443.8620
H	-1.12865	2.95229	2.23821	1446.2110	1447.1648	1447.9637
Ir	-1.62242	-0.71209	-0.22088	1450.8943	1452.9541	1455.1525
C	1.50609	1.01913	-1.31299	1456.4054	1457.7980	1460.3941
C	1.89134	-0.42823	-1.33823	1461.7886	1464.6566	1466.4172
O	1.13893	-1.29143	-1.76246	1470.1819	1472.1501	1473.5740
C	3.19881	-0.88138	-0.75369	1476.5494	1477.3114	1477.5003
C	4.42027	-0.64785	-1.38497	1479.3171	1482.2307	1486.3538
C	3.16413	-1.67547	0.38787	1489.0185	1490.2393	1493.9191
C	5.58996	-1.17829	-0.85158	1498.5048	1504.0104	1506.9680
C	4.32635	-2.21042	0.94659	1510.2858	1513.1405	1529.6051
H	2.19279	-1.86841	0.84632	1545.3174	1554.9921	1667.8824
C	5.53742	-1.94779	0.30664	1682.5280	1692.7252	1707.2595
H	6.54225	-0.99817	-1.35146	1764.3546	1786.5202	1851.3055
H	6.45925	-2.36416	0.71186	3013.6621	3017.7118	3025.8101
O	4.39636	0.10179	-2.52096	3025.9601	3031.1546	3032.9601
H	5.28678	0.18305	-2.87832	3037.0904	3037.3624	3038.4056
C	0.24476	1.31196	-2.02748	3039.2956	3040.6350	3040.7290
C	2.61177	2.02592	-1.41731	3042.7029	3047.7378	3055.9657
C	4.63632	2.66798	-0.39588	3093.3679	3095.4888	3100.9271
H	4.36684	3.73086	-0.42332	3101.9476	3106.6573	3110.6982
H	5.18837	2.44875	-1.32116	3113.0505	3116.3737	3120.7190
C	5.41807	2.29770	0.83764	3121.5023	3122.7575	3122.8669
H	6.37386	2.83088	0.86417	3124.5406	3124.6311	3124.9692
H	4.85479	2.55197	1.74109	3127.6623	3137.0881	3139.7433
H	5.61536	1.21892	0.85184	3141.3251	3141.4870	3143.4050

O	3.44783	1.87770	-0.37798	3145.8717	3147.7257	3153.9923
O	2.74580	2.89427	-2.25066	3154.7797	3155.9669	3163.1955
C	0.16062	2.33075	-3.11767	3172.5875	3173.9566	3174.9171
H	-0.84895	2.31718	-3.53535	3184.5201	3192.9693	3897.0632
H	0.38875	3.32375	-2.71533			
H	0.91912	2.14661	-3.88415			
O	-0.81444	0.74481	-1.71878			
C	4.27806	-3.04984	2.18955			
H	4.94465	-3.91690	2.11373			
H	4.58965	-2.48345	3.07736			
H	3.26534	-3.42275	2.37962			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.772620 Electronic Energy = -2105.65122227
Internal Energy (E)= -2104.82917627 Enthalpy (H)= -2104.82823127
Gibbs Free Energy (G)=-2104.95693327 Gibbs Free Energy of Solvation=-2106.68101398

St.Pt.	General Structure	Ball & Stick model
IX-2		

Cartesian co-ordinate

Atoms	X	Y	Z
H	1.21081	1.02093	-0.20598
C	-2.06648	-1.90714	-1.94951
C	-1.70330	-2.69807	-0.82068
C	-2.65893	-2.41031	0.24052
C	-3.63975	-1.46712	-0.28065
C	-3.25252	-1.12659	-1.62103

Frequencies

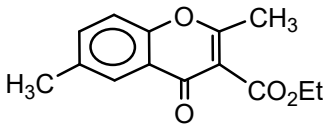
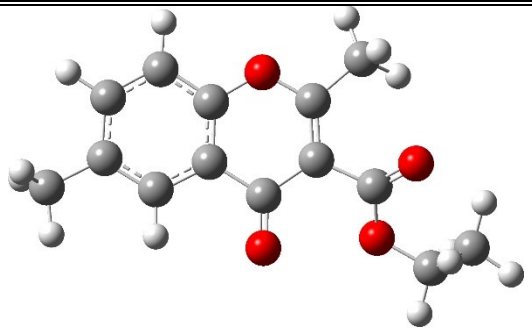
25.9922	30.7813	37.6946
48.6267	52.8946	56.2014
63.3247	67.1827	71.7243
75.6540	81.9482	84.8428
89.3752	92.7026	104.7246
107.5166	114.4212	119.9627
124.0809	127.5273	134.0952
139.7160	145.5510	150.9619
155.7961	161.6810	166.3695
170.7831	184.7615	185.6451

C	-2.74212	2.06602	0.47573	187.3977	197.7223	199.9065
O	-1.97343	1.09916	0.88848	202.3551	206.9121	211.9173
O	-3.65226	1.96436	-0.34065	215.5939	224.3279	231.2881
C	-2.32571	3.42678	1.05063	233.8324	244.1743	248.7046
O	0.03741	-0.77210	1.02163	255.5533	261.6120	264.4716
C	0.45782	0.12098	1.87477	277.6333	278.9827	293.0339
O	0.86484	1.24361	1.58169	298.6323	301.4830	309.9743
C	0.43575	-0.33495	3.34027	313.6370	313.7251	315.9768
C	-4.79610	-0.92273	0.47758	324.1993	327.8381	329.8394
H	-5.67394	-1.57032	0.35613	338.8783	340.0629	345.5170
H	-4.56197	-0.86093	1.54635	348.7352	354.5008	369.7388
H	-5.03420	0.08893	0.13869	371.6989	379.0100	386.9194
C	-3.95206	-0.21032	-2.55841	388.9454	390.2732	393.6869
H	-4.61770	-0.77314	-3.22649	398.8835	411.3071	417.0094
H	-4.52265	0.54233	-2.01190	421.1668	425.3341	436.5740
H	-3.22666	0.33173	-3.17428	451.8814	453.3633	470.1194
C	-2.68949	-3.08586	1.56423	470.8791	517.9525	531.7076
H	-1.68189	-3.15627	1.98795	537.0250	538.4676	546.7864
H	-3.31693	-2.54387	2.27834	557.3636	572.5249	574.2374
H	-3.09013	-4.10343	1.46555	578.5488	588.4110	603.0492
C	-0.52830	-3.60248	-0.69910	603.9976	608.2922	628.8417
H	-0.15299	-3.60636	0.33030	641.0975	675.4066	687.7899
H	-0.79124	-4.63388	-0.96720	742.9557	765.0090	789.8764
H	0.29305	-3.26702	-1.34035	796.0133	799.1315	802.6475
C	-1.39408	-1.87414	-3.27413	805.2956	811.2210	812.4774
H	-0.39306	-2.30682	-3.23658	813.3024	816.6427	855.4465
H	-2.00046	-2.43268	-3.99955	859.7276	902.1528	908.5440
H	-1.29883	-0.84699	-3.64165	913.0563	921.6774	924.4943
C	-1.03147	-0.35385	3.78266	941.6996	949.5542	953.6972
H	-1.11005	-0.73167	4.81122	954.4455	959.0578	961.3826
H	-1.46597	0.65268	3.75072	970.3871	980.7967	986.9962
H	-1.63293	-0.99260	3.12459	997.7417	1012.7788	1015.7244
C	1.22238	0.63553	4.21230	1032.1199	1034.8993	1038.5849
H	1.18465	0.31466	5.26208	1042.8670	1044.1937	1045.0791
H	2.27325	0.68105	3.90217	1046.0472	1047.4414	1048.2550
H	0.81548	1.64941	4.14255	1048.6578	1053.6351	1073.1496
C	1.03469	-1.73436	3.46396	1094.2180	1099.6887	1106.5196
H	0.49235	-2.45533	2.84183	1110.7088	1133.6939	1141.3498
H	2.08704	-1.73908	3.14663	1166.0404	1169.9634	1184.5745
H	0.99711	-2.07322	4.50789	1190.0922	1208.0302	1233.6114
C	-3.46590	4.42591	0.90727	1237.0583	1242.7250	1247.1527
H	-4.33473	4.12326	1.50525	1253.1462	1260.7575	1264.5018
H	-3.14336	5.41743	1.25185	1273.2063	1279.3423	1280.5088
H	-3.79230	4.50177	-0.13453	1283.2629	1307.7376	1323.9568
C	-1.12429	3.87184	0.20419	1355.3801	1359.9884	1364.1392
H	-0.76030	4.84816	0.55173	1369.0868	1373.7157	1375.2760
H	-0.30707	3.14354	0.29259	1375.3051	1379.1528	1385.2527
H	-1.40732	3.96957	-0.85253	1387.2210	1389.2639	1390.7630
C	-1.89144	3.31845	2.51056	1395.7026	1398.3079	1400.1942
H	-1.63796	4.31555	2.89580	1401.0410	1412.5959	1416.2201
H	-2.69698	2.91378	3.13848	1425.6055	1426.8423	1428.7371
H	-1.01026	2.67447	2.60758	1433.8652	1439.7868	1443.7313
Ir	-1.68357	-0.60919	-0.22873	1444.0612	1448.5818	1449.1239
C	1.58481	1.02480	-1.26055	1451.6001	1454.3833	1458.6417
C	2.04236	-0.41256	-1.46545	1461.2147	1461.6047	1462.7769
O	1.33100	-1.18220	-2.08384	1463.1672	1467.5263	1469.9535
C	3.28379	-0.90451	-0.80330	1471.8671	1476.4656	1477.1195
C	4.54712	-0.53001	-1.26052	1478.1917	1479.8134	1481.0666
C	3.16726	-1.82830	0.23083	1482.0817	1487.3840	1488.5295
C	5.68250	-1.05253	-0.65209	1490.4629	1494.6811	1496.3396
C	4.29492	-2.35939	0.85859	1501.3910	1506.6580	1508.6544

H	2.16329	-2.11433	0.55019	1511.0107	1517.4428	1545.0363
C	5.54870	-1.95231	0.40076	1550.9426	1664.2904	1679.2230
H	6.67092	-0.76745	-1.01319	1734.7887	1763.3940	1772.9489
H	6.44490	-2.36025	0.86714	1805.2648	1859.7664	2801.5703
O	4.59283	0.32445	-2.31936	3013.5582	3021.6104	3023.1880
H	5.50825	0.51100	-2.55282	3026.9100	3029.4882	3030.9666
C	0.38460	1.25749	-2.14632	3031.8978	3038.5758	3039.9722
C	2.64064	2.10658	-1.26505	3040.2594	3041.6230	3042.5152
C	4.52252	2.86715	-0.07803	3043.4370	3048.8677	3053.9361
H	4.11823	3.88059	0.03415	3096.0848	3099.1707	3099.7593
H	5.11010	2.85456	-1.00657	3103.2059	3105.6335	3108.2570
C	5.32144	2.42505	1.11935	3110.6300	3112.2938	3114.7794
H	6.18311	3.08285	1.27079	3119.1496	3119.8043	3121.7038
H	4.70241	2.44759	2.02169	3126.8025	3128.5985	3130.8620
H	5.68135	1.39829	0.98164	3132.2729	3133.5745	3134.0969
O	3.43522	1.94620	-0.20734	3135.6348	3144.0861	3147.7810
O	2.73699	3.01747	-2.05461	3149.2653	3150.3816	3151.8112
C	0.57962	1.73543	-3.54318	3161.2674	3164.6138	3167.4263
H	-0.36658	1.69871	-4.08817	3170.2362	3179.2762	3182.7018
H	0.99096	2.74930	-3.53475	3188.7344	3191.7598	3897.5632
H	1.33491	1.10343	-4.02905			
O	-0.73812	0.98837	-1.73385			
C	4.16603	-3.33530	1.99074			
H	4.92269	-4.12569	1.92647			
H	4.29339	-2.84557	2.96543			
H	3.17914	-3.81126	1.99546			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.778500 Electronic Energy = -2105.66028380
Internal Energy (E)= -2104.8317118 Enthalpy (H)= -2104.8307678
Gibbs Free Energy (G)=-2104.9610008 Gibbs Free Energy of Solvation=-2106.68872258

St.Pt.	General Structure	Ball & Stick model
X-2		

Cartesian co-ordinate

Atoms	X	Y	Z
C	1.74593	1.03496	0.11820
C	1.46960	-0.31232	-0.06977
C	0.07974	-0.77208	-0.26136
C	-0.53388	1.60992	-0.03469
O	0.75079	1.97319	0.13177
C	2.53561	-1.21804	-0.08456
C	3.04796	1.49575	0.29447
C	3.84362	-0.79538	0.08694
C	4.08039	0.57768	0.27744
H	2.29262	-2.26785	-0.23996
H	5.10437	0.92371	0.41255
H	3.22094	2.55874	0.43767
O	-0.17853	-1.94378	-0.48691
C	-0.91685	0.30985	-0.19642
C	-1.41353	2.81004	-0.01060
H	-1.68166	3.09932	-1.03196
H	-2.35360	2.61353	0.50737
H	-0.88224	3.63626	0.46780
C	-2.36469	0.03299	-0.38173
C	-4.10214	-1.50402	0.00946
H	-4.09399	-2.59369	0.10253
H	-4.42407	-1.23413	-1.00194
C	-4.98088	-0.85978	1.05398
H	-6.00527	-1.23835	0.97326
H	-4.61182	-1.08292	2.06034
H	-5.00601	0.22557	0.91881
O	-3.13388	0.78056	-0.95174
O	-2.73004	-1.12033	0.18016
C	4.98944	-1.76142	0.06818
H	4.64167	-2.78836	-0.07756
H	5.69451	-1.52887	-0.73900
H	5.55589	-1.72895	1.00667

Frequencies

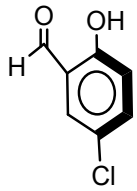
33.0831	36.0553	50.8845
70.6132	86.6112	109.4053
135.3970	148.2641	162.0790
190.1080	206.4316	240.9165
251.0911	286.6228	333.5210
354.6506	359.3151	372.7512
394.4351	431.2323	437.9034
474.4640	539.4242	545.6281
569.5057	592.7356	611.8086
674.7863	691.7016	739.8842
770.9361	788.8425	816.7880
827.2189	838.7873	888.5964
897.1287	919.9141	962.8006
964.8446	1002.0408	1025.3518
1037.5120	1048.9945	1050.7194
1113.2638	1127.0019	1134.5496
1146.6475	1186.4310	1216.2548
1243.9799	1276.7125	1281.9143
1312.8835	1340.5684	1381.7855
1387.6541	1394.1225	1399.9689
1404.9442	1420.8335	1449.7182
1449.9800	1463.3099	1467.0005
1468.4666	1469.7799	1487.2120
1497.3597	1530.9089	1631.7214
1672.7141	1687.7574	1800.9265
1827.7476	3035.7713	3049.6574
3064.2847	3072.3806	3108.1507
3130.4010	3139.9740	3142.6535
3149.0934	3155.9771	3172.4759
3179.2879	3193.1301	3208.3000

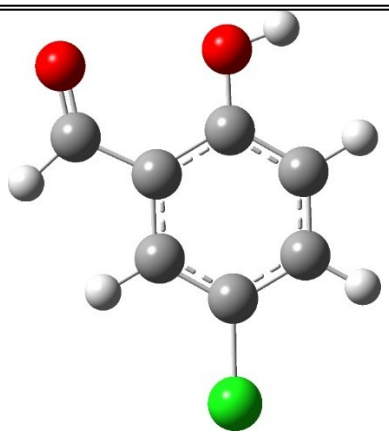
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.253896 Electronic Energy = -842.320820182
Internal Energy (E)= -842.049950182 Enthalpy (H)= -842.049006182
Gibbs Free Energy (G)=-842.112753182 Gibbs Free Energy of Solvation=-842.771267032

St.Pt.	General Structure	Ball & Stick model

S3





Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.18546	0.90192	0.00014
O	-2.46478	1.30913	0.00035
C	-0.12431	1.81072	-0.00016
C	1.19134	1.37309	-0.00032
C	-0.90720	-0.47973	0.00029
C	1.46252	0.00916	-0.00014
C	0.42373	-0.90361	0.00021
H	0.63630	-1.97190	0.00041
H	2.00908	2.08874	-0.00058
C	-1.94216	-1.53035	0.00051
H	-1.49814	-2.55792	0.00152
O	-3.13858	-1.37061	-0.00028
H	-0.33715	2.87914	-0.00028
H	-2.49259	2.27319	0.00070
Cl	3.11757	-0.54745	-0.00032

Frequencies

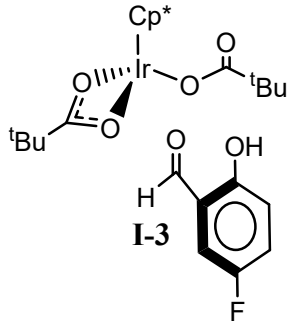
71.0183	118.2841	176.3764
212.0578	261.0385	336.7142
381.1652	397.0581	414.7774
444.0264	448.9050	553.4818
655.0650	713.7400	736.7306
780.5222	814.2674	900.9222
909.0308	938.8747	1016.7546
1113.9573	1129.7446	1173.8617
1218.1126	1299.1763	1339.1466
1377.8481	1412.9873	1463.3934
1534.2871	1646.0001	1671.6174
1857.6825	2837.5932	3166.9990
3179.8043	3209.0734	3874.3383

Statistical Thermodynamic Analysis

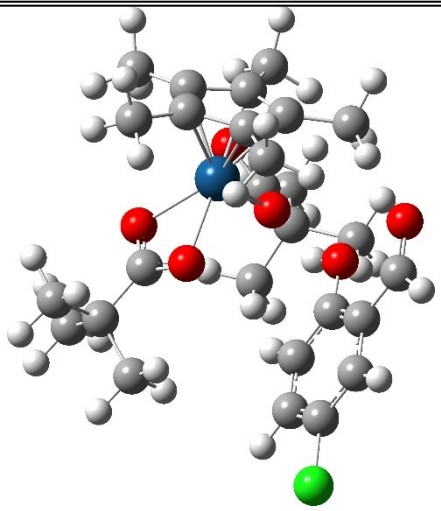
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.104309 Electronic Energy = -880.092861874
Internal Energy (E)= -879.979774874 Enthalpy (H)= -879.978831874
Gibbs Free Energy (G)=-880.023000874 Gibbs Free Energy of Solvation=-880.403593589

St.Pt.	General Structure	Ball & Stick model

I-3



I-3



Cartesian co-ordinate

Atoms	X	Y	Z
C	-2.96370	-1.60092	0.52427
C	-3.24822	-1.26190	-0.85076
C	-2.19201	-1.78527	-1.68554
C	-1.25228	-2.46454	-0.81132
C	-1.72599	-2.35556	0.54501
C	2.56952	-0.80393	0.95529
C	0.28992	2.70242	-2.37871
C	-0.32015	1.57861	-1.56842
O	-1.52134	1.63503	-1.16442
O	0.33352	0.51064	-1.34798
C	-2.05852	-1.63884	-3.16143
H	-2.47432	-0.68329	-3.50131
H	-1.00286	-1.65345	-3.45361
H	-2.57143	-2.44592	-3.69956
C	0.02336	-3.09242	-1.24757
H	0.67881	-3.29841	-0.39476
H	-0.17537	-4.03764	-1.76875
H	0.56302	-2.43257	-1.93768
C	-1.09524	-2.93141	1.76237
H	-0.03381	-3.15132	1.61353
H	-1.17131	-2.23253	2.60364
H	-1.61362	-3.85577	2.04886
C	-3.83555	-1.32683	1.69561
H	-3.24642	-1.24021	2.61301
H	-4.38052	-0.38727	1.57955
H	-4.55716	-2.14420	1.82799
C	-4.38357	-0.40608	-1.28563
H	-4.20429	0.02760	-2.27392
H	-5.31481	-0.98486	-1.32506
H	-4.51997	0.42169	-0.58016
C	-1.32179	1.50642	1.96961
O	-0.52291	0.70616	1.29791
O	-2.53757	1.50721	1.86863
C	-0.57234	2.52535	2.83456
O	1.40026	-1.11771	1.50243
C	0.56436	1.87347	3.61953
H	1.34257	1.46500	2.96567

Frequencies

23.5340	29.0414	39.2109
50.0840	62.7771	68.0357
69.6784	77.0500	88.1668
92.7415	94.5659	100.3786
110.9530	126.1241	139.6646
142.1926	147.3960	154.2965
165.6696	170.0863	178.1501
186.4327	190.3234	198.2429
201.0312	204.4941	210.6003
218.9750	227.0209	239.2958
243.4586	250.9404	252.7605
270.4486	282.4708	290.8219
296.2928	299.9250	309.3223
310.9385	313.0470	318.9652
324.9185	326.6423	339.9904
347.7493	349.2663	361.8232
363.1125	370.4494	388.5867
394.4217	398.8775	410.7295
420.3588	430.0650	442.4786
448.9576	458.3543	460.9939
467.7933	470.3268	483.6932
534.9731	538.9016	548.1907
549.9498	555.4609	570.3966
587.0379	594.5437	606.7247
622.0379	633.4105	654.9251
729.8977	744.1318	787.5767
792.4893	798.5194	808.3498
814.5837	817.2548	831.4774
871.8480	895.8401	910.4755
915.3068	932.9850	938.2534
951.1054	951.8105	954.4267
960.0282	967.1067	974.1357
975.0179	975.8335	994.9617
1020.6746	1037.5912	1038.6640
1041.4456	1042.7398	1044.1847
1049.9464	1051.2839	1052.6868
1055.6796	1096.5193	1099.3858
1108.4323	1123.5992	1155.8388
1187.1057	1191.0002	1210.8075
1229.6167	1236.1278	1243.9808
1254.2137	1261.1136	1266.1201
1268.2955	1346.2765	1357.3437

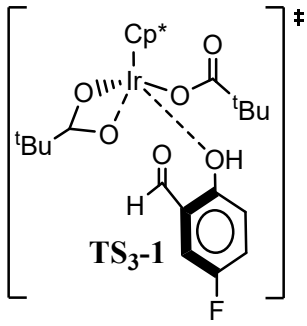
H	1.03843	2.61729	4.27310	1362.0768	1375.6803	1376.2982
H	0.19542	1.05868	4.25564	1384.0601	1388.4950	1389.8165
C	-1.54277	3.19695	3.79767	1390.9594	1401.6390	1404.4450
H	-1.02268	3.97312	4.37406	1409.8239	1410.7241	1411.9504
H	-2.37759	3.65552	3.25952	1414.9222	1417.8693	1437.4469
H	-1.96401	2.47057	4.50277	1442.1762	1446.0805	1448.8969
C	-0.00919	3.56438	1.85830	1450.6649	1454.5508	1456.9487
H	-0.82390	4.06305	1.31647	1460.2929	1461.9625	1463.2332
H	0.56488	4.32899	2.39749	1468.8993	1470.4049	1473.9928
H	0.64937	3.08899	1.11803	1474.6875	1475.9991	1477.5900
C	1.77790	2.83419	-2.06816	1479.4285	1482.4334	1483.8189
H	2.30457	1.88662	-2.22236	1485.5857	1491.1035	1495.3059
H	2.22605	3.59669	-2.71757	1496.5147	1506.0802	1513.0973
H	1.93748	3.14663	-1.02716	1516.9644	1522.9033	1532.3289
C	-0.43255	4.01712	-2.10870	1544.9217	1545.3646	1604.2670
H	0.00086	4.81033	-2.73082	1639.2748	1674.4766	1792.8155
H	-1.50059	3.94043	-2.33506	1827.7320	2843.5575	3018.6971
H	-0.33369	4.31489	-1.05763	3027.8879	3030.3118	3032.5820
C	0.10047	2.29325	-3.84672	3035.2051	3036.5409	3036.7749
H	-0.96339	2.15196	-4.07752	3039.2200	3039.7216	3041.1302
H	0.49309	3.07702	-4.50648	3043.3166	3106.3325	3111.8253
H	0.63148	1.35925	-4.06613	3114.0933	3114.6135	3115.6002
Ir	-1.38201	-0.38946	-0.28454	3116.7286	3117.8357	3119.7562
C	2.89892	0.52127	0.63415	3123.5695	3124.1225	3127.5493
C	4.14230	0.84101	0.12074	3130.2638	3132.9516	3133.5421
C	5.08931	-0.16315	-0.08424	3140.8710	3142.9633	3145.9392
C	3.52287	-1.82066	0.72101	3145.9733	3149.1407	3151.8417
C	4.78342	-1.47519	0.21262	3168.4487	3173.4038	3176.2366
H	4.39013	1.87220	-0.12043	3190.1930	3202.8489	3450.2567
H	5.52197	-2.25870	0.04681			
H	0.79777	-0.33629	1.53872			
H	2.14622	1.29267	0.78971			
C	3.28251	-3.24688	0.96011			
H	4.20572	-3.86156	0.81404			
O	2.23736	-3.78825	1.26020			
Cl	6.66577	0.25080	-0.72054			

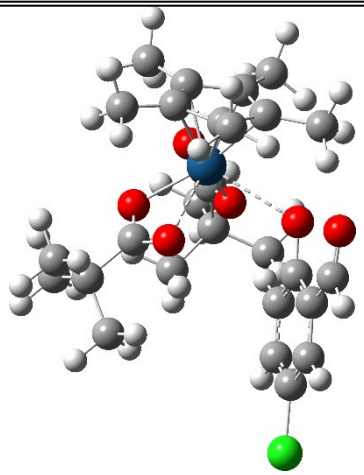
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.605889 Electronic Energy = -2067.07883664
Internal Energy (E)= -2066.43366164 Enthalpy (H)= -2066.43271864
Gibbs Free Energy (G)=-2066.54152164 Gibbs Free Energy of Solvation=-2066.59604993

St.Pt.	General Structure	Ball & Stick model

TS_3-1





Cartesian co-ordinate

Atoms	X	Y	Z
C	3.15243	-0.88429	-0.84588
C	3.26132	-0.80627	0.59862
C	2.39789	-1.83549	1.16730
C	1.75945	-2.51861	0.08602
C	2.20857	-1.92740	-1.16461
C	-2.07349	-0.70883	-1.40562
C	-1.54146	0.66214	2.95520
C	-0.61059	0.20386	1.83702
O	0.48850	0.82348	1.66349
O	-0.89533	-0.81911	1.17453
C	2.19675	-2.08500	2.62032
H	2.14228	-1.14215	3.17604
H	1.26312	-2.62761	2.79851
H	3.02150	-2.67697	3.03642
C	0.75156	-3.60171	0.19995
H	-0.02666	-3.50170	-0.56374
H	1.23219	-4.58062	0.07282
H	0.26072	-3.58120	1.17686
C	1.83420	-2.40666	-2.52277
H	0.79837	-2.75979	-2.54760
H	1.93742	-1.60967	-3.26767
H	2.48676	-3.23391	-2.83121
C	3.89076	-0.04288	-1.82284
H	3.28539	0.13315	-2.71843
H	4.12444	0.93282	-1.38927
H	4.81831	-0.54117	-2.13264
C	4.12648	0.13071	1.35758
H	3.84806	0.15352	2.41554
H	5.17768	-0.17774	1.28528
H	4.01783	1.14281	0.95443
C	1.57502	2.44485	-0.75684
O	0.84757	1.39018	-1.00211
O	2.68223	2.43870	-0.23392
C	0.87555	3.75829	-1.13316
O	-0.81829	-1.12870	-1.67307
C	0.26074	3.68245	-2.52954
H	-0.50360	2.90243	-2.60571
H	-0.20931	4.64241	-2.78087

Frequencies

-79.7869	-30.7123	25.7509
32.1044	37.5201	51.8267
59.5582	61.4635	71.2377
76.2827	84.4547	100.7419
103.7150	117.5512	122.1897
127.9008	141.1200	153.1397
155.9016	162.3089	164.2771
174.3202	178.1279	183.6790
192.1364	200.8076	209.4980
213.1723	214.3680	219.4432
229.8643	238.2434	240.7601
250.6028	260.2281	271.7480
272.8909	282.8368	288.5547
302.7266	305.9184	312.4678
325.1070	332.3659	334.8786
345.5964	347.7641	352.4137
358.8037	362.0832	375.6472
385.7464	388.5535	391.9713
405.4911	418.1691	424.5089
434.4227	447.1227	450.9745
453.4754	456.0450	469.0140
533.3093	538.6296	545.0370
547.0493	553.4076	568.5221
579.6547	585.5107	592.5985
603.7327	619.2407	627.6461
656.9003	727.8661	735.9170
786.4477	788.8295	792.8144
808.2261	810.4742	812.7348
826.7711	849.8094	898.6360
911.3623	912.2449	927.0742
940.7692	949.8458	950.7598
953.1770	957.9163	961.9571
969.9627	970.7979	981.7757
1026.3957	1032.3124	1036.3841
1038.5189	1039.8536	1041.6214
1042.5585	1044.8595	1046.5591
1052.7405	1098.4712	1102.4707
1111.6503	1118.9502	1142.0987
1186.7988	1190.0616	1199.2021
1225.7883	1235.8605	1240.6464
1244.4009	1257.9514	1261.3005
1270.7032	1317.1958	1332.0758
1361.9856	1370.4190	1374.4568

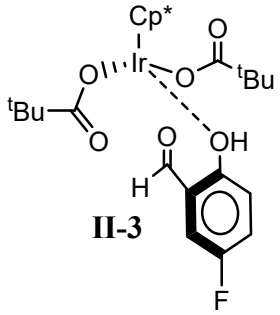
H	1.02636	3.47933	-3.28933	1379.2862	1380.6255	1381.9854
C	1.87314	4.90901	-1.07993	1389.5556	1394.0335	1394.6646
H	1.36566	5.85749	-1.30010	1399.1141	1406.0056	1409.4216
H	2.34055	4.97998	-0.09321	1413.2749	1417.5029	1423.4147
H	2.67489	4.76985	-1.81482	1435.9576	1441.7892	1446.7138
C	-0.22013	3.98029	-0.08300	1449.5819	1450.2446	1455.6807
H	0.22145	4.08380	0.91632	1459.1952	1460.0078	1461.9317
H	-0.78297	4.89587	-0.30865	1462.8052	1465.1069	1466.2780
H	-0.92237	3.13567	-0.04905	1469.0089	1474.0097	1474.4792
C	-2.97902	0.70711	2.44054	1479.1473	1481.2244	1482.7361
H	-3.26145	-0.24052	1.96770	1483.4296	1487.2134	1489.0252
H	-3.66855	0.90851	3.27043	1496.8391	1503.0844	1504.8545
H	-3.10500	1.50854	1.69993	1505.5771	1513.2471	1524.9363
C	-1.13578	2.02590	3.49945	1531.1107	1534.7468	1647.9894
H	-1.81604	2.31948	4.30965	1666.5182	1669.3167	1775.1186
H	-0.11300	2.01394	3.89038	1838.0942	2849.4979	3019.7544
H	-1.18277	2.79421	2.71877	3026.4154	3027.5186	3032.8225
C	-1.42318	-0.39541	4.05922	3035.2566	3035.3973	3036.7134
H	-0.39141	-0.46210	4.43103	3039.6983	3039.9199	3043.5405
H	-2.06939	-0.12943	4.90553	3044.5796	3106.4147	3107.4918
H	-1.72200	-1.38217	3.68779	3110.8956	3114.3339	3114.5037
Ir	1.25750	-0.40608	0.03126	3117.0874	3120.7591	3121.8449
C	-2.34618	0.65319	-1.26802	3124.7430	3125.5998	3126.7462
C	-3.62433	1.08835	-0.96741	3127.0552	3131.6116	3132.6220
C	-4.64739	0.15757	-0.79108	3136.1429	3142.5321	3144.6045
C	-3.10589	-1.64939	-1.24862	3148.2124	3148.9497	3153.4934
C	-4.39318	-1.19217	-0.93413	3159.9073	3173.7497	3173.9959
H	-3.82994	2.14956	-0.84433	3182.2258	3200.6943	3720.5427
H	-5.19620	-1.91663	-0.80458			
H	-0.29280	-0.35499	-1.94181			
H	-1.51670	1.35576	-1.34971			
C	-2.93645	-3.09710	-1.42135			
H	-3.89077	-3.65847	-1.26376			
O	-1.92087	-3.69004	-1.71620			
Cl	-6.24709	0.70907	-0.35320			

Statistical Thermodynamic Analysis

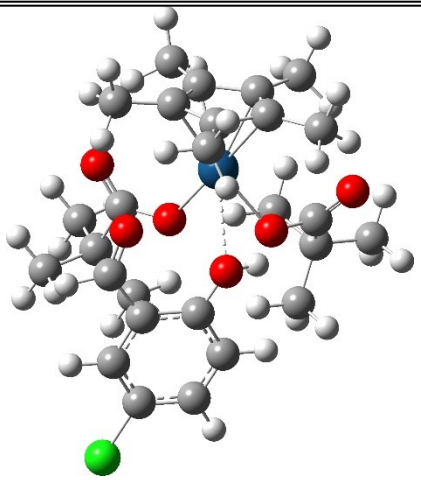
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.602910 Electronic Energy = -2067.05329352
Internal Energy (E)= -2066.41167852 Enthalpy (H)= -2066.41073552
Gibbs Free Energy (G)=-2066.51812052 Gibbs Free Energy of Solvation=-2066.57968923

St.Pt.	General Structure	Ball & Stick model

II-3



II-3



Cartesian co-ordinate

Atoms	X	Y	Z
C	3.14918	-0.52534	-1.26091
C	3.44074	-0.19231	0.10104
C	2.90225	-1.25254	0.95615
C	2.29042	-2.23664	0.11330
C	2.41500	-1.76358	-1.25134
Ir	1.30515	-0.30057	-0.11219
O	-0.43868	-0.19290	0.91786
O	0.51620	1.56816	-0.69077
O	-0.92188	-2.79591	-1.46406
C	-2.08439	-2.50093	-1.28547
H	-2.81271	-3.26841	-0.92277
C	-2.70411	-1.18205	-1.46244
C	-2.00306	-0.02779	-1.86410
C	-4.05614	-1.07339	-1.11094
C	-2.66341	1.20553	-1.86238
C	-4.69406	0.15169	-1.12815
H	-4.59882	-1.96559	-0.79943
C	-3.99547	1.30061	-1.49581
H	-2.10962	2.09531	-2.15535
H	-4.49948	2.26362	-1.49452
O	-0.72248	-0.11909	-2.25316
H	-0.27410	0.73153	-2.04969
C	-0.74563	-0.94588	1.94551
C	-2.04230	-0.54393	2.66537
C	1.21065	2.68050	-0.56150
C	0.57054	3.67926	0.40869
O	2.28510	2.90426	-1.10046
O	-0.08815	-1.89485	2.35033
C	1.91579	-2.45683	-2.46729
H	1.34231	-3.34986	-2.21410
H	1.25296	-1.80850	-3.05068
H	2.76771	-2.73939	-3.09951
C	3.50858	0.26248	-2.46991
H	3.47519	1.33411	-2.25404
H	4.51071	-0.00959	-2.82636
H	2.79849	0.06602	-3.28092
C	4.20084	0.99882	0.55554
H	4.08328	1.16254	1.63106

Frequencies

21.9875	33.4752	36.4102
41.4523	54.9669	58.6396
62.2241	68.5174	75.3167
79.2090	88.0578	91.3854
97.7150	107.1195	117.1024
127.4813	130.4856	134.8881
146.7939	149.9250	159.4902
172.9546	185.7823	193.8602
199.0046	200.3715	209.2072
218.7116	224.3492	228.0366
235.1040	242.7784	245.8195
257.0979	269.6930	273.8063
284.5219	291.9032	297.5085
298.9010	310.7744	316.6585
319.7560	323.3602	329.3058
336.3157	339.7394	350.5537
354.5887	366.8585	381.1513
384.6145	391.3669	395.3202
401.1432	419.3585	428.6345
437.3821	448.6151	453.3949
457.8655	459.5574	465.4605
535.5901	542.3024	550.1807
553.4615	564.4298	572.5438
575.3373	582.9756	600.1584
603.9266	641.2248	651.9378
721.1912	722.3593	750.1608
783.7789	789.4203	797.9285
809.1866	814.3385	817.9982
820.9019	829.7306	888.7882
905.9347	912.4273	920.5222
945.6135	946.7204	948.7191
951.6648	952.6462	955.6285
957.0118	969.4526	986.1352
1029.0165	1031.9090	1037.1689
1039.4363	1041.1695	1042.6907
1045.0508	1047.0292	1048.6692
1051.8975	1100.3471	1101.5980
1116.0035	1121.6481	1137.8880
1188.8691	1195.9810	1202.0706
1223.3910	1229.8359	1233.4304
1238.9011	1239.7318	1264.5005
1268.3050	1326.0278	1337.4752

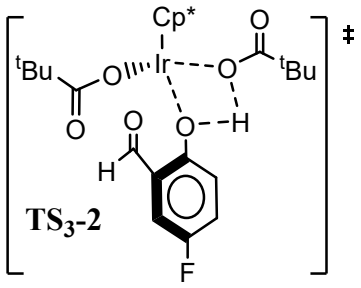
H	5.27031	0.85571	0.35254	1343.8178	1357.1567	1373.2907
H	3.86823	1.89893	0.02463	1374.5830	1377.9812	1382.5984
C	3.00581	-1.29972	2.43593	1383.4241	1389.0302	1393.8249
H	2.12156	-1.78103	2.86319	1395.7910	1399.5152	1405.8750
H	3.90520	-1.85080	2.74020	1410.9687	1412.8311	1415.8311
H	3.07043	-0.28894	2.85398	1425.6368	1434.7076	1437.8513
C	1.70176	-3.53990	0.51509	1442.1437	1446.8215	1450.8627
H	2.38035	-4.35540	0.23112	1454.0122	1457.3540	1459.2659
H	1.51994	-3.57770	1.58949	1462.0979	1462.9534	1464.6863
H	0.74150	-3.69772	0.01532	1467.7657	1471.5602	1473.8966
C	-2.65657	0.73994	2.12201	1476.7709	1477.5163	1477.9297
H	-2.85160	0.67168	1.04644	1478.6877	1480.9952	1491.0177
H	-3.60694	0.94180	2.63471	1492.9378	1497.7552	1498.2582
H	-1.99559	1.60133	2.28392	1506.2428	1509.2855	1517.5274
C	-1.70271	-0.36612	4.14686	1530.5642	1541.2341	1639.6574
H	-2.60872	-0.11423	4.71329	1666.4175	1771.5804	1777.5620
H	-1.27086	-1.28275	4.56068	1836.6004	2856.3269	3014.9432
H	-0.98027	0.44876	4.29079	3019.8738	3025.9251	3031.5729
C	-3.02948	-1.70320	2.50930	3033.4766	3034.2913	3037.8287
H	-2.58928	-2.63951	2.86872	3038.3953	3040.5982	3041.4262
H	-3.94367	-1.49989	3.08200	3046.8128	3096.9790	3098.9664
H	-3.31906	-1.83523	1.45815	3106.8258	3109.4681	3113.5042
C	1.27882	5.02444	0.32331	3115.4947	3119.2559	3120.8295
H	1.18184	5.46136	-0.67754	3121.0762	3121.6952	3130.3062
H	0.84513	5.72513	1.04850	3137.8670	3138.7312	3138.9684
H	2.34859	4.92096	0.53282	3145.0851	3146.2284	3152.6120
C	-0.92099	3.84171	0.12252	3164.2644	3170.2820	3175.3531
H	-1.44158	2.87947	0.18889	3178.2652	3186.7391	3186.8788
H	-1.36687	4.53133	0.85151	3207.1986	3209.5148	3529.5684
H	-1.09011	4.26423	-0.87779			
C	0.75125	3.08069	1.81112			
H	1.81701	2.93758	2.04243			
H	0.33489	3.76198	2.56514			
H	0.24161	2.11210	1.89217			
Cl	-6.37148	0.27366	-0.65689			

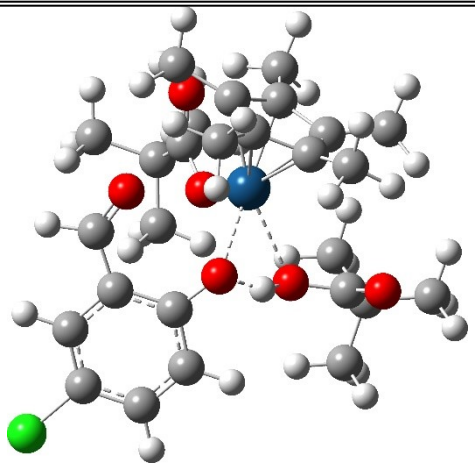
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.603114 Electronic Energy = -2067.06226181
Internal Energy (E)= -2066.41885781 Enthalpy (H)= -2066.41791481
Gibbs Free Energy (G)=-2066.52985281 Gibbs Free Energy of Solvation=-2066.59197018

St.Pt.	General Structure	Ball & Stick model

TS_3-2





Cartesian co-ordinate

Atoms	X	Y	Z
C	2.86615	-0.77697	-1.42271
C	3.22241	-0.31939	-0.10546
C	2.75712	-1.28514	0.86854
C	2.11508	-2.36047	0.13825
C	2.19664	-2.03571	-1.27634
Ir	1.07002	-0.53074	-0.19847
O	-0.53119	-0.24082	1.00230
O	0.40273	1.80240	-0.58281
O	-0.91090	-2.71912	-1.09820
C	-2.06565	-2.35589	-0.98327
H	-2.84782	-3.08248	-0.65245
C	-2.60270	-1.02212	-1.23466
C	-1.82045	0.10515	-1.58426
C	-3.99173	-0.88506	-1.08558
C	-2.47813	1.33681	-1.75438
C	-4.60824	0.33333	-1.27717
H	-4.58402	-1.75828	-0.81354
C	-3.84824	1.45383	-1.61224
H	-1.88341	2.21014	-2.01321
H	-4.33784	2.41334	-1.75814
O	-0.50225	0.04979	-1.78420
H	-0.02594	1.11054	-1.44538
C	-0.76700	-0.83694	2.13925
C	-1.99554	-0.29693	2.88494
C	1.28842	2.77185	-0.71219
C	1.23185	3.75514	0.45611
O	2.04151	2.89689	-1.66391
O	-0.09941	-1.74611	2.61528
C	1.68977	-2.84772	-2.41243
H	1.12920	-3.71883	-2.07177
H	1.02107	-2.25389	-3.04435
H	2.53749	-3.18060	-3.02508
C	3.12367	-0.06385	-2.70319
H	2.99513	1.01896	-2.58730
H	4.14211	-0.26192	-3.06229
H	2.42336	-0.39821	-3.47553
C	3.98011	0.92405	0.18022
H	3.85293	1.25120	1.21704

Frequencies

-155.4538	32.0175	40.7678
43.2500	49.8511	60.6729
67.5080	77.4517	87.4987
88.4538	92.3079	97.6159
106.4276	116.2028	116.7166
126.3738	130.7306	141.0553
149.2744	155.0542	164.8029
174.6598	183.2051	189.8524
198.4169	205.9912	206.8547
214.8800	216.3074	224.4188
232.2159	232.7526	240.8412
245.8747	252.4249	258.4240
272.3747	283.5663	291.6241
295.6369	302.2921	305.9985
306.8545	320.9094	324.7946
329.1011	336.0369	344.2548
356.2646	361.3978	371.9261
383.9518	387.8824	390.7802
392.2035	426.2173	438.7548
445.1416	449.6572	452.4747
465.3817	469.2471	505.5634
533.7175	539.1310	549.3305
557.1971	576.4999	580.1522
582.4252	594.5805	603.9503
624.2585	644.0473	656.5673
720.9681	736.3302	748.1604
786.9706	792.1878	797.0494
810.0361	813.6545	815.7336
817.8402	846.2657	906.4568
917.4227	921.1828	924.7558
944.9433	946.9316	952.4057
957.2367	958.0397	961.5191
964.7782	970.4800	981.7897
1022.8552	1029.0594	1034.9545
1039.6933	1040.8682	1041.7364
1043.8908	1046.5352	1047.0003
1049.2232	1100.0627	1102.7716
1112.2534	1122.5990	1152.4049
1187.7348	1193.0836	1214.0168
1232.4137	1234.8936	1240.0736
1245.8586	1257.9956	1265.2421
1269.2535	1334.1226	1355.9631
1367.3164	1372.8563	1378.5120

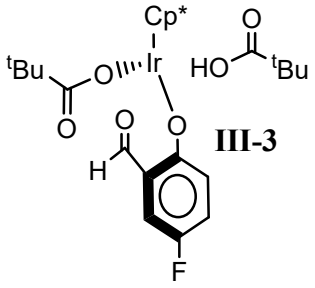
H	5.05044	0.73750	0.01996	1379.5023	1380.2623	1383.9638
H	3.67982	1.73921	-0.48800	1388.4946	1394.4244	1396.0637
C	2.99380	-1.23436	2.33465	1399.2255	1405.7073	1412.3523
H	2.18733	-1.74253	2.86872	1416.3218	1416.3726	1431.0016
H	3.95291	-1.70704	2.58393	1435.9260	1440.5226	1441.6490
H	3.02358	-0.19956	2.69306	1444.8539	1447.8931	1450.6499
C	1.58117	-3.61553	0.72230	1451.6975	1453.0197	1456.5289
H	2.38742	-4.35645	0.80873	1459.0696	1460.8800	1464.3834
H	1.15358	-3.42504	1.70984	1466.0805	1468.3414	1476.0298
H	0.78719	-4.02847	0.09592	1476.7753	1479.1821	1484.4479
C	-2.69829	0.82906	2.13536	1486.8082	1489.2552	1496.9484
H	-3.12161	0.47663	1.18692	1499.1513	1499.8693	1501.6656
H	-3.52093	1.22145	2.74796	1502.7148	1510.0012	1518.1101
H	-2.01177	1.65395	1.90429	1523.6562	1527.0322	1617.2075
C	-1.50760	0.20481	4.24650	1629.8310	1668.3502	1775.1271
H	-2.35997	0.53911	4.85208	1812.0888	1819.9512	2855.0733
H	-0.98218	-0.58968	4.78666	3019.2744	3024.6610	3025.8535
H	-0.82279	1.05592	4.13392	3026.9476	3033.9799	3034.1437
C	-2.95995	-1.46625	3.09035	3036.0943	3039.3097	3040.1115
H	-2.46657	-2.29018	3.61623	3043.7624	3046.0150	3097.0398
H	-3.82924	-1.14136	3.67674	3103.4511	3106.9048	3113.3909
H	-3.33052	-1.84493	2.12774	3115.5374	3118.5063	3118.9394
C	2.44053	4.67928	0.42489	3121.2594	3121.7931	3126.3549
H	2.50111	5.21852	-0.52591	3131.4880	3133.1169	3136.8205
H	2.37688	5.41069	1.24038	3139.1404	3140.6451	3140.7154
H	3.37530	4.11696	0.54391	3141.4395	3150.0156	3151.4675
C	-0.05748	4.56685	0.27029	3171.2481	3175.3761	3179.6524
H	-0.93734	3.91212	0.29498	3188.5725	3190.1110	3204.2025
H	-0.15337	5.30624	1.07570			
H	-0.04933	5.10741	-0.68495			
C	1.15727	3.00066	1.78487			
H	2.06098	2.39952	1.95572			
H	1.07127	3.71477	2.61402			
H	0.29640	2.32210	1.80656			
Cl	-6.34082	0.48321	-1.09497			

Statistical Thermodynamic Analysis

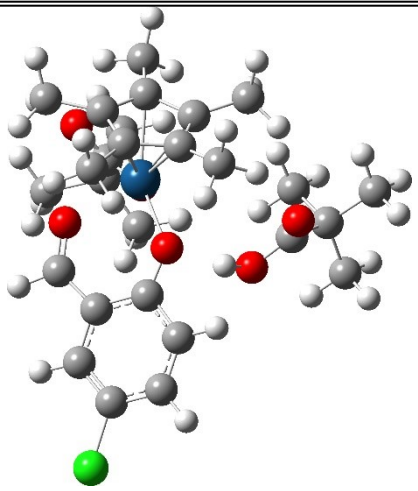
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.599348 Electronic Energy = -2067.05172123
Internal Energy (E)= -2066.41301823 Enthalpy (H)= -2066.41207423
Gibbs Free Energy (G)=-2066.52046123 Gibbs Free Energy of Solvation=-2066.57666134

St.Pt.	General Structure	Ball & Stick model

III-3



III-3



Cartesian co-ordinate

Atoms	X	Y	Z
C	2.59286	-1.00618	-1.60490
C	2.95967	-0.17047	-0.48037
C	2.92075	-0.99289	0.71213
C	2.52065	-2.31274	0.32636
C	2.32193	-2.32812	-1.12151
Ir	0.95385	-0.94686	-0.18264
O	-0.16731	0.25183	1.10104
O	-0.48377	2.45133	-0.91107
O	-0.56618	-2.43325	0.36193
C	-1.79129	-2.31515	0.20898
H	-2.41674	-3.10500	0.66657
C	-2.50558	-1.31122	-0.50705
C	-1.86871	-0.33780	-1.33835
C	-3.91676	-1.37643	-0.42702
C	-2.72725	0.51791	-2.08075
C	-4.69785	-0.49829	-1.12976
H	-4.37658	-2.13035	0.21060
C	-4.09498	0.45304	-1.97070
H	-2.26260	1.25002	-2.73628
H	-4.72413	1.13577	-2.53683
O	-0.58659	-0.18912	-1.48917
H	-0.46119	1.54333	-1.30035
C	-0.28354	-0.06772	2.35446
C	-1.39676	0.69709	3.08966
C	0.63769	3.07296	-1.24372
C	0.90924	4.27862	-0.35904
O	1.37601	2.67809	-2.12886
O	0.39437	-0.89853	2.95303
C	1.91262	-3.51150	-1.92610
H	1.18467	-4.12373	-1.38326
H	1.44704	-3.20637	-2.86855
H	2.77567	-4.14561	-2.16547
C	2.45843	-0.49817	-2.99570
H	2.04768	0.51953	-2.98623
H	3.43924	-0.46808	-3.48758
H	1.79443	-1.12799	-3.59533
C	3.57121	1.18090	-0.56279
H	3.44311	1.73655	0.37159

Frequencies

20.1847	28.8437	42.7805
48.0866	61.5600	67.1311
74.7568	77.8485	81.3336
83.3315	91.5811	102.7815
108.6629	110.3775	128.8277
137.3915	142.2415	147.9707
160.8381	168.1825	169.7897
176.7007	186.4936	193.2626
200.4553	205.5444	216.1359
219.4043	226.5646	231.7409
235.6656	248.9370	258.4138
268.2712	270.4808	277.6760
286.7697	292.9411	304.5365
308.7221	312.2326	316.3843
320.4866	331.0788	332.7945
333.6238	344.0382	349.0882
360.1013	367.2994	382.5168
387.4290	388.3604	397.8822
402.5035	416.9293	431.6745
440.1935	448.6690	450.8193
454.5438	465.0158	533.1176
537.4527	539.5619	540.9444
547.2479	549.6044	572.6120
585.3128	586.3441	595.5536
607.0754	640.4383	664.0382
732.3881	747.8937	775.4759
783.1675	795.6915	803.7154
811.4749	814.5763	818.3144
836.0670	870.1469	892.8116
917.3313	921.3334	943.8969
944.3835	948.8502	952.3529
954.1633	959.8498	962.4483
963.4432	968.6023	986.2748
1007.6897	1036.3854	1038.3559
1039.6934	1041.4088	1044.2265
1046.4633	1047.5990	1048.1243
1051.6006	1093.9229	1104.7737
1114.3348	1115.1078	1147.5725
1186.3242	1193.7134	1215.5383
1233.0854	1240.2218	1244.2495
1245.5339	1248.3706	1261.8894
1268.4594	1336.6970	1356.4907

H	4.65278	1.06887	-0.72478	1375.5194	1379.1333	1381.3898
H	3.15713	1.77948	-1.37774	1382.6186	1383.0910	1385.4415
C	3.28141	-0.52424	2.07615	1388.6383	1390.9352	1399.1229
H	2.80294	-1.12830	2.84926	1403.5471	1405.7860	1411.9591
H	4.37198	-0.54956	2.20438	1415.8288	1427.9777	1430.1937
H	2.94281	0.50673	2.23100	1435.0488	1440.4545	1443.6464
C	2.31493	-3.45057	1.26130	1447.6686	1449.2832	1453.5805
H	3.27629	-3.90595	1.53018	1454.6442	1456.8377	1459.2856
H	1.82210	-3.10139	2.17539	1464.1564	1464.5533	1466.7953
H	1.68151	-4.22423	0.81864	1469.7181	1472.3181	1473.8053
C	-2.25510	1.53859	2.15159	1476.2071	1478.5657	1483.7928
H	-2.77901	0.90956	1.41903	1485.9142	1487.2744	1489.4874
H	-3.01127	2.08649	2.73041	1495.8810	1499.7736	1501.9847
H	-1.65669	2.25909	1.58327	1504.2246	1506.6910	1522.7262
C	-0.72253	1.58786	4.13457	1524.6609	1535.3043	1578.2900
H	-1.47763	2.10615	4.74039	1673.1580	1725.5391	1763.0786
H	-0.08906	0.98969	4.79858	1826.8764	2982.1465	3017.5165
H	-0.09398	2.35143	3.65573	3022.9392	3031.0530	3033.0267
C	-2.27465	-0.34158	3.78893	3034.2299	3036.6999	3037.5884
H	-1.67964	-0.96577	4.46284	3039.1064	3040.0848	3040.8067
H	-3.06715	0.15420	4.36505	3041.8986	3095.3015	3104.5133
H	-2.75984	-0.99939	3.05256	3107.0312	3114.5786	3116.7212
C	2.14720	5.01146	-0.85724	3117.1181	3121.1032	3123.2185
H	2.00860	5.37337	-1.88230	3125.9136	3126.3386	3130.0097
H	2.35707	5.87328	-0.21172	3134.9550	3135.4105	3143.1116
H	3.02559	4.35608	-0.85585	3144.2514	3145.5328	3149.1749
C	-0.29989	5.21571	-0.35983	3150.1755	3151.9442	3165.3544
H	-1.19781	4.71152	0.01192	3184.9718	3187.1008	3190.8430
H	-0.09591	6.07754	0.28821	3199.9077	3213.8806	3470.9127
H	-0.50894	5.59622	-1.36732			
C	1.14083	3.74549	1.06220			
H	1.96659	3.02098	1.08714			
H	1.39473	4.57594	1.73320			
H	0.25052	3.23568	1.44730			
Cl	-6.44057	-0.56173	-1.01143			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm

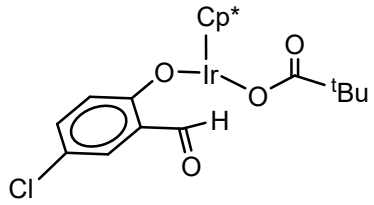
Zero-point correction= 0.604825 Electronic Energy = -2067.07859618

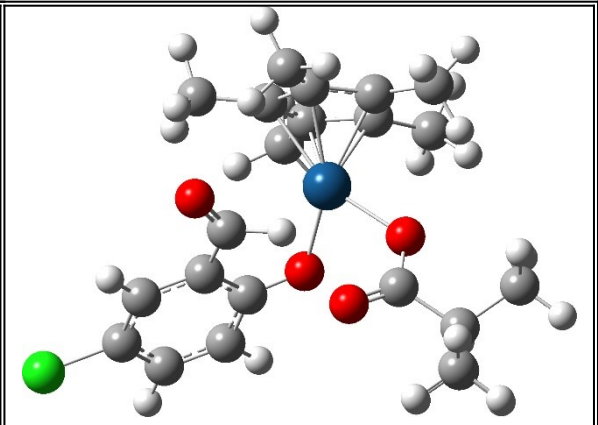
Internal Energy (E)= -2066.43404518 Enthalpy (H)= -2066.43310118

Gibbs Free Energy (G)=-2066.54309018 Gibbs Free Energy of Solvation=-2066.59532349

St.Pt.	General Structure	Ball & Stick model

III'-3





Cartesian co-ordinate

Atoms	X	Y	Z
C	1.29245	-2.38742	-1.00070
C	2.38592	-1.90200	-0.22033
C	1.94243	-1.82750	1.16454
C	0.58328	-2.35515	1.22279
C	0.17790	-2.68813	-0.10627
C	-2.30946	0.27813	-0.47742
Ir	0.69978	-0.55331	0.03324
C	-3.68240	0.27922	-0.78440
C	-4.57948	0.75007	0.14256
C	-1.83739	0.71314	0.79127
C	-4.13453	1.23779	1.38431
C	-2.79608	1.22463	1.70148
H	-2.44007	1.58673	2.66257
H	-4.86447	1.61932	2.09446
H	-0.30143	0.36937	-1.36103
O	1.87748	1.13791	0.02172
C	1.45766	2.24613	-0.53303
C	2.29797	3.46698	-0.14300
O	0.46859	2.34837	-1.24550
H	-4.00379	-0.07883	-1.75979
C	-1.35786	-0.12513	-1.48791
O	-1.56963	-0.73668	-2.51732
O	-0.59031	0.63475	1.15731
C	2.13512	4.56061	-1.19178
H	1.08103	4.81896	-1.32796
H	2.68422	5.46035	-0.88475
H	2.52590	4.23782	-2.16454
C	1.72513	3.94316	1.19714
H	1.82083	3.16463	1.96363
H	2.25957	4.83916	1.53972
H	0.66156	4.19177	1.09532
C	3.77346	3.11281	0.02055
H	4.19296	2.71593	-0.91337
H	4.34547	4.01077	0.28952
H	3.92189	2.36296	0.80474
C	3.71425	-1.42986	-0.69776
H	3.84411	-0.36502	-0.46329
H	4.52307	-1.99215	-0.21560
H	3.81782	-1.54934	-1.77981
C	1.24221	-2.54792	-2.47833

Frequencies

-67.4731	14.9227	31.4032
37.8431	47.0794	66.0333
73.0173	81.7746	90.6800
112.0070	123.2896	153.7593
159.1766	167.9272	175.6855
181.9620	183.4790	187.9798
198.4420	204.9845	213.0170
218.6907	222.2573	232.0124
237.3454	243.1820	259.3269
274.6334	287.6940	292.4271
296.4826	312.7315	316.9190
319.3205	323.8789	328.9831
337.5586	374.1989	392.1303
403.4710	417.8684	426.6998
430.8183	446.6593	457.1117
470.5812	526.9851	536.4959
538.4671	548.3045	572.0780
581.3796	587.3719	593.6065
600.5114	607.8481	641.3163
645.0216	673.3942	736.3713
788.1039	806.9725	811.3998
817.7625	838.8629	853.1770
906.2131	914.4114	916.6203
946.7206	951.3539	953.7264
956.7067	964.9611	969.1551
1036.0328	1038.1724	1042.2601
1044.2633	1046.1434	1048.1184
1050.1062	1075.1728	1090.6540
1091.0059	1095.6345	1106.4719
1132.7686	1178.7184	1183.9128
1189.5093	1235.9658	1241.4368
1244.5634	1266.0307	1339.1908
1355.1361	1375.2189	1377.3694
1379.6706	1383.7066	1387.9526
1393.4765	1400.3529	1402.6096
1413.4780	1428.0466	1432.4893
1438.8216	1440.7719	1449.7887
1451.1125	1452.5212	1454.8843
1458.6656	1461.8183	1463.7934
1467.8411	1469.4732	1472.0748
1473.2122	1474.8256	1476.7378
1481.0518	1487.9817	1499.5365
1501.1671	1515.7221	1522.6734
1543.1230	1594.3118	1668.1367

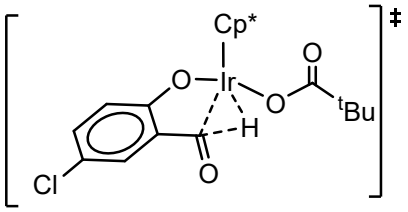
H	2.11904	-2.10243	-2.95666	1781.5798	1803.5129	2306.7591
H	1.20576	-3.61084	-2.74889	3023.8867	3026.3365	3034.7790
H	0.34843	-2.06035	-2.89001	3036.2024	3036.8391	3040.9518
C	-1.11038	-3.30984	-0.51732	3041.3402	3044.6941	3105.2279
H	-1.41265	-2.98074	-1.51602	3114.2948	3115.7777	3117.1668
H	-1.01666	-4.40339	-0.53198	3119.7584	3123.0754	3124.2443
H	-1.92044	-3.05169	0.17281	3126.4837	3130.2716	3134.9045
C	-0.26000	-2.42711	2.44507	3142.8328	3147.0304	3148.4127
H	-1.32151	-2.32628	2.19621	3149.6370	3151.2587	3152.0481
H	-0.11637	-3.38118	2.96678	3190.8828	3206.1111	3207.1632
H	-0.01265	-1.61372	3.13432			
C	2.78665	-1.38773	2.30653			
H	2.17746	-1.11068	3.17190			
H	3.47270	-2.18744	2.61532			
H	3.38431	-0.51294	2.02768			
Cl	-6.29582	0.76060	-0.20813			
Cl	-6.26797	-1.44158	-0.24324			
H	-1.08247	-1.87037	5.35490			
H	-1.25297	-2.79232	3.83883			
Ir	1.41694	-0.21556	-0.32137			
H	-1.49980	0.37953	0.32274			
C	-2.97946	-0.72280	-0.83640			
C	-3.99363	0.00621	-0.20013			
C	-3.32706	-1.69968	-1.79362			
C	-5.32310	-0.22802	-0.49568			
H	-3.72011	0.76531	0.53161			
C	-4.67627	-1.92142	-2.07765			
C	-5.66829	-1.19566	-1.43610			
H	-4.95046	-2.67602	-2.81397			
H	-6.71538	-1.37713	-1.66349			
O	-2.35238	-2.39011	-2.40731			
H	-2.74769	-3.02473	-3.01655			
Cl	-6.57374	0.68394	0.30640			

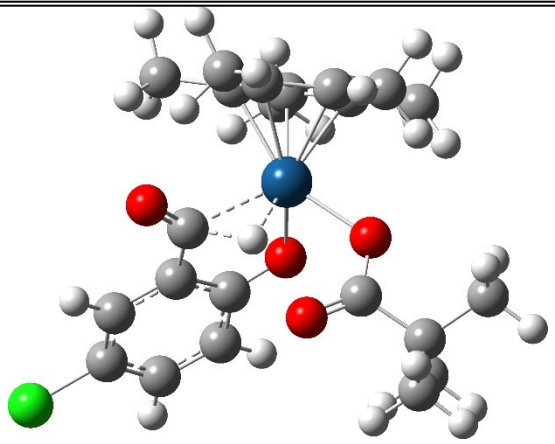
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.452722 Electronic Energy = -1720.21484135
Internal Energy (E)= -1719.73185135 Enthalpy (H)= -1719.73090735
Gibbs Free Energy (G)=-1719.82242935 Gibbs Free Energy of Solvation=-1720.92704411

St.Pt.	General Structure	Ball & Stick model

TS_3-3





Cartesian co-ordinate

Atoms	X	Y	Z
C	1.75033	-2.20391	-0.96907
C	2.69986	-1.36569	-0.30756
C	2.38866	-1.35625	1.11743
C	1.25760	-2.20788	1.32021
C	0.82668	-2.69950	0.03714
C	-2.24614	-0.19827	-0.32270
Ir	0.70566	-0.48401	-0.02403
C	-3.58940	-0.30994	-0.71483
C	-4.56121	0.20626	0.10984
C	-1.87624	0.40790	0.89648
C	-4.21811	0.84024	1.31682
C	-2.90134	0.94505	1.70837
H	-2.62512	1.43089	2.64047
H	-5.01011	1.24732	1.94108
H	-0.10972	0.30124	-1.28255
O	1.53013	1.42298	0.03788
C	0.91596	2.38668	-0.59027
C	1.41043	3.77984	-0.19193
O	-0.01973	2.23962	-1.36944
H	-3.83418	-0.79011	-1.65887
C	-1.17070	-0.69620	-1.16278
O	-1.27931	-1.35860	-2.17097
O	-0.62730	0.45244	1.26906
C	1.10713	4.77577	-1.30464
H	0.04232	4.77270	-1.55461
H	1.39474	5.78741	-0.99004
H	1.66413	4.53225	-2.21769
C	0.60561	4.13579	1.06446
H	0.78643	3.40542	1.86239
H	0.89091	5.13237	1.42601
H	-0.46923	4.14050	0.84463
C	2.90211	3.78447	0.12755
H	3.49737	3.48513	-0.74510
H	3.21739	4.79555	0.41671
H	3.13662	3.10112	0.95044
C	3.82086	-0.60124	-0.91627
H	3.77723	0.45002	-0.60578
H	4.78658	-1.01379	-0.59788
H	3.77853	-0.62839	-2.00869

Frequencies

-198.2276	23.5785	31.5928
32.9292	58.0770	67.6457
83.8881	94.5091	111.8183
123.4661	132.4889	143.0756
149.8510	155.8344	158.5344
170.9120	175.1471	182.0647
186.8156	194.8720	209.5628
211.2447	215.0188	218.2742
226.8256	229.4534	250.6609
259.3422	280.8372	283.7024
287.9490	299.2520	314.5810
316.6493	321.1041	345.4996
348.2390	357.8094	371.6648
391.9516	407.4578	414.9446
428.4544	432.8134	440.0660
471.4026	493.7762	535.3419
540.1219	542.2598	547.1980
569.2873	590.1828	596.4429
605.6739	631.3475	643.1342
652.2209	669.6107	714.2605
763.2110	793.0840	809.4732
812.9561	819.6964	829.7387
856.9504	891.0139	903.4917
921.5161	926.7986	939.6891
949.4760	951.3220	952.9128
958.4653	959.1598	1033.6583
1036.9502	1038.7523	1038.8622
1042.3850	1046.2067	1048.6753
1085.4560	1088.0608	1090.5333
1106.0755	1130.0416	1182.6369
1184.2704	1190.6474	1234.8130
1236.5761	1247.5918	1264.0188
1347.2327	1357.0633	1373.4124
1375.0210	1378.0112	1378.4852
1393.2069	1394.5222	1396.0955
1397.5354	1408.2484	1435.2244
1438.8543	1441.9841	1443.0450
1445.2414	1446.0932	1452.2170
1454.1475	1454.9482	1458.5358
1461.6481	1465.0388	1468.0227
1470.0046	1472.7122	1475.0167
1481.9034	1485.7523	1504.4611
1509.5731	1520.0576	1521.5086
1543.6039	1608.8899	1661.5231

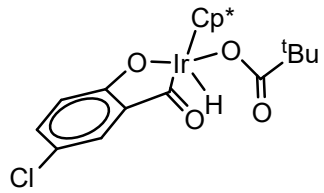
C	1.69971	-2.54748	-2.41520	1726.2927	1783.5510	1852.9548
H	2.44939	-1.99025	-2.98382	3025.8798	3029.2858	3035.2432
H	1.89016	-3.61847	-2.55895	3037.1297	3037.2400	3037.9548
H	0.71324	-2.31480	-2.83013	3044.0099	3046.7784	3106.5726
C	-0.26702	-3.67989	-0.20518	3115.2408	3115.6964	3118.0944
H	-0.69787	-3.54998	-1.20218	3119.3696	3120.6188	3127.5040
H	0.11304	-4.70655	-0.12491	3129.6282	3132.6495	3134.9973
H	-1.07717	-3.56236	0.52270	3142.1511	3146.1073	3148.6167
C	0.55630	-2.44937	2.60830	3149.0567	3149.5205	3160.3079
H	-0.52557	-2.52760	2.45693	3199.5727	3213.6168	3214.5308
H	0.90237	-3.38303	3.06897			
H	0.72729	-1.63265	3.31546			
C	3.15825	-0.60118	2.14381			
H	2.63416	-0.58168	3.10367			
H	4.14587	-1.05156	2.30680			
H	3.30537	0.43759	1.82727			
Cl	-6.25211	0.08693	-0.33553			
Cl	-6.26797	-1.44158	-0.24324			
H	-1.08247	-1.87037	5.35490			
H	-1.25297	-2.79232	3.83883			
Ir	1.41694	-0.21556	-0.32137			
H	-1.49980	0.37953	0.32274			
C	-2.97946	-0.72280	-0.83640			
C	-3.99363	0.00621	-0.20013			
C	-3.32706	-1.69968	-1.79362			
C	-5.32310	-0.22802	-0.49568			
H	-3.72011	0.76531	0.53161			
C	-4.67627	-1.92142	-2.07765			
C	-5.66829	-1.19566	-1.43610			
H	-4.95046	-2.67602	-2.81397			
H	-6.71538	-1.37713	-1.66349			
O	-2.35238	-2.39011	-2.40731			
H	-2.74769	-3.02473	-3.01655			
Cl	-6.57374	0.68394	0.30640			

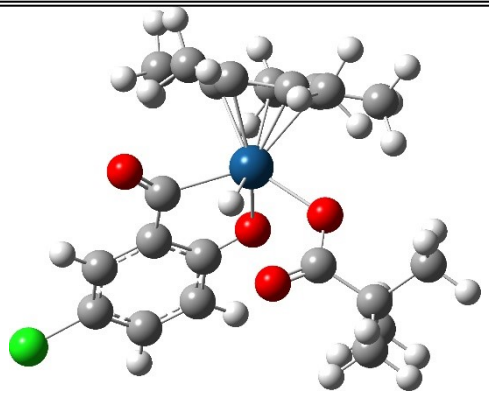
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.448860 Electronic Energy = -1720.20980032
Internal Energy (E)= -1719.73027632 Enthalpy (H)= -1719.72933232
Gibbs Free Energy (G)=-1719.82092532 Gibbs Free Energy of Solvation=-1720.91955669

St.Pt.	General Structure	Ball & Stick model

IV-3





Cartesian co-ordinate

Atoms	X	Y	Z
C	0.99152	-2.37668	-1.02128
C	2.22483	-1.68160	-0.70478
C	2.42414	-1.72175	0.73670
C	1.28791	-2.29711	1.31116
C	0.34926	-2.64551	0.23329
C	-2.33854	0.20117	-0.33243
Ir	0.47606	-0.48500	-0.06914
C	-3.61246	0.48599	-0.83740
C	-4.62834	0.75028	0.05674
C	-2.07845	0.17369	1.04829
C	-4.39407	0.72840	1.43912
C	-3.13707	0.44313	1.93741
H	-2.94496	0.42814	3.00694
H	-5.21707	0.94204	2.11729
H	1.02428	0.17083	-1.41920
O	1.04487	1.45140	0.42085
C	1.77932	2.12449	-0.41665
C	2.25894	3.46860	0.14265
O	2.11819	1.73433	-1.53372
H	-3.77493	0.49623	-1.91231
C	-1.20362	-0.12279	-1.20662
O	-1.26864	-0.23751	-2.40837
O	-0.86699	-0.10894	1.47103
C	-0.94543	-3.34730	0.45745
H	-1.57367	-3.32636	-0.43852
H	-0.78200	-4.39612	0.73683
H	-1.50805	-2.86444	1.26453
C	0.53456	-2.75488	-2.38611
H	1.22071	-3.48983	-2.82418
H	-0.46620	-3.19521	-2.36208
H	0.47799	-1.88084	-3.04410
C	3.26306	-1.24836	-1.68031
H	4.09029	-1.96984	-1.69799
H	2.84842	-1.17007	-2.68957
H	3.65859	-0.26072	-1.42124
C	3.58438	-1.09015	1.41996
H	4.53210	-1.51267	1.06408
H	3.60883	-0.01126	1.21382
H	3.53839	-1.21951	2.50469
C	0.94939	-2.42115	2.75020
H	1.79004	-2.14630	3.39289

Frequencies

11.1822	19.7416	30.1100
48.2653	59.6344	71.5644
90.7160	103.0286	114.2643
140.5039	148.5290	153.3481
159.2250	168.6797	174.1535
184.4109	189.4887	193.3048
196.3117	201.7892	214.6036
221.2944	228.5176	232.7815
234.3006	244.9539	268.2287
276.6012	277.9965	290.4832
298.3086	303.7381	320.5208
330.5467	335.0293	347.7361
348.6980	369.0026	376.8014
390.4045	414.9166	422.5384
431.1063	436.2000	447.0282
474.5817	533.1396	535.2247
535.7834	552.9458	568.6833
594.8774	613.1819	618.2189
632.8271	646.5685	647.8677
661.0255	679.9341	746.2236
788.2842	805.7080	811.0534
813.9736	824.6514	833.5378
869.4661	908.4585	909.5578
932.5788	942.5648	947.3552
948.7067	951.8933	953.7441
954.9258	967.8025	1027.4771
1034.8891	1036.3012	1045.0119
1046.2195	1048.8001	1054.2253
1083.9913	1087.6365	1088.8142
1106.1421	1125.1800	1174.5655
1183.0057	1189.9061	1236.9771
1240.3870	1246.7225	1268.2796
1338.5828	1360.1395	1364.0014
1373.3845	1374.5700	1380.0028
1388.6818	1392.1849	1394.7685
1397.9048	1414.6346	1429.3192
1433.4400	1435.9764	1442.4289
1447.6074	1448.8828	1449.7622
1452.5871	1455.0171	1457.3664
1458.5488	1462.7558	1463.5990
1470.5863	1471.1772	1475.5513
1477.1320	1483.7120	1490.6074
1507.1418	1511.7422	1517.5942
1586.3056	1619.1718	1655.5225
1727.9408	1813.7606	2073.8590

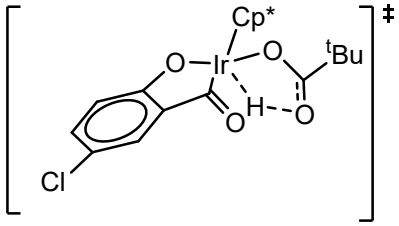
H	0.10572	-1.75636	2.98425	3018.9710	3031.7112	3032.1271
H	0.64524	-3.44584	2.99604	3034.4779	3037.1248	3037.5015
C	3.32237	3.15329	1.19962	3042.2173	3043.8731	3101.4690
H	3.72261	4.08516	1.61962	3103.2258	3109.0057	3113.7416
H	2.89891	2.55850	2.01730	3119.5273	3123.1998	3130.0532
H	4.16166	2.59845	0.75669	3131.1688	3132.7140	3140.6448
C	2.87345	4.30224	-0.97482	3140.6662	3146.7052	3148.1428
H	2.13727	4.51710	-1.75752	3150.0032	3150.9114	3154.0909
H	3.23602	5.25626	-0.57068	3194.2026	3209.0765	3211.7259
H	3.71162	3.77983	-1.44715			
C	1.09830	4.22376	0.78696			
H	1.45503	5.18489	1.17972			
H	0.30848	4.43256	0.05507			
H	0.65682	3.65164	1.60813			
Cl	-6.23876	1.12282	-0.52719			
Cl	-6.26797	-1.44158	-0.24324			
H	-1.08247	-1.87037	5.35490			
H	-1.25297	-2.79232	3.83883			
Ir	1.41694	-0.21556	-0.32137			
H	-1.49980	0.37953	0.32274			
C	-2.97946	-0.72280	-0.83640			
C	-3.99363	0.00621	-0.20013			
C	-3.32706	-1.69968	-1.79362			
C	-5.32310	-0.22802	-0.49568			
H	-3.72011	0.76531	0.53161			
C	-4.67627	-1.92142	-2.07765			
C	-5.66829	-1.19566	-1.43610			
H	-4.95046	-2.67602	-2.81397			
H	-6.71538	-1.37713	-1.66349			
O	-2.35238	-2.39011	-2.40731			
H	-2.74769	-3.02473	-3.01655			
Cl	-6.57374	0.68394	0.30640			

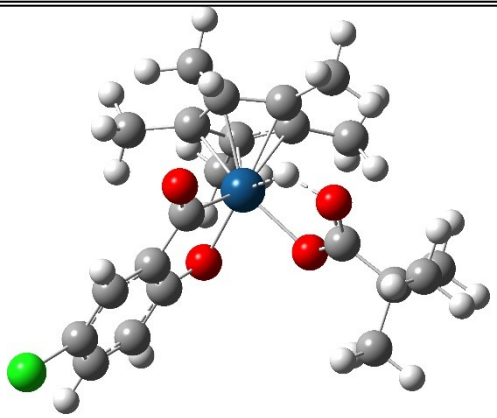
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.450933 Electronic Energy = -1720.21743674
Internal Energy (E)= -1719.73563074 Enthalpy (H)= -1719.73468774
Gibbs Free Energy (G)=-1719.82803874 Gibbs Free Energy of Solvation=-1720.92836427

St.Pt.	General Structure	Ball & Stick model

TS_3-4





Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.17525	-2.21306	1.17458
C	-2.34565	-1.48280	0.74369
C	-2.51186	-1.67655	-0.69293
C	-1.40497	-2.38855	-1.16166
C	-0.51769	-2.66644	-0.02202
C	2.31531	0.13105	0.30512
Ir	-0.51276	-0.49389	0.01369
C	3.58459	0.41714	0.82025
C	4.62963	0.58479	-0.06395
C	2.08918	0.00380	-1.07646
C	4.42866	0.46655	-1.44669
C	3.17631	0.17947	-1.95513
H	3.01014	0.08891	-3.02534
H	5.27374	0.60613	-2.11688
H	-1.03927	0.43113	1.28556
O	-1.00795	1.45629	-0.60426
C	-1.51629	2.21588	0.30372
C	-2.00566	3.57432	-0.18913
O	-1.65752	1.87042	1.49068
H	3.72025	0.50412	1.89554
C	1.14298	-0.08130	1.16544
O	1.17209	-0.08562	2.37586
O	0.88200	-0.27863	-1.50851
C	0.72936	-3.47848	-0.10842
H	1.35799	-3.33490	0.77614
H	0.50124	-4.54876	-0.19574
H	1.32421	-3.18727	-0.98168
C	-0.77886	-2.45454	2.58825
H	-1.52121	-3.09157	3.08453
H	0.19353	-2.95072	2.65138
H	-0.68702	-1.51287	3.14064
C	-3.37783	-0.88528	1.63657
H	-4.18369	-1.60781	1.82212
H	-2.94938	-0.58912	2.59842
H	-3.82197	0.01125	1.19022
C	-3.60819	-1.04862	-1.47903
H	-4.59010	-1.41475	-1.15367
H	-3.60234	0.04176	-1.34235
H	-3.50809	-1.24724	-2.54959
C	-1.02967	-2.68371	-2.56831

Frequencies

-319.8117	19.5398	31.6874
40.1012	54.6574	71.2226
82.5111	101.5312	106.2509
139.1360	144.5249	147.4426
150.7457	161.6117	166.5917
172.8620	185.1469	198.7793
203.3064	210.3522	213.4183
221.1985	230.0931	232.9039
234.9665	243.3101	246.6536
264.6994	280.3400	289.6293
299.0575	306.2800	314.1692
327.9555	331.4304	334.2948
347.8454	351.7407	373.2777
392.3633	414.1284	421.7338
430.5658	437.3487	444.5812
475.8478	502.2960	533.9825
535.9568	538.7581	552.1597
593.6165	612.6175	621.2761
622.1680	636.7664	646.4852
655.2173	660.5868	690.0968
748.7933	792.3421	810.1831
812.2346	833.1358	836.3994
863.7353	890.9269	910.1809
939.4432	946.3473	949.6750
953.6119	954.3368	955.8360
957.4973	961.1055	1034.0811
1038.7530	1042.0058	1045.2866
1047.4278	1052.3882	1058.0455
1083.9716	1087.0601	1088.2144
1105.5904	1125.5968	1175.1611
1181.7364	1189.1013	1236.3194
1241.6851	1253.5616	1267.5097
1340.2602	1367.2306	1372.9981
1377.8478	1380.0891	1380.2774
1389.0019	1395.6719	1399.8920
1400.5446	1424.1113	1428.1182
1437.8715	1438.6692	1443.1655
1448.5531	1451.0342	1453.4176
1455.6652	1456.3982	1459.5038
1459.7321	1464.0681	1465.6059
1466.9134	1469.2295	1474.1803
1480.8576	1483.4351	1501.7202
1503.6574	1511.7993	1516.0956
1585.3149	1591.8249	1621.0729

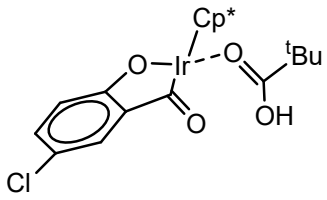
H	-1.83464	-2.43996	-3.26704	1655.8470	1769.9451	1816.7794
H	-0.14602	-2.08916	-2.84330	3015.9542	3019.6772	3029.6247
H	-0.77343	-3.74259	-2.69412	3034.2431	3037.0529	3038.2179
C	-3.24196	3.30209	-1.05404	3040.2601	3045.1274	3098.4515
H	-3.66025	4.24951	-1.41674	3098.7441	3106.4835	3116.3150
H	-2.98714	2.68201	-1.92121	3117.2304	3119.5165	3125.4894
H	-4.02322	2.79166	-0.47354	3127.2661	3129.5626	3140.0199
C	-2.38246	4.46211	0.98964	3142.6849	3145.3470	3147.9027
H	-1.51892	4.64930	1.63732	3149.8743	3150.0435	3156.1601
H	-2.75306	5.42715	0.62142	3196.8017	3205.9782	3210.5312
H	-3.16197	3.99915	1.60347			
C	-0.92103	4.24259	-1.03297			
H	-1.28868	5.20578	-1.40949			
H	-0.01995	4.43627	-0.43853			
H	-0.63793	3.61775	-1.88522			
Cl	6.23700	0.95422	0.53318			
Cl	-6.26797	-1.44158	-0.24324			
H	-1.08247	-1.87037	5.35490			
H	-1.25297	-2.79232	3.83883			
Ir	1.41694	-0.21556	-0.32137			
H	-1.49980	0.37953	0.32274			
C	-2.97946	-0.72280	-0.83640			
C	-3.99363	0.00621	-0.20013			
C	-3.32706	-1.69968	-1.79362			
C	-5.32310	-0.22802	-0.49568			
H	-3.72011	0.76531	0.53161			
C	-4.67627	-1.92142	-2.07765			
C	-5.66829	-1.19566	-1.43610			
H	-4.95046	-2.67602	-2.81397			
H	-6.71538	-1.37713	-1.66349			
O	-2.35238	-2.39011	-2.40731			
H	-2.74769	-3.02473	-3.01655			
Cl	-6.57374	0.68394	0.30640			

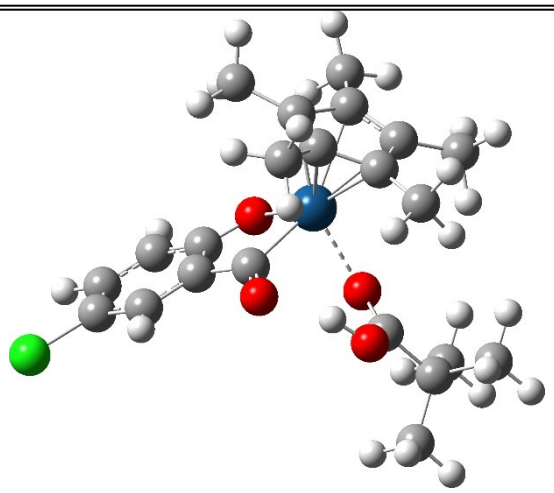
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.449259 Electronic Energy = -1720.21689034
Internal Energy (E)= -1719.73737434 Enthalpy (H)= -1719.73643034
Gibbs Free Energy (G)=-1719.82699334 Gibbs Free Energy of Solvation=-1720.92444819

St.Pt.	General Structure	Ball & Stick model

V-3





Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.98114	-2.06537	1.41697
C	-2.15354	-1.31323	1.07432
C	-2.54684	-1.69089	-0.29088
C	-1.58451	-2.55865	-0.81002
C	-0.53462	-2.72826	0.20659
C	2.30353	0.23038	0.20969
Ir	-0.44407	-0.63284	-0.09998
C	3.51991	0.67643	0.74336
C	4.63065	0.68603	-0.07020
C	2.18319	-0.17368	-1.14217
C	4.54313	0.28055	-1.41262
C	3.34248	-0.13680	-1.95009
H	3.26759	-0.43943	-2.99150
H	5.43961	0.30531	-2.02821
H	-0.55231	1.61708	1.67828
O	-1.05058	1.40911	-0.69153
C	-1.42710	2.29773	0.08309
C	-2.24871	3.47257	-0.41307
O	-1.20855	2.31149	1.37060
H	3.56335	1.00244	1.77991
C	1.04039	0.23553	0.93255
O	0.87455	0.78360	2.03368
O	1.01982	-0.54074	-1.60490
C	0.63481	-3.63922	0.05731
H	1.41448	-3.40685	0.79055
H	0.34691	-4.69125	0.18509
H	1.08174	-3.52559	-0.93664
C	-0.33568	-2.10848	2.75686
H	-0.88479	-2.77927	3.42932
H	0.69712	-2.46522	2.68893
H	-0.30073	-1.11004	3.20598
C	-2.99049	-0.51518	2.01528
H	-3.80528	-1.11976	2.43716
H	-2.39111	-0.13478	2.84929
H	-3.44772	0.34966	1.51910
C	-3.72431	-1.10451	-0.98768
H	-4.66024	-1.38891	-0.48916
H	-3.67478	-0.00647	-0.98318

Frequencies

22.4986	41.5952	61.3718
65.7985	75.5771	81.0349
101.5729	120.8198	124.4874
135.0278	145.4749	154.4271
158.5175	161.9580	168.9678
175.7581	179.9019	190.5603
201.9352	206.7917	219.6653
230.6513	238.8125	249.5675
257.4923	277.3835	287.4748
289.2708	297.9627	307.5608
311.7111	316.7373	325.3800
328.4663	335.9091	340.6287
357.4154	370.2823	390.3778
397.6847	408.4007	413.1420
422.7748	431.8432	461.7291
486.7414	533.0041	534.0070
537.9104	546.2828	554.1676
593.8669	604.1980	611.2612
624.6509	639.8558	652.9445
670.6153	697.4792	753.6567
781.2911	787.1060	802.2076
809.8154	836.7902	868.6583
895.1665	909.0667	919.5898
950.5207	953.0473	953.5243
959.1468	960.2108	960.2966
964.4518	1029.4590	1041.1133
1043.4385	1044.6053	1047.6126
1048.1005	1051.0751	1077.9993
1085.9602	1090.8967	1104.2853
1127.9550	1176.7618	1184.1618
1190.6288	1229.2071	1238.7439
1248.1360	1260.8163	1333.4424
1348.6580	1368.5439	1376.0127
1381.9755	1386.3560	1391.1329
1391.2519	1403.1493	1403.8231
1417.9279	1428.1897	1434.2706
1445.6682	1449.7805	1451.4943
1452.8995	1455.2960	1455.4905
1458.7006	1459.2361	1461.8503
1467.4326	1468.1323	1470.2645
1473.4785	1477.6340	1482.7510
1484.7284	1491.2122	1506.5123

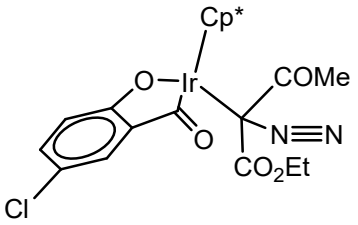
H	-3.78340	-1.42650	-2.03139	1511.0333	1516.1263	1519.5498
C	-1.48953	-3.12252	-2.18371	1594.6950	1604.8717	1657.8776
H	-2.32544	-2.80326	-2.81319	1665.1020	1742.3163	3022.8659
H	-0.56182	-2.79882	-2.67217	3029.2482	3030.5455	3033.1600
H	-1.48510	-4.21995	-2.15863	3033.3809	3038.7521	3042.4335
C	-3.63947	3.35405	0.22401	3048.4019	3089.8415	3103.1868
H	-4.26693	4.18601	-0.11775	3105.6816	3113.1721	3115.6473
H	-4.13482	2.41998	-0.07548	3123.8344	3126.8416	3135.2513
H	-3.58625	3.38729	1.31726	3136.9976	3138.9522	3140.3733
C	-1.58516	4.77915	0.02990	3141.9069	3143.0936	3145.7845
H	-0.58070	4.88013	-0.39825	3147.4121	3149.8270	3153.6652
H	-2.18556	5.62737	-0.32059	3186.9518	3202.3708	3204.9306
H	-1.50246	4.84072	1.11916			
C	-2.36834	3.42830	-1.93098			
H	-2.97186	4.27768	-2.27261			
H	-1.38634	3.48666	-2.41227			
H	-2.84888	2.50387	-2.26931			
Cl	6.18267	1.22054	0.55617			
Cl	-6.26797	-1.44158	-0.24324			
H	-1.08247	-1.87037	5.35490			
H	-1.25297	-2.79232	3.83883			
Ir	1.41694	-0.21556	-0.32137			
H	-1.49980	0.37953	0.32274			
C	-2.97946	-0.72280	-0.83640			
C	-3.99363	0.00621	-0.20013			
C	-3.32706	-1.69968	-1.79362			
C	-5.32310	-0.22802	-0.49568			
H	-3.72011	0.76531	0.53161			
C	-4.67627	-1.92142	-2.07765			
C	-5.66829	-1.19566	-1.43610			
H	-4.95046	-2.67602	-2.81397			
H	-6.71538	-1.37713	-1.66349			
O	-2.35238	-2.39011	-2.40731			
H	-2.74769	-3.02473	-3.01655			
Cl	-6.57374	0.68394	0.30640			

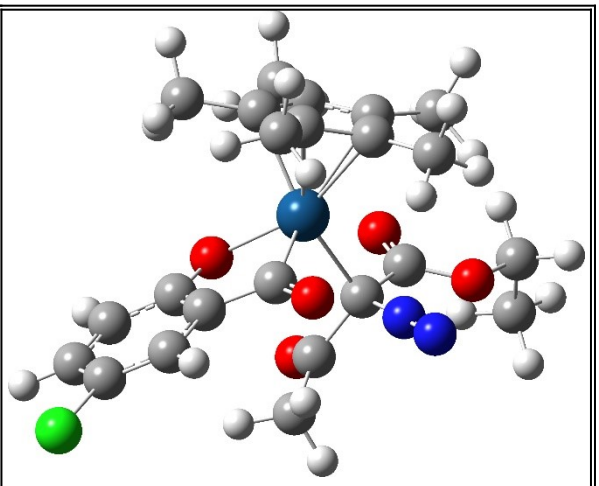
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.455379 Electronic Energy = -1720.25157292
Internal Energy (E)= -1719.76589792 Enthalpy (H)= -1719.76495392
Gibbs Free Energy (G)=-1719.85480592 Gibbs Free Energy of Solvation=-1720.94254088

St.Pt.	General Structure	Ball & Stick model

V'-3





Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.19155	-2.71278	0.57379
C	-1.41852	-2.14034	1.05794
C	-2.26695	-1.88057	-0.10297
C	-1.53834	-2.15091	-1.27324
C	-0.21069	-2.60809	-0.86124
C	2.49381	0.19201	0.26122
Ir	-0.28181	-0.59533	-0.03648
C	2.18852	0.40985	-1.10136
C	3.22698	0.84351	-1.95570
C	3.77780	0.40986	0.77266
C	4.49757	1.04071	-1.45009
C	4.77011	0.82474	-0.09030
H	3.96547	0.25371	1.83278
H	5.30255	1.37178	-2.10270
H	3.00277	1.02462	-3.00390
C	-1.13527	1.42083	0.24844
C	-2.55466	1.49417	-0.26883
C	-0.23768	2.52058	-0.36922
O	-0.54404	2.98267	-1.43626
N	-1.09470	1.43170	1.63631
N	-0.99335	1.40933	2.75649
C	-3.68057	-1.42857	-0.00807
H	-4.04150	-1.00812	-0.95123
H	-4.32521	-2.27680	0.25739
H	-3.81057	-0.67208	0.77629
C	-1.80557	-2.04247	2.49415
H	-2.65326	-1.36158	2.63506
H	-2.09280	-3.01666	2.91231
H	-0.96522	-1.65243	3.08383
C	0.88895	-3.28130	1.42429
H	0.98431	-2.72496	2.36245
H	0.67064	-4.32947	1.66633
H	1.86116	-3.24541	0.92122
C	0.86166	-3.03070	-1.80351
H	1.82129	-3.15308	-1.29069
H	0.60807	-3.98318	-2.28656
H	1.00212	-2.27701	-2.58650
C	-1.96522	-1.93796	-2.68419

Frequencies

18.3677	25.7075	36.3789
50.9811	70.4543	79.3879
83.7297	90.7587	103.5241
109.2380	125.2950	131.2903
137.7850	144.8290	147.9051
153.5822	161.1317	166.2820
182.5181	186.8564	194.0690
200.0559	202.6229	206.7200
214.8361	219.1434	219.6806
229.2510	234.4247	239.0834
264.8658	267.1547	282.6697
297.5322	316.5093	329.2733
333.6255	340.0224	341.1833
356.6352	361.2405	367.8811
382.6204	385.5241	406.1936
411.7231	433.4992	439.4790
455.1461	481.3511	493.9596
503.6264	529.2655	534.0021
534.4096	538.8605	549.9038
587.3079	594.6237	599.1994
610.2677	624.5894	636.1553
655.6269	671.8064	688.0291
752.6251	753.6898	778.5979
810.7679	814.1615	822.2714
833.4756	866.8526	876.6599
899.3151	935.2639	953.2108
956.2321	958.2685	969.8343
983.0098	1017.0465	1037.1647
1044.6708	1046.6634	1050.1696
1051.1644	1055.9005	1080.8687
1088.5909	1090.3420	1094.5444
1110.3360	1120.7795	1124.9575
1169.9593	1175.3589	1182.9615
1187.4818	1195.1504	1232.9888
1263.4334	1321.6837	1345.2418
1368.0213	1377.9138	1378.9324
1380.0682	1385.0719	1397.4978
1404.8427	1405.4244	1412.6342
1431.4268	1434.8136	1439.1324
1446.4109	1448.2556	1452.0492
1453.0169	1459.0599	1462.3986
1465.9393	1466.8144	1471.7487
1474.3822	1477.0539	1487.5765

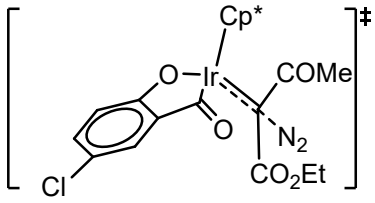
H	-2.35863	-2.85803	-3.13729	1488.6686	1493.2090	1506.0857
H	-2.73180	-1.15950	-2.75342	1508.2693	1510.7946	1515.6262
H	-1.11884	-1.60182	-3.29391	1568.6720	1606.0952	1656.2654
C	1.33773	-0.16055	1.09588	1739.5246	1854.5008	1894.1991
O	0.96062	0.25661	-1.52481	2256.7245	3026.2216	3030.9720
O	1.35876	-0.21139	2.31974	3034.5886	3037.8687	3038.4285
O	-2.85712	1.26563	-1.40839	3053.8257	3054.3661	3076.5892
C	-4.76945	2.10759	0.28437	3101.9853	3105.5151	3110.9882
H	-5.35523	1.99692	1.20132	3117.8242	3120.4168	3127.6001
H	-5.06328	1.32754	-0.42618	3134.6920	3141.2891	3141.3554
O	-3.40618	1.87227	0.69871	3144.2024	3144.7336	3146.9527
C	-4.90486	3.48315	-0.31902	3150.9319	3159.9553	3175.8617
H	-4.30871	3.56012	-1.23344	3190.1809	3201.3095	3206.0769
H	-5.95082	3.68186	-0.57381			
H	-4.57148	4.25107	0.38625			
C	0.94055	3.01649	0.42183			
H	1.79833	3.09172	-0.25432			
H	0.70321	4.02978	0.76731			
H	1.22135	2.40272	1.28030			
Cl	6.39997	1.09526	0.50572			
H	-1.25297	-2.79232	3.83883			
Ir	1.41694	-0.21556	-0.32137			
H	-1.49980	0.37953	0.32274			
C	-2.97946	-0.72280	-0.83640			
C	-3.99363	0.00621	-0.20013			
C	-3.32706	-1.69968	-1.79362			
C	-5.32310	-0.22802	-0.49568			
H	-3.72011	0.76531	0.53161			
C	-4.67627	-1.92142	-2.07765			
C	-5.66829	-1.19566	-1.43610			
H	-4.95046	-2.67602	-2.81397			
H	-6.71538	-1.37713	-1.66349			
O	-2.35238	-2.39011	-2.40731			
H	-2.74769	-3.02473	-3.01655			
Cl	-6.57374	0.68394	0.30640			

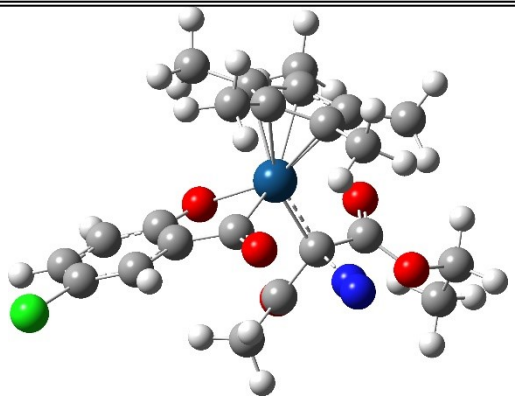
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.451025 Electronic Energy = -1941.67714017
Internal Energy (E)= -1941.19203617 Enthalpy (H)= -1941.19109217
Gibbs Free Energy (G)=-1941.29008517 Gibbs Free Energy of Solvation=-1942.54651426

St.Pt.	General Structure	Ball & Stick model

TS_3-5





Cartesian co-ordinate

Atoms	X	Y	Z
C	0.13305	-2.75099	0.42287
C	-1.04336	-2.29223	1.12098
C	-2.06570	-2.02474	0.12244
C	-1.51042	-2.23105	-1.16830
C	-0.12882	-2.63145	-0.97704
C	2.45114	0.32263	0.24262
Ir	-0.28872	-0.58029	-0.05521
C	2.13995	0.51521	-1.12191
C	3.17022	0.95056	-1.98467
C	3.73412	0.56184	0.74802
C	4.44055	1.16638	-1.48591
C	4.72025	0.97111	-0.12451
H	3.92755	0.42425	1.80954
H	5.23978	1.49640	-2.14601
H	2.94169	1.11418	-3.03473
C	-1.23103	1.21460	0.21117
C	-2.69090	1.31011	-0.19296
C	-0.53368	2.47562	-0.33470
O	-0.99435	2.97921	-1.33328
N	-1.24344	1.42394	1.83592
N	-0.92269	1.21706	2.88820
C	-3.47992	-1.68647	0.44734
H	-4.00316	-1.26317	-0.41382
H	-4.01694	-2.58796	0.76934
H	-3.54397	-0.96317	1.27113
C	-1.21769	-2.27563	2.60113
H	-2.14189	-1.76064	2.88677
H	-1.26639	-3.29186	3.01383
H	-0.38399	-1.74798	3.08248
C	1.38287	-3.24048	1.06933
H	1.54233	-2.75524	2.03786
H	1.32934	-4.32350	1.24049
H	2.26679	-3.04264	0.45339
C	0.82661	-2.90434	-2.08573
H	1.85596	-2.97668	-1.72011
H	0.57841	-3.84447	-2.59466
H	0.79627	-2.09783	-2.82713
C	-2.17828	-2.07326	-2.48968
H	-2.53955	-3.03559	-2.87778
H	-3.02243	-1.38180	-2.42667

Frequencies

-400.5922	17.8949	32.1004
40.7618	56.4677	61.3532
71.9910	73.1581	87.1705
95.7648	115.9362	121.5605
134.8469	140.1917	144.7738
152.1346	156.7455	166.1937
180.3457	180.5206	184.9033
194.5456	199.0447	202.0493
214.8512	216.9323	218.7376
227.5989	231.7732	235.7155
254.3910	271.8009	278.5072
290.4042	297.8474	306.1924
317.5761	324.9140	330.0616
331.8576	341.3602	343.2703
357.1895	359.3687	402.9785
407.4907	411.1660	422.6476
433.6535	437.1789	459.0589
481.3860	518.4705	533.1152
534.3205	538.6381	543.6215
546.8359	590.1448	597.2253
603.8276	623.4850	638.5080
655.6523	668.2957	683.3787
703.5864	749.6658	756.0717
808.9768	811.5413	813.1437
831.6245	865.6320	890.1785
896.6961	902.2511	933.4224
952.9620	954.0014	956.2365
960.8570	1015.5705	1022.4654
1035.7081	1042.2334	1043.9960
1046.4395	1049.7991	1080.8088
1083.2381	1087.0148	1088.4092
1106.9980	1124.2753	1125.3255
1175.5149	1179.7224	1186.2162
1188.2372	1198.7342	1232.2833
1281.3317	1316.0683	1344.0107
1371.6550	1378.1393	1380.1948
1380.7494	1384.3938	1396.4640
1400.3886	1401.4715	1413.2199
1433.0366	1433.9472	1441.5543
1447.4505	1451.2895	1455.2212
1458.2791	1463.7268	1465.6576
1466.1970	1468.7327	1473.7132
1476.8417	1478.6469	1479.9106
1487.5397	1494.8436	1496.2762
1501.2013	1510.6185	1521.5971

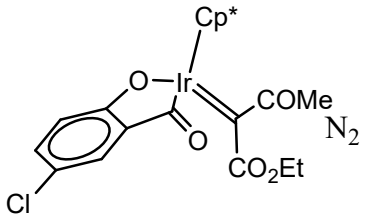
H	-1.48219	-1.65708	-3.22665	1548.2505	1605.6657	1654.8480
C	1.30150	-0.03304	1.08314	1730.7731	1832.1722	1871.8390
O	0.91397	0.33468	-1.54046	2253.4291	3025.5179	3029.7620
O	1.32343	-0.04782	2.30734	3032.5579	3036.2060	3039.5645
O	-3.09739	0.87537	-1.23942	3053.3343	3057.1381	3074.3336
C	-4.78847	2.26242	0.29362	3099.9225	3102.5320	3112.8534
H	-5.32377	2.43625	1.23140	3114.7488	3119.7476	3125.6630
H	-5.20366	1.37462	-0.19697	3134.4177	3137.3726	3140.3996
O	-3.43369	1.97525	0.69974	3143.6305	3145.9028	3153.9773
C	-4.81182	3.46818	-0.61219	3158.9090	3159.7790	3184.2507
H	-4.24669	3.27079	-1.52840	3191.3389	3203.4543	3207.7419
H	-5.84222	3.71622	-0.88688			
H	-4.37040	4.33529	-0.11050			
C	0.66884	3.04754	0.36008			
H	1.48632	3.10775	-0.36722			
H	0.42412	4.07225	0.66056			
H	1.01624	2.48595	1.22878			
Cl	6.34981	1.26013	0.46070			
H	-1.25297	-2.79232	3.83883			
Ir	1.41694	-0.21556	-0.32137			
H	-1.49980	0.37953	0.32274			
C	-2.97946	-0.72280	-0.83640			
C	-3.99363	0.00621	-0.20013			
C	-3.32706	-1.69968	-1.79362			
C	-5.32310	-0.22802	-0.49568			
H	-3.72011	0.76531	0.53161			
C	-4.67627	-1.92142	-2.07765			
C	-5.66829	-1.19566	-1.43610			
H	-4.95046	-2.67602	-2.81397			
H	-6.71538	-1.37713	-1.66349			
O	-2.35238	-2.39011	-2.40731			
H	-2.74769	-3.02473	-3.01655			
Cl	-6.57374	0.68394	0.30640			

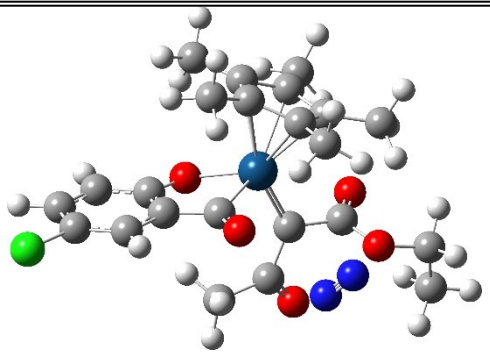
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.448863 Electronic Energy = -1941.67108018
Internal Energy (E)= -1941.18818918 Enthalpy (H)= -1941.18724518
Gibbs Free Energy (G)=-1941.28606318 Gibbs Free Energy of Solvation=-1942.53794957

St.Pt.	General Structure	Ball & Stick model

VI-3





Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.49897	2.39271	0.92702
C	0.70594	1.87049	1.53126
C	1.77620	1.99484	0.56400
C	1.21999	2.55027	-0.63768
C	-0.17774	2.78603	-0.40378
C	-2.44079	-0.58857	0.16436
Ir	0.25665	0.47028	-0.14186
C	-2.32466	-0.19141	-1.17957
C	-3.48085	-0.19389	-1.98412
C	-3.65977	-1.01049	0.70698
C	-4.68715	-0.60007	-1.44510
C	-4.77432	-1.00769	-0.10540
H	-3.70801	-1.32005	1.74813
H	-5.58530	-0.60910	-2.05805
H	-3.40178	0.11232	-3.02402
C	1.35663	-1.01505	-0.57662
C	2.84168	-0.82967	-0.65652
C	1.02926	-2.39786	-1.07609
O	1.93971	-3.04360	-1.57301
N	1.35022	-2.53311	2.14464
N	1.74530	-1.93347	2.98440
C	3.22419	1.81204	0.85731
H	3.79749	1.64197	-0.05896
H	3.61890	2.71091	1.34799
H	3.39597	0.96237	1.52795
C	0.85307	1.47341	2.95812
H	1.81388	0.98104	3.13675
H	0.79900	2.35756	3.60675
H	0.06585	0.77343	3.25723
C	-1.81352	2.53588	1.61709
H	-1.93742	1.77235	2.39258
H	-1.89393	3.51801	2.10071
H	-2.65435	2.43420	0.92236
C	-1.13122	3.27722	-1.43516
H	-2.15393	3.32364	-1.04948
H	-0.85194	4.27968	-1.78072
H	-1.13498	2.60340	-2.30165
C	1.96115	2.85493	-1.89227
H	2.44888	3.83756	-1.83415
H	2.72822	2.09761	-2.08405
H	1.28460	2.86804	-2.75293
C	-1.20100	-0.52109	0.94870

Frequencies

24.4589	28.3216	36.9410
50.6980	64.0030	75.0848
81.6601	89.5123	93.3095
101.5125	120.5038	122.1033
129.9297	141.1312	146.7574
153.2183	156.0689	159.7813
171.4641	176.6668	180.6787
188.9794	190.4895	197.5785
203.3676	214.2976	219.8953
227.1598	233.2642	238.0933
242.9136	275.1694	284.4973
290.4777	295.4096	297.7635
309.3548	315.0011	320.8661
331.8487	334.9689	346.6905
352.1080	361.3249	372.6654
377.9673	401.7782	412.8177
429.5772	434.1950	441.2401
474.1250	480.7500	531.8837
538.0397	541.0057	550.0066
574.5719	588.5817	603.4218
604.1010	631.1273	651.7312
657.8178	673.1522	685.4405
730.3606	747.6950	757.6211
812.9417	815.5860	818.4047
838.5352	862.1436	885.0180
907.2451	921.0161	956.4189
960.6703	963.3911	967.3725
1009.4423	1033.0714	1037.9999
1042.5576	1047.0647	1048.4671
1050.5907	1051.3400	1082.7548
1088.1544	1095.4394	1107.2960
1112.2947	1125.5146	1127.0939
1177.9914	1180.3554	1187.2032
1188.8116	1230.8790	1244.2510
1295.3656	1326.2998	1335.3652
1378.8039	1380.8453	1382.9371
1384.0287	1387.1493	1394.0102
1402.9872	1406.2972	1419.2779
1439.7314	1440.2638	1446.1050
1449.0012	1453.5680	1454.5155
1462.6402	1463.0125	1465.9911
1471.5668	1472.0947	1473.6264
1478.4919	1482.0551	1485.4451
1492.6479	1496.9011	1501.7067
1504.9340	1507.3385	1518.3425
1536.0578	1615.7410	1652.8088

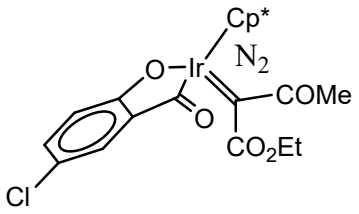
O	-1.14756	0.14912	-1.65411	1779.2026	1801.9678	1819.2934
O	-1.09581	-0.87121	2.10243	2469.7860	3034.4297	3036.0776
O	3.39177	-0.20924	-1.54110	3038.0366	3039.1990	3042.2000
C	4.91366	-1.45220	0.28509	3054.5187	3060.1253	3066.8347
H	5.24147	-1.59602	1.31921	3114.0685	3117.8647	3120.1655
H	5.28008	-0.48306	-0.07272	3121.5001	3123.0176	3128.2887
O	3.47598	-1.41189	0.36585	3136.9603	3144.0685	3145.0837
C	5.36061	-2.57735	-0.61490	3147.9748	3149.2953	3153.1498
H	5.03256	-2.39908	-1.64298	3162.3574	3167.6814	3175.3746
H	6.45307	-2.65478	-0.60703	3191.9801	3205.9612	3208.4001
H	4.94048	-3.53053	-0.27967			
C	-0.35657	-2.94705	-0.98037			
H	-1.04137	-2.33475	-1.57651			
H	-0.35324	-3.97175	-1.35756			
H	-0.71599	-2.93671	0.05500			
Cl	-6.32861	-1.50480	0.53243			
H	-1.25297	-2.79232	3.83883			
Ir	1.41694	-0.21556	-0.32137			
H	-1.49980	0.37953	0.32274			
C	-2.97946	-0.72280	-0.83640			
C	-3.99363	0.00621	-0.20013			
C	-3.32706	-1.69968	-1.79362			
C	-5.32310	-0.22802	-0.49568			
H	-3.72011	0.76531	0.53161			
C	-4.67627	-1.92142	-2.07765			
C	-5.66829	-1.19566	-1.43610			
H	-4.95046	-2.67602	-2.81397			
H	-6.71538	-1.37713	-1.66349			
O	-2.35238	-2.39011	-2.40731			
H	-2.74769	-3.02473	-3.01655			
Cl	-6.57374	0.68394	0.30640			

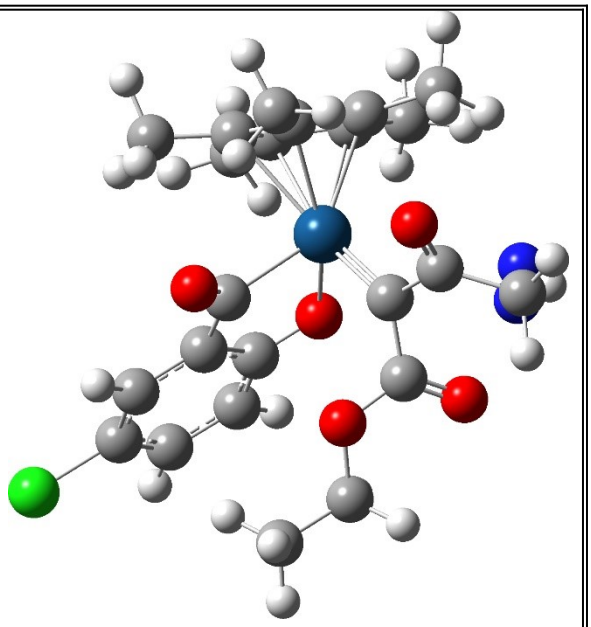
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.450296 Electronic Energy = -1941.72063755
Internal Energy (E)= -1941.23542455 Enthalpy (H)= -1941.23448055
Gibbs Free Energy (G)=-1941.33522455 Gibbs Free Energy of Solvation=-1942.58727243

St.Pt.	General Structure	Ball & Stick model

VI'-3





Cartesian co-ordinate

Atoms	X	Y	Z
C	1.09649	-2.61164	-0.32074
C	2.13706	-1.85628	-0.99414
C	2.89764	-1.17420	0.01898
C	2.27121	-1.44258	1.29547
C	1.17540	-2.34439	1.07036
C	-2.08840	-0.49712	-0.27695
Ir	0.82363	-0.31044	-0.02919
C	-1.83216	0.03968	0.99982
C	-2.92374	0.23406	1.87312
C	-3.38191	-0.83605	-0.69114
C	-4.19864	-0.11301	1.46947
C	-4.42490	-0.65038	0.19268
H	-3.53921	-1.23712	-1.68974
H	-5.04308	0.02534	2.14072
H	-2.73924	0.65623	2.85786
C	0.99390	1.45546	-0.70823
C	2.17837	1.91459	-1.49162
C	0.02001	2.50971	-0.30576
C	-2.21402	3.21559	-0.32125
H	-2.33503	3.04029	0.75675
H	-1.85991	4.24503	-0.45055
C	-3.47582	2.93280	-1.08993
H	-4.27382	3.60527	-0.75939
H	-3.32017	3.08436	-2.16291
H	-3.80925	1.90111	-0.93299
O	-1.19985	2.31302	-0.80120
O	0.32886	3.44036	0.40960
C	4.17302	-0.43537	-0.17705
H	4.29871	0.36049	0.56659
H	5.02229	-1.12308	-0.07379
H	4.22402	0.01618	-1.17077
C	2.43175	-1.95179	-2.45042
H	3.12877	-1.17487	-2.76924
H	2.85289	-2.93621	-2.69480

Frequencies

29.8473	31.1268	37.1341
52.4440	59.2953	62.1180
74.4024	85.8627	99.5464
105.7965	109.3202	122.4073
130.1614	135.1096	140.8645
146.1898	157.1445	163.1781
168.1040	172.2304	176.5510
186.6622	194.3443	204.2613
211.3930	216.4347	223.0657
230.1131	234.5622	239.1473
239.8591	244.7162	254.2517
273.9324	282.6351	292.0139
294.2915	304.0594	314.0592
320.3494	326.3214	338.4687
340.8372	348.0952	361.7764
368.9436	401.1607	406.8228
415.3949	426.5163	432.9095
474.0490	517.3029	532.0842
533.1825	541.2941	551.6743
580.1886	587.3629	600.9604
608.9707	630.2883	644.6437
654.4050	659.4844	675.4052
742.2669	751.0731	799.3291
806.9013	811.2055	819.4351
833.9595	863.1447	888.8806
906.7480	920.6621	938.3602
954.9011	961.9661	968.6685
1015.7034	1022.1907	1031.2091
1034.7529	1037.5071	1040.1944
1051.9225	1069.4584	1090.8606
1092.1489	1094.0325	1107.8104
1109.5712	1129.0442	1139.9908
1169.3662	1180.3811	1183.9297
1187.3884	1239.7346	1244.4482
1288.5185	1312.0744	1342.5235
1375.2204	1377.6418	1379.5845
1381.2408	1383.7047	1394.0313
1398.7329	1402.6309	1419.5894

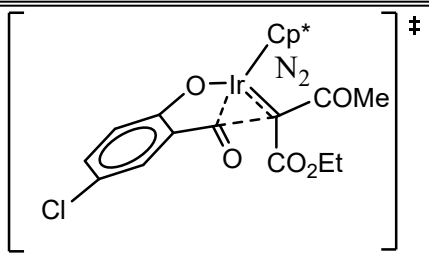
H	1.51320	-1.81562	-3.03215	1436.4481	1439.4647	1444.6696
C	0.17221	-3.56019	-0.99740	1445.7161	1449.2464	1454.8338
H	-0.04805	-3.23696	-2.01853	1455.2831	1460.5966	1461.0039
H	0.63572	-4.55408	-1.04937	1461.6031	1462.9720	1468.2125
H	-0.77976	-3.66109	-0.46483	1472.2824	1472.7330	1481.0440
C	0.24747	-2.82364	2.13211	1485.2228	1495.1713	1496.5041
H	-0.63355	-3.31309	1.70557	1508.2393	1512.4639	1518.1972
H	0.74344	-3.54041	2.79888	1548.9253	1612.8226	1653.2003
H	-0.10432	-1.98323	2.74329	1779.3473	1815.5152	1832.5098
C	2.72000	-0.99148	2.64141	2466.5587	3028.4430	3038.3073
H	3.25773	-1.79418	3.16420	3039.9037	3040.7967	3043.8094
H	3.38636	-0.12542	2.58213	3045.5786	3055.7971	3061.1624
H	1.85885	-0.71085	3.26025	3101.9346	3103.5758	3114.4738
C	-0.92305	-0.63940	-1.15276	3118.2909	3118.6255	3130.2653
O	-0.61002	0.35836	1.34538	3142.6778	3145.7501	3146.7143
O	-0.93519	-0.98242	-2.30697	3148.1471	3156.0207	3156.8950
N	2.30376	2.29145	2.37534	3175.9615	3178.0405	3183.9840
N	1.61006	2.49016	3.21215	3192.8930	3203.8140	3206.4534
C	2.79990	3.24034	-1.14466			
H	2.98237	3.31979	-0.06797			
H	3.72953	3.34481	-1.70903			
H	2.12056	4.06297	-1.39345			
O	2.64213	1.21319	-2.37688			
Cl	-6.05900	-1.08536	-0.26997			
H	-1.25297	-2.79232	3.83883			
Ir	1.41694	-0.21556	-0.32137			
H	-1.49980	0.37953	0.32274			
C	-2.97946	-0.72280	-0.83640			
C	-3.99363	0.00621	-0.20013			
C	-3.32706	-1.69968	-1.79362			
C	-5.32310	-0.22802	-0.49568			
H	-3.72011	0.76531	0.53161			
C	-4.67627	-1.92142	-2.07765			
C	-5.66829	-1.19566	-1.43610			
H	-4.95046	-2.67602	-2.81397			
H	-6.71538	-1.37713	-1.66349			
O	-2.35238	-2.39011	-2.40731			
H	-2.74769	-3.02473	-3.01655			
Cl	-6.57374	0.68394	0.30640			

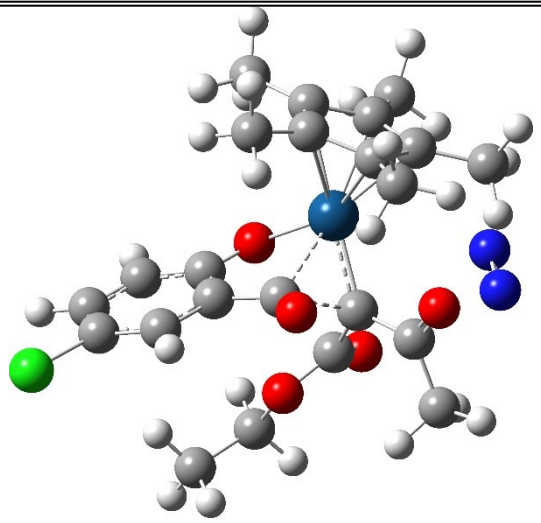
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.449576 Electronic Energy = -1941.72761241
Internal Energy (E)= -1941.24281441 Enthalpy (H)= -1941.24187041
Gibbs Free Energy (G)=-1941.34321441 Gibbs Free Energy of Solvation=-1942.59698151

St.Pt.	General Structure	Ball & Stick model

TS_3-6





Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.33102	-2.50705	0.40490
C	-2.17578	-1.60550	1.18569
C	-3.02100	-0.90247	0.27804
C	-2.66724	-1.33632	-1.07004
C	-1.67161	-2.37244	-0.96453
C	1.98491	-0.44344	0.36222
Ir	-0.94193	-0.36358	-0.17332
C	1.79388	-0.38764	-1.04174
C	2.92001	-0.61673	-1.86472
C	3.23219	-0.75021	0.92405
C	4.14643	-0.91637	-1.30667
C	4.30023	-0.98870	0.08698
H	3.33813	-0.78270	2.00564
H	5.00822	-1.10465	-1.94290
H	2.79036	-0.55848	-2.94244
C	-0.36731	1.37514	0.49985
C	-1.00037	2.00775	1.69121
C	0.41879	2.30436	-0.37701
C	2.52958	3.12379	-1.00524
H	2.35365	2.74487	-2.02115
H	2.19255	4.16731	-0.98282
C	3.96267	2.96606	-0.57355
H	4.62170	3.54242	-1.23060
H	4.10226	3.32336	0.45195
H	4.26766	1.91396	-0.61428
O	1.72562	2.35358	-0.09715
O	-0.11295	3.00468	-1.20995
C	-4.09196	0.05651	0.66068
H	-4.45897	0.61769	-0.20419
H	-4.94579	-0.47585	1.09948
H	-3.71375	0.76985	1.40328
C	-2.22434	-1.56952	2.67252
H	-3.00820	-0.89648	3.02517
H	-2.42526	-2.57764	3.05834
H	-1.28105	-1.21230	3.09823
C	-0.31756	-3.42540	0.99431
H	0.07120	-3.02680	1.93676

Frequencies

-260.7073	28.3380	32.6726
46.5217	55.4294	69.3184
78.0343	83.8080	88.3508
101.7496	110.3964	112.0196
116.1701	125.8345	133.4652
133.9158	148.6023	153.0383
160.3362	164.4004	176.3515
182.4264	189.0728	191.2959
194.2931	197.8808	208.9604
215.8907	223.4146	234.4709
241.5171	246.0491	268.2308
281.2919	283.1123	292.1522
300.5225	302.4750	312.5496
318.4858	327.5016	338.5382
349.3337	362.9566	383.9785
397.7656	401.2323	404.6527
410.3455	424.3079	445.9810
460.7486	473.3544	520.5657
536.9928	541.7716	554.4981
557.9445	575.4957	592.3672
600.9895	609.1383	620.5141
642.4824	661.5034	681.3979
725.3291	743.6127	811.4680
812.0581	818.9497	821.1968
835.8602	843.0855	891.2568
903.6162	908.0537	930.8824
957.4346	959.3185	972.0344
1019.2502	1027.6877	1032.8630
1042.8750	1044.2064	1046.6573
1048.7629	1054.5314	1089.4627
1090.2265	1097.7649	1108.0410
1115.5434	1125.5924	1140.2117
1169.3421	1179.8610	1183.1929
1190.8409	1235.9000	1244.7564
1279.5708	1308.8567	1339.9161
1369.6595	1379.8637	1381.3460
1383.0331	1389.6495	1400.1806
1401.7642	1403.0153	1421.6880
1433.5691	1434.2973	1440.2658
1446.4205	1449.3839	1451.3864
1452.5090	1454.3587	1465.6183

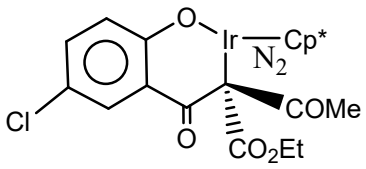
H	-0.76338	-4.40631	1.20587	1467.7081	1471.4090	1471.8775
H	0.53309	-3.58094	0.32221	1473.1433	1476.4581	1481.4779
C	-1.00557	-3.03787	-2.11735	1488.8846	1501.5447	1513.8995
H	-0.05219	-3.48697	-1.82085	1524.5672	1530.0292	1531.4027
H	-1.63780	-3.83008	-2.53732	1555.8635	1598.5980	1655.3475
H	-0.79200	-2.31650	-2.91397	1775.7631	1831.4041	1841.6041
C	-3.30449	-0.88546	-2.33693	2468.5796	3035.0592	3037.0478
H	-4.12527	-1.55704	-2.62352	3038.2660	3040.9707	3043.8541
H	-3.71440	0.12511	-2.24461	3047.2529	3050.7352	3052.8552
H	-2.57970	-0.87019	-3.15763	3096.7485	3111.8661	3118.6605
C	0.86192	-0.10477	1.22884	3119.9213	3121.4734	3141.1940
O	0.62845	-0.11000	-1.56048	3141.3380	3142.8001	3145.0442
O	0.79910	-0.19879	2.42445	3147.4991	3149.9559	3155.9196
N	-3.09338	3.16457	-0.60534	3157.9802	3178.9970	3179.4036
N	-3.36061	2.75670	-1.59682	3193.9790	3206.6739	3208.1320
C	-0.73406	3.46924	1.93744			
H	-1.05246	4.06728	1.07585			
H	-1.27166	3.78909	2.83201			
H	0.34205	3.63905	2.07027			
O	-1.71065	1.35858	2.44237			
Cl	5.87301	-1.37956	0.75318			
H	-1.25297	-2.79232	3.83883			
Ir	1.41694	-0.21556	-0.32137			
H	-1.49980	0.37953	0.32274			
C	-2.97946	-0.72280	-0.83640			
C	-3.99363	0.00621	-0.20013			
C	-3.32706	-1.69968	-1.79362			
C	-5.32310	-0.22802	-0.49568			
H	-3.72011	0.76531	0.53161			
C	-4.67627	-1.92142	-2.07765			
C	-5.66829	-1.19566	-1.43610			
H	-4.95046	-2.67602	-2.81397			
H	-6.71538	-1.37713	-1.66349			
O	-2.35238	-2.39011	-2.40731			
H	-2.74769	-3.02473	-3.01655			
Cl	-6.57374	0.68394	0.30640			

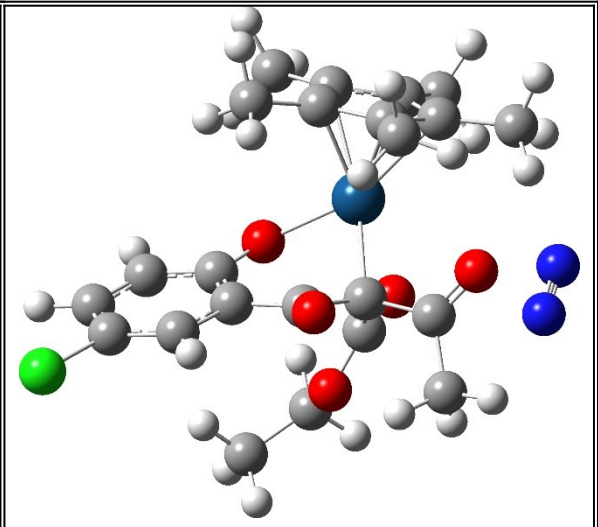
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.449051 Electronic Energy = -1941.70809433
Internal Energy (E)= -1941.22435333 Enthalpy (H)= -1941.22340933
Gibbs Free Energy (G)=-1941.32330433 Gibbs Free Energy of Solvation=-1942.57847799

St.Pt.	General Structure	Ball & Stick model

VII-3





Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.09575	-2.38239	0.49141
C	-1.91669	-1.55532	1.35339
C	-2.96632	-0.99746	0.55014
C	-2.83404	-1.55101	-0.79370
C	-1.72015	-2.42749	-0.82643
C	2.28225	-0.01560	0.51080
Ir	-0.99844	-0.40769	-0.22925
C	1.99236	-0.53527	-0.77729
C	3.05558	-1.11109	-1.50782
C	3.57322	-0.12685	1.04000
C	4.33304	-1.18871	-0.98528
C	4.58669	-0.69643	0.29681
H	3.75380	0.25521	2.04178
H	5.13932	-1.64227	-1.55736
H	2.82940	-1.50860	-2.49520
C	0.03356	1.20049	0.72619
C	-0.75637	2.04492	1.73303
C	0.09728	1.84659	-0.60765
C	1.40590	2.76898	-2.34869
H	0.98667	1.93042	-2.91555
H	0.86172	3.67950	-2.62538
C	2.89522	2.89794	-2.52229
H	3.13795	3.07745	-3.57432
H	3.29149	3.72828	-1.92970
H	3.39502	1.97615	-2.20229
O	1.17537	2.51417	-0.94183
O	-0.86956	1.65386	-1.36750
C	-4.10084	-0.17187	1.04520
H	-4.63449	0.30327	0.21690
H	-4.82227	-0.79777	1.58731
H	-3.74267	0.61205	1.71922
C	-1.69170	-1.35783	2.81091
H	-2.32848	-0.56282	3.20297
H	-1.90859	-2.28870	3.35111
H	-0.65294	-1.07627	3.02474
C	0.09806	-3.16571	0.90971
H	0.58656	-2.70348	1.77407

Frequencies

25.9056	43.4439	45.7983
63.0768	65.6951	74.5869
84.9657	89.6204	96.8819
103.3794	110.7151	112.7451
117.9764	125.2360	134.5468
144.6628	149.2900	155.2397
164.6068	166.2908	168.0550
171.8753	180.6909	183.1439
196.0809	210.8484	216.3152
222.4827	226.4379	230.3966
243.2602	249.7458	257.4332
272.2763	282.1762	286.7917
303.8004	304.3251	308.6230
327.0072	339.8161	352.6662
356.2239	391.3927	397.1621
408.7387	412.0771	421.8705
425.5235	448.8475	474.0177
498.2800	522.0015	535.8265
540.4752	543.8650	548.2400
555.2071	586.0696	597.0527
608.8726	625.2200	654.4196
663.9080	695.4061	723.7651
748.2651	797.4797	806.2101
812.5265	815.7384	827.7466
840.5750	864.3925	890.3946
906.9280	925.2172	947.5882
954.8290	971.3711	989.9900
1015.2118	1035.7823	1039.1103
1044.4272	1045.8877	1048.4961
1053.2807	1081.4607	1090.9460
1094.4785	1106.7325	1109.6358
1126.3549	1131.0229	1159.4072
1177.1732	1181.1636	1189.2319
1206.1872	1241.3310	1267.8713
1287.1662	1339.6591	1354.1902
1368.8749	1370.7135	1376.2109
1382.5826	1393.2480	1396.8253
1400.4824	1402.2321	1425.4317
1436.4831	1437.8358	1441.7467
1443.5331	1447.0230	1447.6363
1452.6907	1457.4383	1459.8361

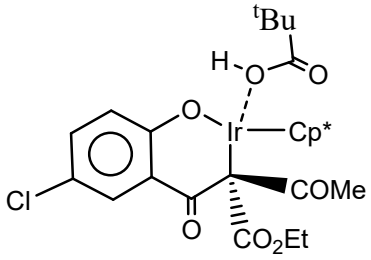
H	-0.18465	-4.19064	1.18457	1461.7878	1462.8223	1468.7491
H	0.83657	-3.22096	0.10229	1472.3046	1474.9495	1475.0493
C	-1.14245	-3.14787	-1.99298	1487.6145	1496.4547	1500.0807
H	-0.10908	-2.81742	-2.16743	1506.9786	1516.8506	1536.5775
H	-1.13121	-4.23130	-1.82055	1551.5042	1605.1531	1657.5500
H	-1.71128	-2.95726	-2.90772	1676.8877	1737.9269	1848.4611
C	-3.70646	-1.16218	-1.93508	2467.0763	3029.4755	3034.5295
H	-4.69089	-1.64123	-1.85726	3036.0931	3041.5009	3042.8500
H	-3.86413	-0.07691	-1.94433	3045.4224	3046.2847	3065.0102
H	-3.26414	-1.44145	-2.89562	3105.9044	3110.1981	3115.7479
C	1.27013	0.65498	1.35606	3121.3495	3125.2260	3133.6073
O	0.79880	-0.52629	-1.32998	3133.7331	3138.1128	3139.7511
O	1.40181	0.72928	2.57678	3142.7730	3150.3318	3152.1681
N	-2.98502	3.29649	-0.13152	3175.1294	3176.1406	3182.9033
N	-3.78221	2.69397	-0.60287	3186.9019	3201.7683	3209.7244
C	-0.14741	3.38295	2.04707			
H	-0.15347	4.01419	1.14844			
H	-0.71853	3.87548	2.83707			
H	0.89567	3.25680	2.35515			
O	-1.79862	1.68565	2.23374			
Cl	6.20708	-0.80990	0.96052			
H	-1.25297	-2.79232	3.83883			
Ir	1.41694	-0.21556	-0.32137			
H	-1.49980	0.37953	0.32274			
C	-2.97946	-0.72280	-0.83640			
C	-3.99363	0.00621	-0.20013			
C	-3.32706	-1.69968	-1.79362			
C	-5.32310	-0.22802	-0.49568			
H	-3.72011	0.76531	0.53161			
C	-4.67627	-1.92142	-2.07765			
C	-5.66829	-1.19566	-1.43610			
H	-4.95046	-2.67602	-2.81397			
H	-6.71538	-1.37713	-1.66349			
O	-2.35238	-2.39011	-2.40731			
H	-2.74769	-3.02473	-3.01655			
Cl	-6.57374	0.68394	0.30640			

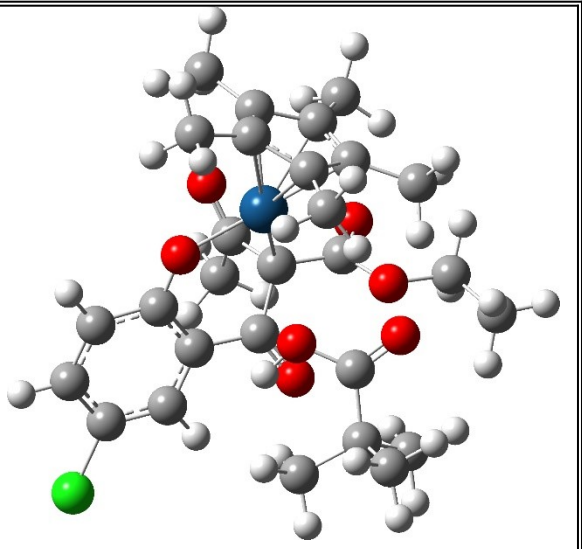
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.450524 Electronic Energy = -1941.74712506
Internal Energy (E)= -1941.26159006 Enthalpy (H)= -1941.26064606
Gibbs Free Energy (G)=-1941.36131406 Gibbs Free Energy of Solvation=-1942.61195894

St.Pt.	General Structure	Ball & Stick model

VII'-3





Cartesian co-ordinate

Atoms	X	Y	Z
C	2.66893	-1.33340	-1.88578
C	2.54319	0.08842	-1.85531
C	2.95253	0.57205	-0.53914
C	3.26783	-0.56197	0.26465
C	3.03872	-1.74902	-0.55556
O	-0.91702	1.32734	-1.51315
C	-0.89414	2.65484	-1.29008
O	0.17064	3.22909	-1.28265
C	-2.22300	3.39209	-1.12716
C	-1.61491	-1.83536	-0.63998
H	-1.81182	0.96584	-1.42063
C	2.11327	0.97669	-2.96466
H	1.58799	1.85471	-2.57230
H	2.98996	1.32117	-3.53017
H	1.44069	0.45963	-3.65626
C	3.09500	2.01050	-0.19688
H	3.87240	2.46541	-0.82502
H	2.15537	2.54906	-0.37024
H	3.38919	2.14463	0.84817
C	3.23202	-3.15040	-0.10784
H	2.65519	-3.84233	-0.72969
H	4.29271	-3.42767	-0.17596
H	2.90218	-3.27198	0.92732
C	2.31861	-2.25184	-3.00422
H	1.99294	-1.69447	-3.88713
H	3.17842	-2.86786	-3.29405
H	1.49813	-2.92047	-2.71544
C	3.79244	-0.58324	1.65506
H	4.87592	-0.76009	1.65001
H	3.59382	0.35463	2.18207
H	3.31353	-1.37615	2.23852
Ir	1.18965	-0.71671	-0.34307
C	-2.31503	4.37502	-2.29938
H	-2.38099	3.84974	-3.26088
H	-3.21420	4.99380	-2.19095
H	-1.43891	5.03075	-2.32337

Frequencies

27.2175	37.3969	42.7862
57.8166	60.9563	68.0893
72.6512	78.8888	86.1301
89.3833	94.1185	98.8943
109.4684	115.2622	118.3602
120.6806	127.9444	135.9739
140.5444	145.5359	150.9743
156.4113	159.3738	168.7626
183.3495	185.1132	191.1845
207.6482	211.8038	218.1814
224.2393	233.6679	239.6447
250.5455	262.0943	269.5798
277.1301	281.2784	287.1329
290.9953	298.2429	302.5598
307.0470	316.6434	320.4336
330.6808	331.7725	339.2497
345.7562	357.0039	369.5675
373.6461	392.8437	396.7140
399.7269	415.3575	428.1075
431.8696	442.7390	450.5332
459.4069	486.9312	498.1654
527.7674	532.9917	533.5476
542.6233	545.9201	547.9595
554.7174	576.6525	585.6682
591.1064	607.1621	631.8033
645.5314	678.6514	706.1885
724.8977	771.0603	772.1933
783.7621	798.4654	807.5557
813.1168	815.5065	839.9428
872.4758	881.1000	885.9466
900.7521	932.1997	941.8281
949.3728	956.1623	963.9755
966.5803	968.8440	971.5234
999.0369	1010.2226	1032.2371
1037.2651	1038.8882	1045.6723
1048.4147	1048.4885	1049.6342
1063.9415	1094.4509	1098.5047
1102.3413	1107.2500	1110.3090
1121.8519	1138.4251	1151.3566
1166.9332	1184.5109	1187.2143

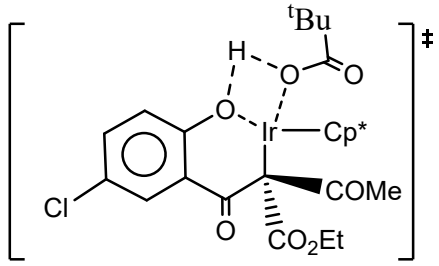
C	-3.44046	2.47226	-1.12421	1192.5580	1194.5097	1228.5679
H	-3.42408	1.78864	-0.26610	1242.7548	1251.8172	1260.2944
H	-4.35082	3.07669	-1.03809	1268.6988	1277.0285	1296.8686
H	-3.53560	1.90029	-2.05876	1330.9986	1369.7213	1375.6544
C	-2.15389	4.16275	0.19200	1378.3835	1380.5726	1381.3987
H	-2.00539	3.47542	1.03388	1384.5350	1385.1817	1386.2942
H	-1.32648	4.87992	0.16915	1397.6052	1404.6527	1410.8804
H	-3.09024	4.71316	0.34644	1414.7430	1418.6014	1430.8798
O	-0.36537	-1.80214	-1.04740	1432.4445	1435.7755	1441.5919
C	-2.18709	-0.94744	0.30396	1448.5386	1450.6377	1452.6375
C	-3.56585	-1.00435	0.56954	1456.3545	1457.5564	1459.7179
C	-2.46532	-2.78433	-1.25204	1462.3589	1465.6195	1470.1651
C	-4.36412	-1.94052	-0.05146	1471.5672	1476.0499	1476.9365
C	-3.81267	-2.84392	-0.96448	1477.1429	1479.4191	1479.8826
C	-1.40831	0.05502	1.07945	1490.1453	1491.7579	1494.7685
O	-1.96914	1.05939	1.50384	1497.2865	1501.8600	1505.0539
H	-2.01763	-3.46170	-1.97488	1511.9389	1525.5776	1552.0782
H	-4.45066	-3.58175	-1.44468	1602.4289	1658.5201	1754.6441
H	-3.98102	-0.30384	1.29131	1792.7588	1823.1495	1862.7278
C	0.01766	-0.28790	1.41333	3021.5907	3032.0968	3036.4813
C	0.03797	-1.58000	2.27197	3037.4768	3038.8954	3039.0733
C	0.71442	0.74966	2.23188	3040.7300	3042.2917	3045.5561
C	1.30639	2.98239	2.54784	3047.4483	3056.4572	3094.8989
H	2.37751	2.74389	2.61814	3108.1572	3116.3150	3117.0717
H	0.90723	2.91661	3.56694	3126.0872	3128.4133	3130.1274
C	1.06910	4.33289	1.93008	3131.2543	3134.0484	3135.2377
H	1.64055	5.09591	2.46887	3136.2218	3144.2977	3145.2852
H	1.36924	4.34452	0.87666	3146.4764	3149.9268	3161.4884
H	0.00984	4.60070	1.98028	3162.8288	3164.9563	3168.6167
O	0.66341	1.99391	1.73027	3173.9110	3174.5409	3195.5338
O	1.32138	0.48706	3.25585	3198.9928	3210.4507	3791.0028
O	0.82552	-2.48296	2.07611			
C	-0.96686	-1.64851	3.38984			
H	-0.70978	-2.46922	4.06264			
H	-1.00466	-0.70212	3.93875			
H	-1.96643	-1.82964	2.97364			
Cl	-6.07711	-2.01513	0.30862			

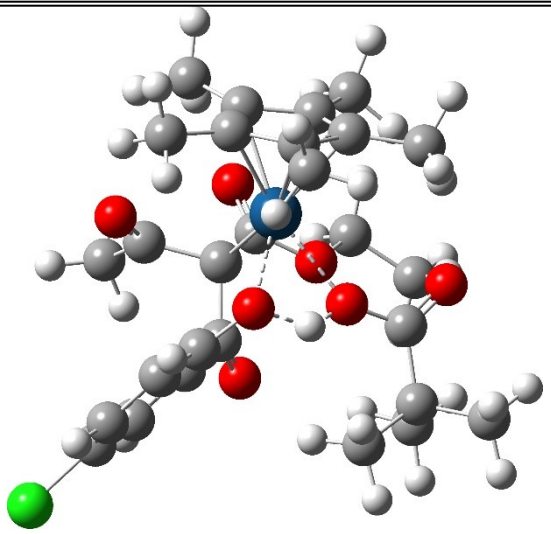
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.592873 Electronic Energy = -2179.11747833
Internal Energy (E)= -2178.48370633 Enthalpy (H)= -2178.48276333
Gibbs Free Energy (G)=-2178.59485233 Gibbs Free Energy of Solvation=-2180.0379367

St.Pt.	General Structure	Ball & Stick model

TS_3-7





Cartesian co-ordinate

Atoms	X	Y	Z
C	1.88011	-2.05795	-1.86354
C	2.82362	-1.17718	-1.27971
C	2.81786	-1.38473	0.16580
C	1.91102	-2.47215	0.45302
C	1.26506	-2.82872	-0.78711
O	0.53681	1.34185	-1.03480
C	1.08340	2.55889	-1.04709
O	2.25332	2.71641	-0.77382
C	0.14253	3.71771	-1.37040
C	-2.19100	-0.33375	-1.12516
H	-0.35905	0.89202	-1.49642
C	3.63490	-0.13256	-1.95819
H	3.48880	0.84287	-1.47710
H	4.70154	-0.38659	-1.90435
H	3.36311	-0.03134	-3.01307
C	3.74016	-0.71342	1.12058
H	4.74067	-1.16466	1.07840
H	3.83742	0.35104	0.87297
H	3.37136	-0.79371	2.14860
C	0.23788	-3.88198	-0.99635
H	-0.44875	-3.59394	-1.80107
H	0.71372	-4.82964	-1.28229
H	-0.35837	-4.03400	-0.09542
C	1.47985	-2.15056	-3.29348
H	1.93108	-1.35182	-3.88939
H	1.78612	-3.11187	-3.72528
H	0.39159	-2.06617	-3.39590
C	1.74914	-3.13365	1.77425
H	2.61645	-3.78049	1.96106
H	1.69171	-2.39513	2.58212
H	0.84462	-3.74515	1.80934
Ir	0.83789	-0.77662	-0.36792
C	0.81381	4.58960	-2.43140
H	0.89544	4.06263	-3.39081
H	0.21977	5.49697	-2.59597
H	1.81936	4.88270	-2.11416

Frequencies

-886.8923	-82.8894	-19.2444
13.3790	25.9366	31.4025
52.3488	59.8864	73.3765
75.5702	88.0795	92.8310
102.3175	109.3346	113.4088
120.5302	122.8476	127.3460
136.3723	138.9427	144.8546
147.0558	151.8958	161.6222
171.1023	177.9199	183.3442
185.7386	190.5720	201.6103
212.5701	217.1999	227.4983
231.5922	235.5984	251.8782
257.4789	263.3457	264.2401
272.3018	278.5507	289.4273
294.3691	305.9901	308.7886
324.1922	331.1057	334.4978
348.1335	358.6134	370.6962
372.6138	383.6406	389.8624
395.1513	403.9970	407.8343
417.3079	429.5204	436.1274
446.9553	457.5969	496.8328
526.8883	535.2485	536.1864
546.2751	554.9388	561.2907
578.5437	585.5925	588.4843
601.8948	605.7325	624.7839
650.8300	672.2943	702.6717
722.8605	769.3431	775.0148
799.5072	803.6558	805.9680
812.4078	829.2373	835.0065
866.5837	878.3506	891.9038
894.2986	928.0918	939.8088
945.7337	946.9787	952.9056
955.7620	956.0741	971.2982
997.7402	1014.6526	1031.1470
1032.6888	1035.4462	1036.7604
1039.0893	1044.2219	1046.7495
1051.3347	1089.1431	1089.7674
1096.0819	1100.0711	1108.6517
1115.8560	1135.7687	1148.8266
1173.2865	1175.5113	1184.3113
1185.4041	1194.8280	1219.7368

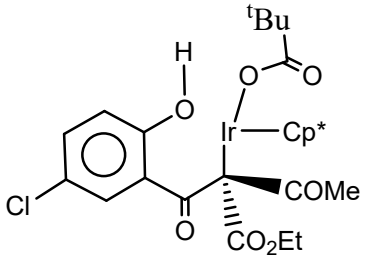
C	-1.23570	3.27025	-1.84634	1233.8976	1238.7351	1255.9645
H	-1.78382	2.74132	-1.05636	1263.1001	1293.2393	1312.1351
H	-1.82823	4.15335	-2.11364	1319.3741	1344.5372	1352.4489
H	-1.18385	2.63113	-2.73830	1373.3825	1373.9827	1374.7861
C	-0.00949	4.50655	-0.06335	1374.9083	1382.6494	1383.8883
H	-0.43251	3.87516	0.72964	1387.7740	1398.7928	1400.0814
H	0.96140	4.88794	0.27181	1411.8546	1422.7698	1433.2210
H	-0.68360	5.35668	-0.22760	1437.3750	1439.9042	1442.0371
O	-0.94145	-0.29951	-1.62062	1442.8641	1443.0292	1445.2161
C	-2.50182	0.27229	0.10402	1446.0458	1450.8220	1455.5570
C	-3.83113	0.36824	0.51977	1456.3413	1457.3696	1460.1698
C	-3.21887	-0.89676	-1.88665	1463.7972	1464.9357	1467.5691
C	-4.83292	-0.19699	-0.25157	1471.5566	1477.8614	1479.2991
C	-4.53386	-0.84083	-1.44991	1483.0145	1484.2151	1490.6953
C	-1.45252	0.79255	1.02732	1499.8511	1505.3917	1507.0670
O	-1.60135	1.87111	1.57707	1515.8885	1521.4394	1554.8504
H	-2.96181	-1.36095	-2.83606	1621.8621	1656.7018	1774.1206
H	-5.33426	-1.28236	-2.03785	1783.7779	1828.9148	1829.9453
H	-4.06132	0.87127	1.45654	2026.2936	3019.8416	3023.8639
C	-0.33880	-0.18230	1.36661	3029.1863	3032.7601	3036.7900
C	-1.07395	-1.38455	1.99502	3036.9621	3039.0813	3039.7542
C	0.68631	0.34943	2.31513	3051.3533	3052.9250	3054.1374
C	2.09456	2.11867	2.92998	3099.8996	3100.9339	3108.8225
H	2.99508	1.49183	2.89485	3108.8482	3110.3247	3114.7526
H	1.70169	2.05770	3.95225	3116.8998	3118.5617	3120.3237
C	2.37925	3.53309	2.50614	3126.8729	3133.5072	3139.4132
H	3.14083	3.97399	3.15771	3142.1065	3142.5027	3143.5767
H	2.73883	3.55568	1.47227	3146.9346	3147.9346	3161.1596
H	1.47302	4.14464	2.57042	3162.0278	3168.7270	3194.2019
O	1.11537	1.58204	2.02813	3206.4050	3208.6152	3211.7406
O	1.15163	-0.30104	3.23976			
O	-1.22417	-2.44186	1.41798			
C	-1.67977	-1.16181	3.35678			
H	-2.51066	-1.85634	3.50186			
H	-0.91017	-1.35667	4.11110			
H	-2.00962	-0.12599	3.49814			
Cl	-6.49615	-0.10816	0.28690			

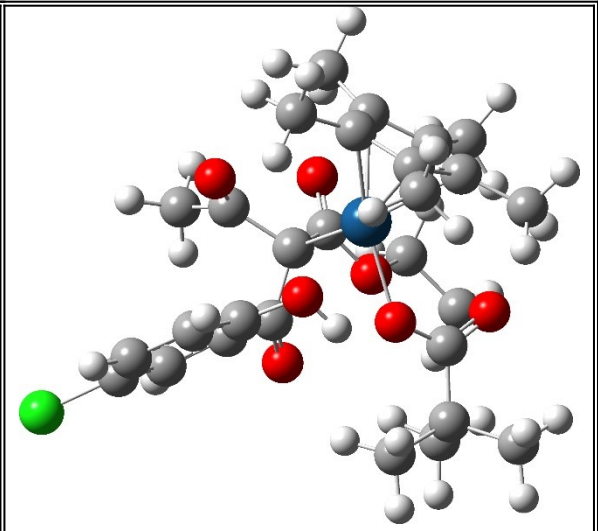
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.585908 Electronic Energy = -2179.10664954
Internal Energy (E)= -2178.48131654 Enthalpy (H)= -2178.48037254
Gibbs Free Energy (G)=-2178.59031954 Gibbs Free Energy of Solvation=-2180.02277798

St.Pt.	General Structure	Ball & Stick model

VIII-3





Cartesian co-ordinate

Atoms	X	Y	Z
C	1.90196	-2.19687	-1.63843
C	2.84001	-1.30673	-1.06142
C	2.71203	-1.40579	0.39159
C	1.77121	-2.48022	0.68481
C	1.21774	-2.90507	-0.55979
O	0.56231	1.15338	-1.10622
C	1.38978	2.16156	-1.02027
O	2.51277	2.10595	-0.53801
C	0.82739	3.48238	-1.56205
C	-2.39412	-0.36510	-1.22951
H	-0.72202	0.31200	-1.91195
C	3.75594	-0.39736	-1.79892
H	4.02299	0.47256	-1.19546
H	4.66639	-0.93719	-2.09075
H	3.28000	-0.01481	-2.70879
C	3.55293	-0.68303	1.38034
H	4.53331	-1.16639	1.48624
H	3.70295	0.35411	1.05685
H	3.06444	-0.67436	2.36177
C	0.16745	-3.93407	-0.78158
H	-0.60923	-3.54915	-1.45309
H	0.60292	-4.83097	-1.24180
H	-0.32472	-4.21269	0.15182
C	1.62536	-2.40101	-3.08575
H	1.99155	-1.56455	-3.68888
H	2.11404	-3.31493	-3.44878
H	0.55083	-2.50575	-3.27025
C	1.49821	-3.05315	2.02904
H	2.33540	-3.69830	2.32656
H	1.38391	-2.26947	2.78579
H	0.58551	-3.65527	2.02723
Ir	0.82009	-0.78341	-0.31403
C	1.83108	4.05341	-2.56257
H	1.91753	3.41348	-3.45123
H	1.50743	5.04784	-2.89638
H	2.82267	4.14169	-2.10713

Frequencies

30.7069	55.8270	60.2408
69.4488	75.3417	79.6877
84.7054	89.4116	96.7855
108.9986	114.0726	120.5139
128.3737	129.7622	133.3001
141.7183	146.4183	155.0680
164.0954	167.7612	175.0270
184.4877	192.5049	196.9907
198.6622	199.1576	208.8824
216.9780	227.4754	229.3009
240.1617	245.0966	257.9179
266.3292	272.2958	274.1394
282.9867	293.5362	295.5757
306.0499	309.7594	314.7201
323.6815	330.9533	337.6656
354.5469	357.6257	367.5132
370.8992	378.5170	380.8137
393.6802	397.4893	403.4966
404.8440	408.1348	423.6928
426.0819	429.1483	459.2705
467.3722	475.8462	507.2949
533.6992	536.8106	544.1897
549.9730	565.4267	581.8213
585.9456	591.9035	592.4075
602.7652	632.3418	643.1050
658.6113	692.2589	708.3125
762.8005	790.2546	796.9586
807.7908	808.9476	810.6880
814.0795	827.1475	839.3299
857.2923	876.7234	883.6652
895.0774	927.1567	928.2938
951.3239	953.3345	955.5677
960.8399	961.7925	978.7641
993.4410	1014.4353	1019.9786
1037.8293	1038.8820	1039.7583
1048.9749	1055.5476	1058.3325
1058.7996	1090.2221	1095.4476
1098.7510	1101.0397	1112.1554
1113.6658	1138.5918	1154.0698
1174.4466	1187.0041	1190.3835
1201.4141	1225.9872	1237.1908

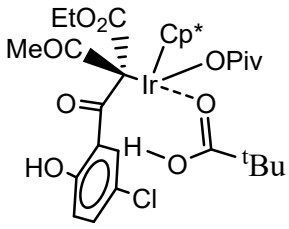
C	-0.53887	3.32165	-2.21949	1245.1402	1250.3206	1262.2666
H	-1.28302	2.95428	-1.50215	1269.6975	1283.6470	1322.2326
H	-0.88445	4.29452	-2.59283	1341.9574	1363.2135	1364.1281
H	-0.50139	2.63401	-3.07496	1378.2510	1379.1651	1380.4692
C	0.69845	4.42295	-0.35988	1384.3010	1384.9254	1389.7338
H	0.06026	3.97865	0.41641	1396.4232	1404.2936	1404.7609
H	1.68314	4.62739	0.07395	1416.5341	1426.7314	1434.3706
H	0.25342	5.37510	-0.67775	1441.7397	1442.0869	1444.6766
O	-1.13086	-0.57132	-1.74485	1446.5506	1451.6635	1453.8278
C	-2.58542	0.43785	-0.10336	1455.8724	1456.3589	1458.9078
C	-3.88956	0.71515	0.30876	1463.9768	1464.9922	1466.1835
C	-3.47081	-0.94235	-1.88753	1469.5763	1470.7134	1477.0942
C	-4.96247	0.13884	-0.35532	1483.8167	1490.5958	1493.3271
C	-4.76519	-0.70486	-1.44275	1496.2011	1499.8123	1503.6006
C	-1.47694	0.97808	0.76229	1508.7482	1510.9431	1522.1376
O	-1.51912	2.14370	1.10640	1529.1205	1531.2413	1558.3177
H	-3.27991	-1.55989	-2.76123	1633.7955	1667.7616	1767.7065
H	-5.61842	-1.15240	-1.94455	1776.5334	1791.6572	1827.8203
H	-4.04825	1.37001	1.16248	3022.9895	3027.3984	3033.3073
C	-0.49912	-0.05310	1.28450	3037.8181	3038.3492	3038.9985
C	-1.35617	-1.20839	1.83108	3040.2194	3040.4520	3044.6239
C	0.43488	0.44162	2.34236	3048.8222	3053.0475	3095.1700
C	1.88273	2.12158	3.09625	3103.5871	3106.8197	3113.1422
H	2.67037	1.36815	3.21878	3117.8999	3118.4440	3119.4163
H	1.37667	2.21433	4.06580	3128.0567	3128.5422	3129.9147
C	2.43697	3.42965	2.60259	3139.3244	3140.7100	3141.2661
H	3.20700	3.79343	3.29115	3145.1678	3149.7111	3157.6252
H	2.87663	3.29704	1.60747	3159.5442	3162.7977	3166.3777
H	1.65050	4.18843	2.53336	3176.3594	3186.6245	3201.3099
O	0.93432	1.65561	2.12550	3207.1976	3216.4650	3453.8951
O	0.76317	-0.23519	3.30769			
O	-1.51516	-2.25083	1.22740			
C	-2.08060	-0.96173	3.13047			
H	-2.99327	-1.56271	3.15390			
H	-1.42726	-1.26536	3.95498			
H	-2.31345	0.09903	3.28176			
Cl	-6.58881	0.47501	0.18622			

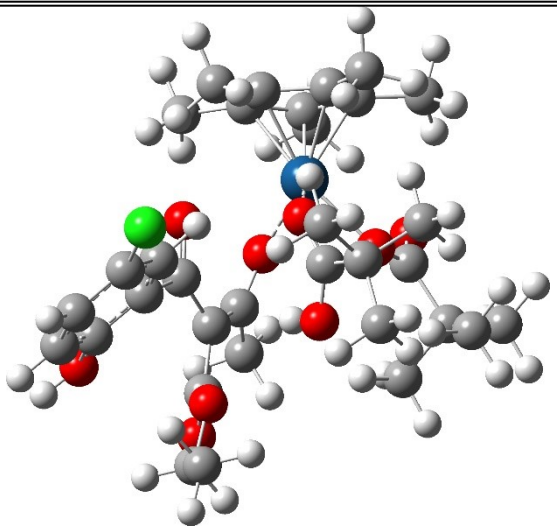
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.594975 Electronic Energy = -2179.11961790
Internal Energy (E)= -2178.4852439 Enthalpy (H)= -2178.4842999
Gibbs Free Energy (G)=-2178.5910479 Gibbs Free Energy of Solvation=-2179.99034476

St.Pt.	General Structure	Ball & Stick model

VIII'-3





Cartesian co-ordinate

Atoms	X	Y	Z
H	0.79429	1.32672	0.56003
C	-2.12557	-2.22131	-1.87626
C	-1.62743	-2.85409	-0.69793
C	-2.50853	-2.51794	0.41464
C	-3.56773	-1.68746	-0.09520
C	-3.30747	-1.44938	-1.50647
C	-2.81504	1.86556	0.59724
O	-1.87257	0.99622	0.81384
O	-3.76063	1.72222	-0.17243
C	-2.61054	3.18760	1.35425
O	0.12747	-0.81963	1.18825
C	0.60788	0.03846	1.92887
O	0.95112	1.23959	1.53182
C	0.85999	-0.24571	3.39800
C	-4.71867	-1.14767	0.67217
H	-5.58929	-1.80612	0.55414
H	-4.48538	-1.08067	1.73991
H	-4.97182	-0.14307	0.32251
C	-4.15621	-0.62804	-2.40788
H	-5.06385	-1.17632	-2.69253
H	-4.43531	0.30224	-1.90141
H	-3.61568	-0.36252	-3.32101
C	-2.36380	-3.02669	1.80383
H	-1.31880	-2.97210	2.12906
H	-2.96240	-2.43669	2.50563
H	-2.68951	-4.07247	1.87564
C	-0.39542	-3.67926	-0.59301
H	-0.03041	-3.70415	0.43865
H	-0.59620	-4.71105	-0.90850
H	0.40334	-3.26037	-1.21165
C	-1.51731	-2.27343	-3.23059
H	-0.43886	-2.43590	-3.16736
H	-1.96901	-3.07966	-3.82247
H	-1.67207	-1.32969	-3.76276
C	-0.51664	-0.43356	4.04508
H	-0.39305	-0.69935	5.10216

Frequencies

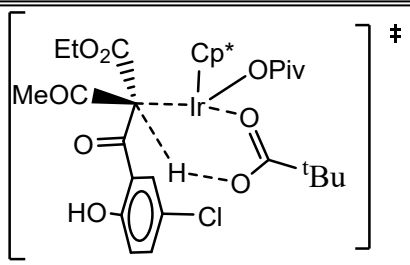
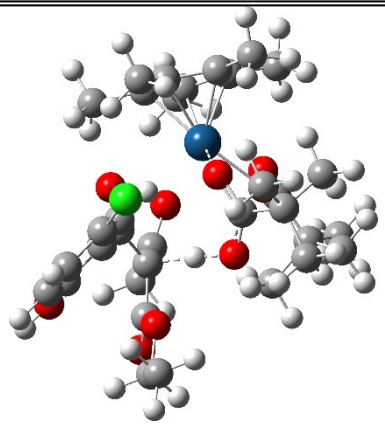
6.7977	30.9764	34.3262
42.3937	48.1557	53.1796
57.7765	63.2363	70.5002
76.1286	80.2591	87.9160
92.2436	98.0214	102.8716
109.0209	111.5860	121.0785
124.9946	131.8856	136.3048
142.7389	148.0441	153.7563
162.4303	167.9033	173.7349
180.1801	181.2480	187.7825
191.3380	196.1583	200.3868
206.5399	208.0367	213.8988
222.4451	225.5948	227.5218
234.7290	235.9882	246.2688
258.7195	263.2389	268.9030
271.7148	276.4133	288.2496
292.8997	297.1623	300.9030
303.2221	316.4387	318.6146
321.9882	323.2108	328.7435
339.7234	343.1074	348.0539
352.2939	352.6036	358.1472
373.3719	374.2236	382.0130
389.2705	390.5371	398.9397
399.8876	405.5867	414.0450
426.8894	432.3020	441.1059
453.3803	465.4517	480.7965
503.5517	535.0153	538.1386
540.3698	541.8726	547.4232
570.7152	581.7980	583.3397
595.1479	597.9340	602.4199
616.9273	622.6357	631.3040
647.5572	656.8953	694.5745
722.4109	770.3952	777.8885
787.2048	788.1194	792.9433
800.1116	806.7852	811.0254
817.0488	819.9679	834.4936
861.5192	896.3244	902.3846
906.8531	910.5192	916.2404
946.7639	947.9805	952.8861
958.2713	958.7954	960.4908
965.4740	971.1116	986.7956

H	-1.11057	0.48636	3.98625	1008.4484	1031.1766	1031.8381
H	-1.07715	-1.23055	3.54471	1037.3938	1037.7599	1042.9049
C	1.61221	0.88608	4.08782	1045.0544	1047.4865	1047.7286
H	1.76622	0.62864	5.14296	1049.7471	1052.6676	1053.8516
H	2.59349	1.05200	3.62954	1093.2801	1099.0835	1100.2931
H	1.05483	1.82796	4.04265	1111.3510	1121.4998	1133.0165
C	1.66716	-1.54302	3.49036	1144.4373	1162.7687	1167.2221
H	1.14860	-2.37254	2.99574	1184.9496	1190.3581	1191.3974
H	2.65440	-1.43374	3.02194	1233.5596	1239.4181	1242.3027
H	1.82163	-1.80778	4.54329	1250.3935	1251.5903	1269.4873
C	-3.94573	3.90655	1.50443	1272.5054	1282.1885	1289.3826
H	-4.63554	3.32834	2.13190	1291.7788	1314.5967	1319.1153
H	-3.79788	4.88725	1.97553	1363.1426	1365.6234	1369.2069
H	-4.42429	4.04776	0.53080	1372.6079	1374.1216	1374.6876
C	-1.66689	4.02597	0.48505	1375.3884	1383.1932	1386.5257
H	-1.47749	4.99929	0.95681	1387.9026	1391.2238	1394.8961
H	-0.70009	3.51890	0.35214	1403.0568	1406.5466	1408.7760
H	-2.10669	4.20497	-0.50441	1412.0884	1417.7812	1429.2691
C	-1.97253	2.97146	2.72321	1433.6684	1436.6509	1437.5326
H	-1.85370	3.93551	3.23599	1439.6199	1447.5562	1449.3781
H	-2.59925	2.33025	3.35784	1449.6209	1452.5189	1454.3646
H	-0.98477	2.50725	2.62528	1456.6317	1457.2190	1459.3249
Ir	-1.68722	-0.71041	-0.39017	1459.7932	1465.6176	1467.0963
C	1.18594	1.30903	-1.50849	1469.4089	1472.5213	1472.8889
C	1.61686	-0.07281	-1.42633	1474.1112	1475.3973	1476.0941
O	0.86370	-1.03607	-1.61801	1479.6499	1482.7484	1483.9807
C	3.04490	-0.44576	-1.10779	1489.0949	1492.4100	1493.9585
C	4.16069	-0.00098	-1.82752	1494.5645	1500.9809	1509.2939
C	3.22965	-1.38753	-0.09996	1515.1838	1519.2987	1529.2031
C	5.43417	-0.46494	-1.50834	1537.5912	1578.8894	1651.2760
C	4.50605	-1.82905	0.22362	1662.5924	1705.3970	1760.7277
H	2.35659	-1.76791	0.42867	1764.9186	1834.5388	3020.8801
C	5.61665	-1.37689	-0.47361	3024.4951	3027.2314	3031.8664
H	6.29388	-0.11437	-2.07950	3033.7920	3040.8558	3041.2614
H	6.60889	-1.73999	-0.22060	3041.5607	3042.3046	3042.9704
O	3.94700	0.88274	-2.83424	3045.3897	3046.1647	3046.9512
H	4.78403	1.11741	-3.24858	3059.3031	3087.6027	3100.5545
C	-0.13883	1.59681	-1.96882	3110.3259	3111.8994	3115.5487
C	2.14675	2.42123	-1.38909	3120.3173	3123.6396	3125.8301
C	4.10301	3.09197	-0.24370	3127.6668	3128.4980	3129.4742
H	3.71879	4.11040	-0.10683	3133.1301	3133.2115	3133.8777
H	4.68233	3.09134	-1.17955	3134.8496	3136.8827	3142.4744
C	4.91745	2.61900	0.93258	3147.7438	3147.9134	3149.0454
H	5.78869	3.26338	1.08786	3153.6853	3157.2475	3157.8774
H	4.31083	2.62952	1.84442	3163.9410	3168.8672	3171.4674
H	5.26570	1.59181	0.77045	3172.3737	3175.0483	3207.4404
O	3.01368	2.18424	-0.37476	3215.0757	3475.8370	3900.5362
O	2.17554	3.45614	-2.02232			
C	-0.46184	2.87925	-2.68158			
H	-1.53097	2.88340	-2.90914			
H	-0.20506	3.74875	-2.06949			
H	0.13751	2.97647	-3.59202			
O	-1.12343	0.82046	-1.82749			
Cl	4.71368	-3.00029	1.51293			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm

Zero-point correction= 0.741483	Electronic Energy = -2525.94478986
Internal Energy (E)= -2525.15342386	Enthalpy (H)= -2525.15247986
Gibbs Free Energy (G)=-2525.28395086	Gibbs Free Energy of Solvation=-2527.01556611

St.Pt.	General Structure	Ball & Stick model
TS_3-8		

Cartesian co-ordinate

Atoms	X	Y	Z
H	0.97705	1.31239	0.14999
C	-1.98488	-2.29108	-1.81584
C	-1.49528	-2.90347	-0.62469
C	-2.43462	-2.60438	0.45173
C	-3.52007	-1.83093	-0.10533
C	-3.22174	-1.58420	-1.49995
C	-3.03991	1.77940	0.39545
O	-2.10461	0.97344	0.79836
O	-3.90873	1.51659	-0.43246
C	-2.92577	3.19574	0.98178
O	0.03301	-0.73299	1.14584
C	0.43818	0.25522	1.81081
O	0.78646	1.37357	1.32225
C	0.55727	0.09020	3.32122
C	-4.70605	-1.33134	0.63635
H	-5.54494	-2.02956	0.52077
H	-4.48624	-1.23468	1.70488
H	-4.99624	-0.34434	0.26641
C	-4.06395	-0.83991	-2.47183
H	-4.73332	-1.52267	-3.01164
H	-4.64791	-0.06985	-1.96409
H	-3.43198	-0.32460	-3.20243
C	-2.31584	-3.10521	1.84598
H	-1.28931	-2.98781	2.21107
H	-2.97654	-2.55650	2.52452
H	-2.57832	-4.16957	1.90156
C	-0.23495	-3.67842	-0.47191
H	0.13086	-3.62439	0.55877
H	-0.39701	-4.73569	-0.71796

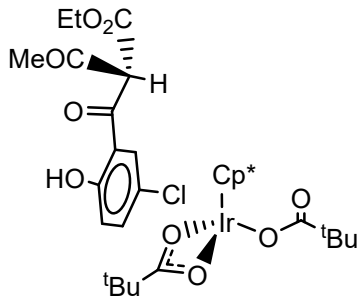
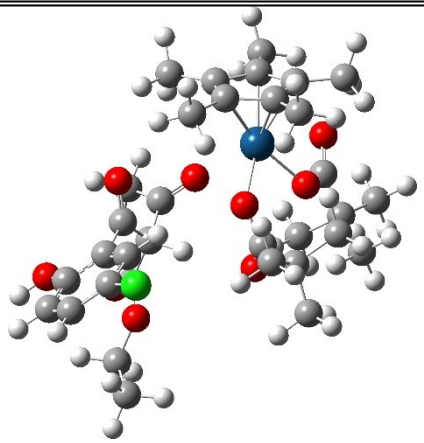
Frequencies

-313.3372	-167.9220	-132.7116
-58.5965	-28.1614	12.8041
32.1508	36.6499	44.5373
46.4505	58.5831	61.6260
67.5709	76.8195	81.0299
89.5879	95.9224	97.5214
105.5163	108.8407	117.3577
121.2490	134.9706	137.5634
141.9531	146.5473	150.6814
152.4956	155.9706	164.5466
167.6985	175.3658	179.2488
190.1402	191.6765	196.6796
198.1789	201.3759	206.1664
217.8558	221.6564	222.5324
225.4073	228.8161	231.3845
234.3903	246.9781	262.4838
266.7880	277.5293	289.8165
293.4134	297.3646	304.6030
306.7391	309.9591	310.8575
326.9960	331.6654	333.4361
336.8064	341.4318	349.0751
352.5975	365.3907	374.5790
379.8391	392.8753	395.2758
399.9379	406.8275	421.9964
428.7355	433.5573	444.4181
453.4808	462.4023	468.0403
473.1434	514.7727	533.3591
537.0108	538.0467	546.4339
559.4054	568.5465	585.4681
587.3336	597.7879	602.7040
609.3284	622.9798	630.0364
648.2286	682.6021	691.3890
737.0791	771.5786	792.0596
794.7089	800.6008	803.2670

H	0.55080	-3.27540	-1.11768	806.4626	807.8635	809.3770
C	-1.34727	-2.32844	-3.15719	816.7948	824.4081	849.6835
H	-0.27351	-2.51051	-3.08362	892.2578	897.9786	907.5070
H	-1.80479	-3.11984	-3.76509	911.7134	913.4795	923.2692
H	-1.48411	-1.37815	-3.68233	935.1315	937.5206	943.5543
C	-0.85596	-0.11982	3.87210	945.9349	949.2976	957.7206
H	-0.81763	-0.22791	4.96350	964.2484	971.7478	973.1266
H	-1.50913	0.72563	3.62223	1006.5272	1028.6158	1030.8104
H	-1.30887	-1.02303	3.44867	1032.4640	1033.3104	1035.5834
C	1.20004	1.31278	3.96572	1036.9163	1037.4119	1037.7521
H	1.29599	1.15195	5.04713	1042.8113	1044.7107	1054.6513
H	2.19782	1.50220	3.55249	1093.3364	1093.6328	1095.0299
H	0.60087	2.21549	3.80555	1108.2791	1114.7432	1131.6630
C	1.41834	-1.14660	3.59318	1146.2049	1164.7873	1175.3699
H	0.99093	-2.04247	3.12876	1181.7756	1185.3458	1189.5033
H	2.43453	-1.01024	3.19967	1234.5766	1236.1691	1247.0435
H	1.49592	-1.31765	4.67415	1248.3954	1256.0049	1261.4185
C	-4.28745	3.87915	0.95281	1263.2512	1268.6390	1279.9757
H	-5.00058	3.36384	1.60852	1283.3150	1308.8460	1319.4221
H	-4.19666	4.91688	1.30014	1360.2203	1367.3056	1368.1298
H	-4.70542	3.87830	-0.05789	1368.4640	1369.2472	1375.8034
C	-1.95078	3.93617	0.05887	1377.2187	1380.8770	1382.0048
H	-1.82936	4.97683	0.38778	1383.4604	1384.8131	1392.4004
H	-0.96156	3.45657	0.08006	1394.1876	1398.5188	1401.8381
H	-2.32189	3.94253	-0.97441	1407.0591	1415.5850	1423.0079
C	-2.36478	3.19930	2.39913	1424.5098	1430.9038	1431.9688
H	-2.31645	4.22909	2.77813	1434.7414	1435.5066	1437.6597
H	-2.99973	2.62168	3.08423	1442.2839	1445.9019	1446.5230
H	-1.35374	2.77905	2.41811	1446.7481	1448.6184	1451.9929
Ir	-1.66919	-0.76962	-0.29536	1453.4079	1457.4707	1460.9976
C	1.25181	1.29283	-1.24006	1463.4617	1464.5733	1465.8750
C	1.75447	-0.09706	-1.36347	1467.6875	1471.6157	1473.3288
O	1.04415	-1.03528	-1.70054	1474.9511	1475.3178	1480.9176
C	3.17351	-0.44608	-1.00800	1482.4138	1487.2273	1488.6184
C	4.27244	0.00077	-1.74673	1489.0411	1500.9517	1501.7839
C	3.36598	-1.35335	0.02685	1510.6506	1528.2745	1530.7245
C	5.55279	-0.44326	-1.43257	1539.8925	1546.6495	1654.5031
C	4.65215	-1.77126	0.35029	1665.0732	1674.9939	1726.1504
H	2.50014	-1.71734	0.58139	1758.6941	1780.5771	1847.6278
C	5.74877	-1.32713	-0.37454	3016.3132	3017.1783	3023.0676
H	6.40484	-0.09917	-2.01858	3026.2687	3029.0859	3032.7753
H	6.74727	-1.67255	-0.12118	3037.0549	3037.4715	3041.3252
O	4.02111	0.86214	-2.76613	3042.6560	3043.2827	3045.0374
H	4.84649	1.11915	-3.19064	3050.6597	3058.3617	3084.7120
C	-0.02856	1.53725	-1.91517	3100.3591	3101.7115	3110.8897
C	2.23141	2.41159	-1.16183	3112.3794	3112.6017	3113.5274
C	4.24076	3.05621	-0.10541	3123.1044	3123.5698	3124.2351
H	3.85072	4.03437	0.20227	3124.6915	3125.1148	3131.1358
H	4.70209	3.19284	-1.09484	3132.7644	3134.7078	3143.6192
C	5.20198	2.46646	0.89462	3143.9583	3144.9330	3145.8383
H	6.07540	3.11493	1.01778	3147.4022	3148.9702	3152.0283
H	4.71946	2.34544	1.87030	3153.4006	3161.6315	3166.0197
H	5.54505	1.47828	0.56084	3174.4345	3177.2347	3193.4584
O	3.15632	2.13662	-0.22361	3196.8982	3214.5920	3899.9676
O	2.20891	3.46517	-1.76115			
C	-0.23050	2.68653	-2.85025			
H	-1.24407	2.63440	-3.25506			
H	-0.07402	3.63476	-2.32739			
H	0.51996	2.66827	-3.64719			
O	-1.00713	0.79077	-1.74203			
Cl	4.88706	-2.89570	1.67105			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.732978 Electronic Energy = -2525.93066911
Internal Energy (E)= -2525.15005811 Enthalpy (H)= -2525.14911411
Gibbs Free Energy (G)=-2525.27543411 Gibbs Free Energy of Solvation=-2527.00338967

St.Pt.	General Structure	Ball & Stick model
IX-3		

Cartesian co-ordinate

Atoms	X	Y	Z
H	1.07024	1.24830	-0.12154
C	-1.97693	-1.73329	-2.20542
C	-1.47505	-2.61795	-1.20727
C	-2.41571	-2.60012	-0.09624
C	-3.52186	-1.72362	-0.45508
C	-3.23137	-1.15603	-1.74224
C	-3.06150	1.74701	0.74702
O	-2.15753	0.85092	1.02207
O	-3.94646	1.63895	-0.09647
C	-2.85609	3.05417	1.52475
O	0.07136	-0.76616	0.88352
C	0.38310	0.07383	1.83569
O	0.68235	1.25281	1.65559
C	0.39518	-0.52473	3.24817
C	-4.70410	-1.42925	0.39561
H	-5.53320	-2.10534	0.15111
H	-4.46095	-1.55459	1.45663
H	-5.01877	-0.39198	0.25242
C	-4.07513	-0.23019	-2.54263
H	-4.57292	-0.77352	-3.35738
H	-4.82300	0.26202	-1.91980
H	-3.46178	0.56385	-2.98269

Frequencies

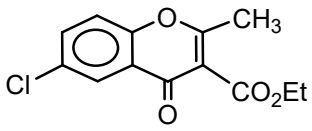
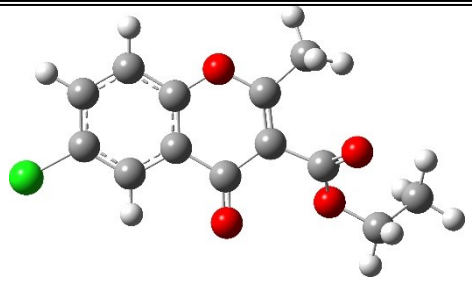
23.1263	33.7342	40.3935
46.1555	49.0061	59.0877
64.4298	67.2785	71.8282
72.8419	80.2864	84.6936
87.1198	96.1440	101.3768
103.8491	110.5123	111.3296
114.9406	121.2896	129.9342
133.7129	139.0297	141.5364
144.8319	156.9111	157.4286
163.2423	170.5240	177.3730
179.7001	186.8733	192.0660
197.4591	206.4579	216.5766
223.6322	236.3060	237.6136
239.8572	255.3898	259.6920
263.7928	265.9986	273.9743
278.4883	287.1204	289.8438
300.2409	306.1723	314.1889
315.5726	319.3446	323.7970
334.6703	336.3445	337.5321
338.9313	340.0410	343.2727
345.9650	350.7643	354.2456
379.9889	381.3171	385.4411
386.7902	389.4868	397.7331
407.5406	415.5080	423.1195
430.2078	438.7683	443.8961
448.5154	456.6917	466.0724
510.7702	518.8832	536.0226

C	-2.30742	-3.45974	1.11125	536.3979	545.5572	554.2530
H	-1.28702	-3.44200	1.50901	566.8623	574.0991	580.6224
H	-2.98603	-3.13391	1.90504	586.2106	600.3463	603.9069
H	-2.55446	-4.49970	0.85953	605.8049	631.2313	642.2884
C	-0.20200	-3.38786	-1.22106	661.4636	671.0798	705.9751
H	0.27504	-3.33906	-0.23442	752.0109	788.9321	789.3257
H	-0.38242	-4.44437	-1.45787	799.9006	802.5710	808.5598
H	0.50803	-2.97601	-1.94495	809.7056	813.5956	814.1292
C	-1.37449	-1.42582	-3.52845	816.5257	854.8380	861.1277
H	-0.38015	-1.86059	-3.64100	886.9705	901.5084	909.0119
H	-2.02673	-1.81453	-4.32146	913.7929	922.9795	940.5387
H	-1.27988	-0.34460	-3.67322	943.8984	949.7173	955.3622
C	-1.05033	-0.85783	3.62915	958.2459	962.2493	965.2773
H	-1.08111	-1.28269	4.64159	967.3070	971.0670	1003.6456
H	-1.68244	0.03772	3.60427	1009.7429	1032.2149	1033.1678
H	-1.48071	-1.58615	2.93252	1038.0361	1041.7758	1043.3614
C	0.96857	0.47851	4.24111	1044.3266	1045.0692	1045.5241
H	0.97687	0.04474	5.24996	1050.6961	1051.3888	1070.4816
H	1.99507	0.75619	3.97516	1093.1581	1097.5624	1108.1503
H	0.37398	1.39815	4.26349	1109.0580	1114.8591	1130.7238
C	1.24059	-1.79764	3.25863	1139.6458	1169.5256	1173.2320
H	0.85028	-2.54689	2.55909	1184.3990	1188.5315	1230.3047
H	2.28170	-1.58557	2.97898	1233.1723	1239.6849	1245.0804
H	1.24980	-2.23696	4.26489	1250.0330	1261.7704	1262.5053
C	-4.16209	3.83600	1.58032	1272.7021	1274.9765	1280.0204
H	-4.92190	3.29604	2.15943	1282.8966	1290.6416	1321.0342
H	-3.99958	4.81077	2.05902	1356.7399	1362.2962	1366.6853
H	-4.56474	3.99644	0.57541	1371.4945	1372.1643	1375.0125
C	-1.80875	3.83667	0.71964	1375.9024	1379.8348	1385.0771
H	-1.61790	4.80809	1.19531	1386.2701	1387.7505	1390.3570
H	-0.86367	3.27895	0.67833	1393.1746	1395.2001	1399.1988
H	-2.16112	4.01776	-0.30430	1412.4368	1417.7108	1424.1133
C	-2.31782	2.80880	2.93146	1426.8429	1427.9580	1429.2373
H	-2.20177	3.76707	3.45593	1437.9255	1440.4626	1443.7228
H	-3.00454	2.18649	3.52134	1450.3142	1451.5341	1452.8358
H	-1.34119	2.31330	2.89164	1453.4958	1453.7713	1457.1916
Ir	-1.68522	-0.64235	-0.32342	1457.6146	1461.9358	1465.3700
C	1.40468	1.40292	-1.17879	1468.8563	1470.6195	1471.8284
C	1.94664	0.04159	-1.57929	1472.6749	1473.5932	1475.3110
O	1.30343	-0.68354	-2.31220	1480.9546	1481.9817	1482.6343
C	3.22617	-0.45205	-0.97937	1485.1963	1489.7468	1493.8056
C	4.45804	0.01701	-1.44041	1496.6175	1499.6243	1508.1118
C	3.17632	-1.45896	-0.02294	1516.9267	1526.5957	1532.9806
C	5.63955	-0.50581	-0.92756	1545.2636	1657.1523	1673.1571
C	4.36516	-1.97494	0.48152	1732.2160	1760.4830	1771.4577
H	2.20692	-1.81089	0.32943	1812.5071	1865.2475	2781.3852
C	5.59474	-1.50532	0.03957	3017.8197	3023.1538	3024.2082
H	6.59945	-0.13886	-1.28986	3030.5247	3031.1490	3035.5652
H	6.51218	-1.92482	0.44284	3036.4665	3038.1863	3038.5582
O	4.42130	0.98181	-2.39648	3038.8867	3039.0121	3042.2063
H	5.31482	1.22763	-2.65882	3045.3405	3051.6385	3097.9051
C	0.15418	1.67374	-1.98183	3098.4781	3106.6998	3107.5012
C	2.42083	2.52007	-1.08838	3110.2028	3112.5282	3118.4659
C	4.31998	3.18761	0.13330	3119.0097	3120.2662	3123.4297
H	3.92480	4.20224	0.26232	3124.6806	3125.0464	3126.2925
H	4.93154	3.18812	-0.78065	3126.5020	3128.2596	3137.4303
C	5.08256	2.70272	1.33777	3142.8238	3143.5576	3144.7496
H	5.94370	3.34955	1.53298	3148.0670	3152.5367	3153.2662
H	4.43966	2.70198	2.22341	3159.6626	3167.6855	3169.3456
H	5.44243	1.67884	1.18039	3173.4967	3181.9685	3205.9581
O	3.22797	2.28134	-0.05392	3208.0389	3212.0735	3897.7099

O	2.49314	3.49736	-1.79561
C	0.24950	2.36838	-3.29491
H	-0.73729	2.42825	-3.75973
H	0.70229	3.35721	-3.17318
H	0.93875	1.79484	-3.93057
O	-0.92513	1.25581	-1.57657
Cl	4.31619	-3.25778	1.66855

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.740942 Electronic Energy = -2525.93844601
Internal Energy (E)= -2525.14767801 Enthalpy (H)= -2525.14673401
Gibbs Free Energy (G)=-2525.27712301 Gibbs Free Energy of Solvation=-2527.00824365

St.Pt.	General Structure	Ball & Stick model
X-3		

Cartesian co-ordinate

Atoms	X	Y	Z
C	1.36249	1.25626	0.10723
C	1.17535	-0.10614	-0.09170
C	-0.18017	-0.65807	-0.29467
C	-0.95529	1.66996	-0.03289
O	0.30574	2.12113	0.12575
C	2.28939	-0.94912	-0.10763
C	2.62991	1.80264	0.29174
C	3.54647	-0.41145	0.07874
C	3.72724	0.96169	0.27791
H	2.12833	-2.01182	-0.26972
H	4.72916	1.35705	0.41899
H	2.73272	2.87347	0.44118
O	-0.34936	-1.83987	-0.54463
C	-1.24852	0.34847	-0.20550
C	-1.91307	2.80662	0.01086
H	-2.15962	3.12585	-1.00753
H	-2.85666	2.52251	0.47829
H	-1.45582	3.64411	0.54316
C	-2.67531	-0.03437	-0.37530
C	-4.27740	-1.71582	0.00717

Frequencies

36.1097	41.9415	68.5190
83.0060	102.8029	133.7843
138.0399	151.7872	180.0934
189.0060	235.7565	250.6920
278.5045	310.9833	353.3898
359.2878	362.6424	393.3119
402.3150	439.5135	478.9014
520.4291	544.8407	559.8704
590.5372	593.6383	668.7026
685.4624	701.8716	760.9837
772.8551	813.4604	832.9692
837.8626	878.6661	897.3228
927.1524	943.9291	963.7081
1011.3149	1043.6801	1049.4769
1086.9422	1114.3562	1126.9601
1131.7552	1166.1057	1195.4814
1230.4367	1244.9315	1274.9484
1313.5087	1339.8010	1380.2651
1390.0347	1391.9913	1407.0744
1422.5899	1447.3646	1450.3399
1466.6711	1472.5608	1482.6747
1488.8931	1503.2727	1629.9504
1668.6954	1678.0022	1803.9944
1828.3541	3048.9908	3063.9380
3074.5395	3131.3368	3139.7081

H	-4.17514	-2.80298	0.06771	3147.5441	3154.9489	3186.8133
H	-4.63783	-1.44581	-0.99091	3203.4419	3212.8313	3215.8210
C	-5.18822	-1.17759	1.08322			
H	-6.18027	-1.63398	1.00225			
H	-4.78802	-1.40208	2.07723			
H	-5.30190	-0.09413	0.98375			
O	-3.50659	0.66400	-0.91901			
O	-2.93880	-1.22184	0.16923			
Cl	4.94823	-1.45165	0.06528			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.217125 Electronic Energy = -1262.60023117
Internal Energy (E)= -1262.36680717 Enthalpy (H)= -1262.36586317
Gibbs Free Energy (G)=-1262.42801817 Gibbs Free Energy of Solvation=-1263.08796695

Combined PES associated to the conversion from I to VI for S4 and S5 of first part of C-H activation

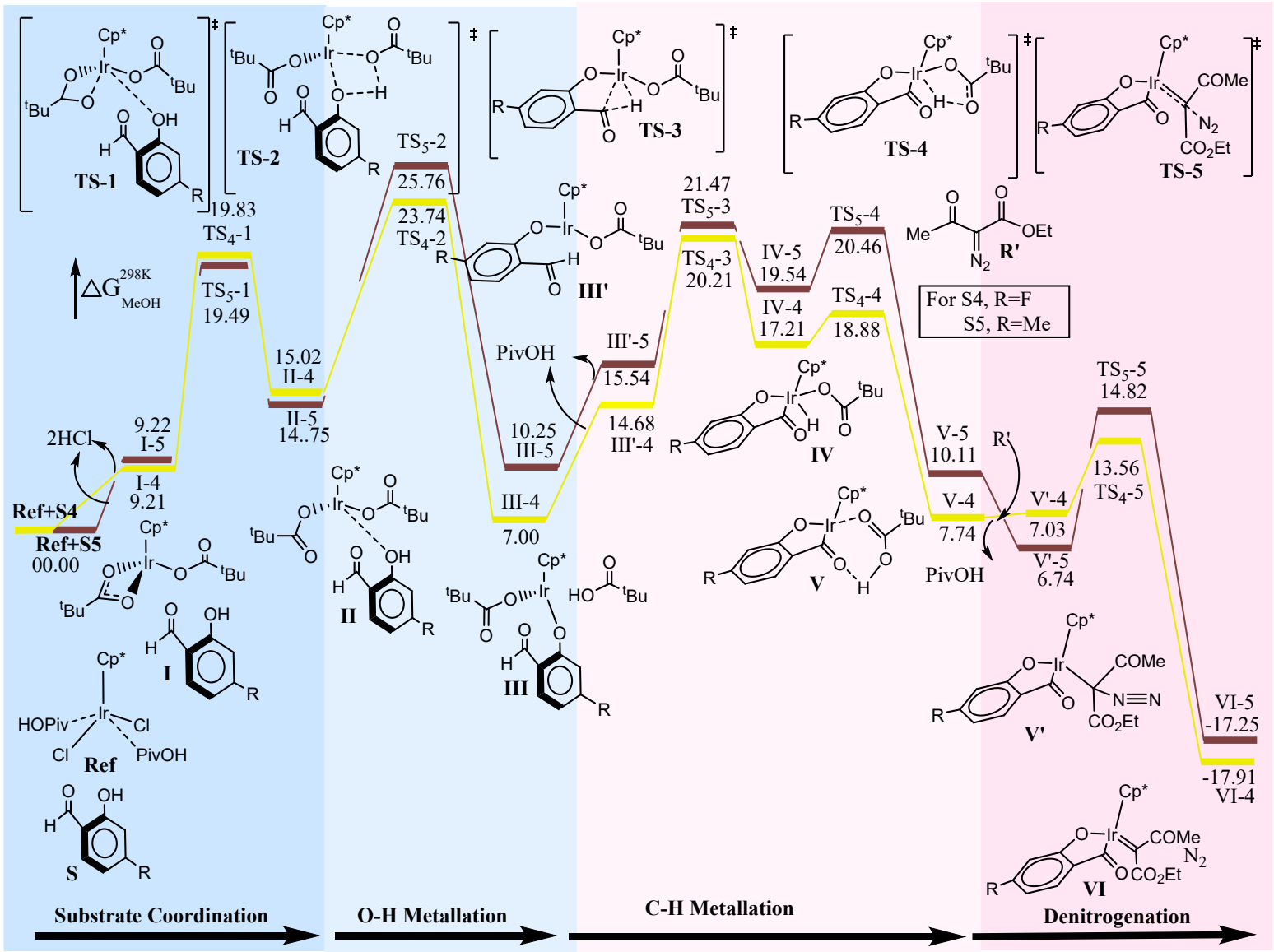


Fig-15: PES with Gibbs free energy (kcal/mol) and the structures of the stationary points of first part of path using M06L functional & 6-311++G(d,p) basis set for non-metals and triple-zeta SDD for metal. (Yellow colour for S4 and Brown colour for S5)

Combined PES associated to the conversion from VI to X for S4 and S5 of first part of C-H activation

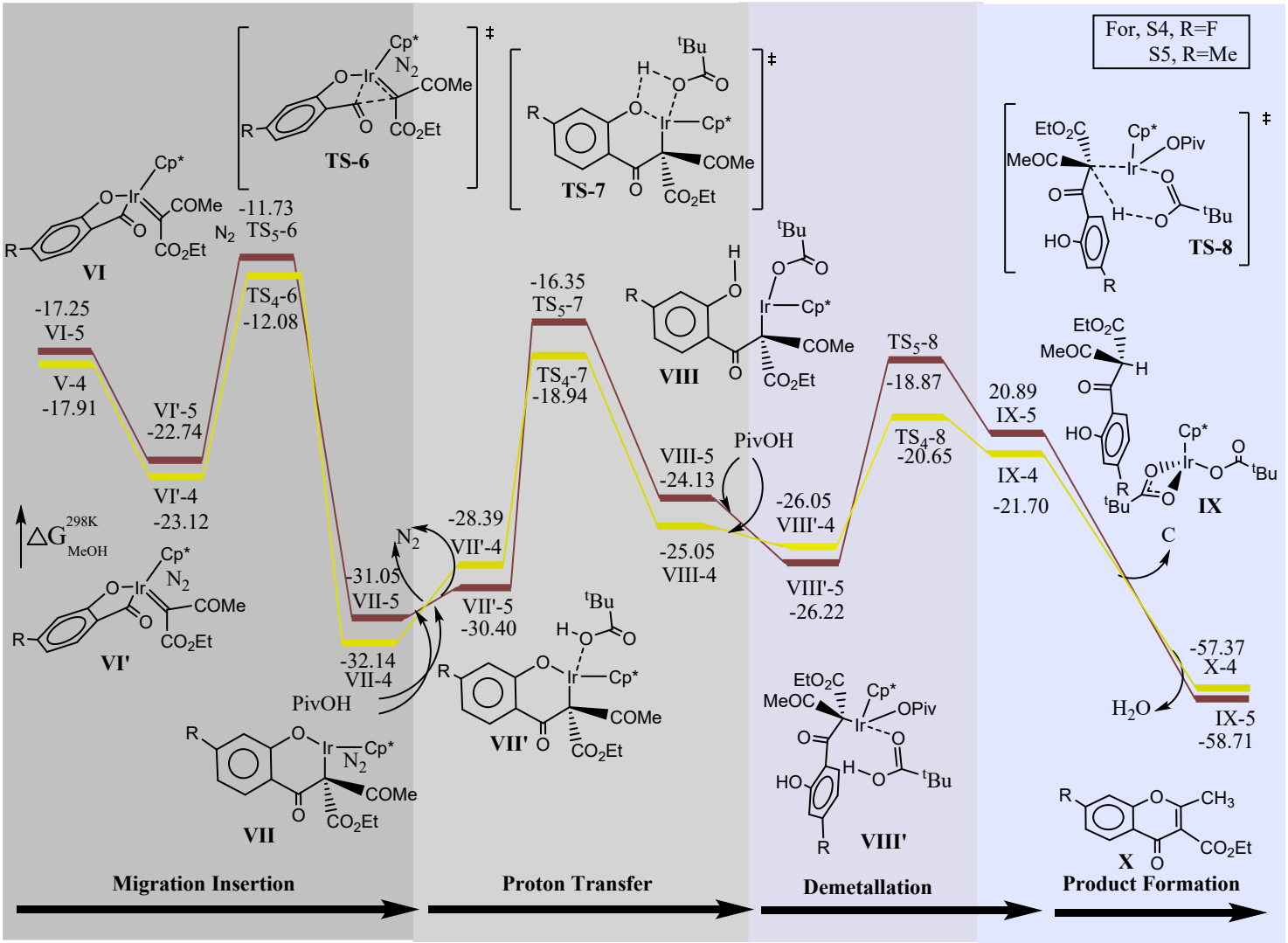
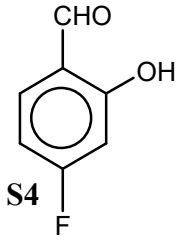
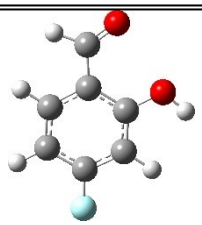


Fig-16: PES with Gibbs free energy (kcal/mol) and the structures of the stationary points of first part of path using M06L functional & 6-311++G(d,p) basis set for non-metals and triple-zeta SDD for metal. (Yellow colour for S4 and Brown colour for S5)

St.Pt.	General Structure	Ball & Stick model
S4		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.35035	0.82555	0.00003
O	-1.23633	1.83213	0.00014
C	1.02321	1.06756	-0.00025
C	1.89938	-0.00438	-0.00035
C	-0.82619	-0.50364	0.00020
C	1.47252	-1.32423	-0.00020
C	0.10628	-1.54552	0.00008
H	-0.27316	-2.56684	0.00022
H	2.19926	-2.12948	-0.00030
C	-2.25173	-0.86559	0.00050
H	-2.40098	-1.97576	0.00064
O	-3.19720	-0.11334	0.00051
H	1.42079	2.08031	-0.00039
H	-0.76480	2.67353	0.00014
F	3.20537	0.25217	-0.00061

Frequencies

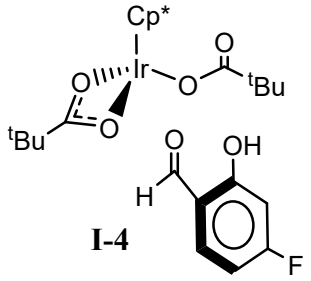
80.3891	185.8014	212.7594
221.1941	321.5240	339.7674
384.7734	425.4629	467.7012
485.9805	545.3134	632.3784
642.6338	703.3649	762.2783
797.9469	811.5415	812.5547
945.1105	1011.5663	1023.7296
1112.5921	1164.6375	1227.2503
1235.7327	1303.3158	1358.2397
1402.8883	1425.0077	1498.1503
1564.8465	1662.2411	1686.9657
1854.3290	2832.0008	3174.6666
3192.2500	3228.7382	3875.8454

Statistical Thermodynamic Analysis

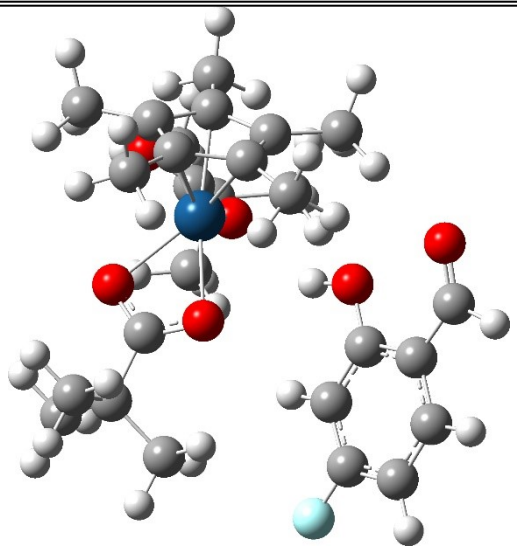
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.106193 Electronic Energy = -519.737181697
Internal Energy (E)= -519.622738697 Enthalpy (H)= -519.621794697
Gibbs Free Energy (G)=-519.664159697 Gibbs Free Energy of Solvation=-519.683348235

St.Pt.	General Structure	Ball & Stick model

I-4



I-4



Cartesian co-ordinate

Atoms	X	Y	Z
C	2.89322	-1.05009	-0.93918
C	3.32477	-0.75596	0.40156
C	2.54439	-1.55673	1.32609
C	1.62666	-2.34801	0.53416
C	1.83287	-2.03619	-0.86023
C	-2.70104	-1.13278	-0.82503
C	-0.87002	2.10461	2.78450
C	-0.09795	1.24472	1.80723
O	1.05556	1.58866	1.40539
O	-0.54264	0.11393	1.43229
C	2.67249	-1.56868	2.80937
H	2.97852	-0.58637	3.18587
H	1.71683	-1.81642	3.28341
H	3.41474	-2.30471	3.14362
C	0.58543	-3.26677	1.06391
H	-0.27164	-3.32497	0.38353
H	0.99357	-4.27875	1.18120
H	0.22252	-2.93055	2.04085
C	1.14229	-2.64533	-2.02807
H	0.17594	-3.08463	-1.76152
H	0.95198	-1.88982	-2.79908
H	1.77705	-3.42356	-2.47211
C	3.46862	-0.49198	-2.19088
H	2.72029	-0.46932	-2.98915
H	3.81075	0.53572	-2.04946
H	4.30855	-1.11285	-2.52972
C	4.32589	0.28309	0.76007
H	4.20643	0.60779	1.79811
H	5.34768	-0.09541	0.63163
H	4.19542	1.16355	0.12137
C	0.72688	1.85376	-1.77539
O	0.11223	0.86458	-1.16839
O	1.91952	2.09446	-1.66739
C	-0.21132	2.74315	-2.59834
O	-1.51527	-1.23280	-1.41231
C	-1.15959	1.90309	-3.45295

Frequencies

22.3048	42.8337	47.5040
54.7203	68.3514	71.6657
76.2831	89.4365	93.5344
97.0830	99.2584	105.5202
111.1279	114.2399	122.7147
131.6585	153.8116	160.3043
165.2508	168.7204	175.8074
183.3010	185.0905	190.6618
195.3691	200.6125	202.5697
213.3622	225.9097	227.2796
231.5416	234.9045	242.6336
245.4817	250.8118	269.6703
287.2739	294.3913	296.7241
304.3857	311.1734	316.7436
320.7316	324.0394	330.0204
335.4680	345.7718	349.9205
357.5579	374.6834	380.1762
390.9831	393.0227	397.0606
411.0468	417.7380	429.7786
452.9334	457.9204	463.3469
486.8336	510.7695	532.6979
537.1345	542.7116	547.5342
549.4394	568.7693	583.5612
587.4824	602.8229	622.9773
632.4765	633.0146	655.5730
729.6793	763.0804	785.8731
799.8409	804.0735	805.8281
809.7072	815.9790	822.1419
834.2307	904.4476	913.3914
929.9030	937.4989	940.5831
943.4950	945.0707	950.3694
951.3582	953.7888	954.5714
965.4483	969.1727	1019.8520
1032.2851	1033.0910	1034.4693
1036.4527	1036.8533	1040.8454
1042.1033	1043.6556	1051.7136
1056.4414	1090.6206	1091.6808
1105.3614	1117.1198	1182.7895
1186.8153	1210.6834	1230.7160
1237.4503	1238.9595	1243.7745

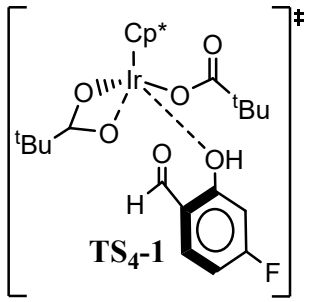
H	-1.83698	1.28965	-2.84793	1254.3176	1262.4913	1265.1107
H	-1.77854	2.55878	-4.07893	1268.0210	1343.3978	1357.9472
H	-0.60346	1.23275	-4.12154	1373.6426	1378.0150	1379.0775
C	0.61226	3.65979	-3.49513	1380.8575	1384.9417	1388.8430
H	-0.05003	4.32698	-4.06172	1389.2510	1397.7513	1401.2330
H	1.30526	4.26736	-2.90524	1405.9760	1410.5009	1412.9695
H	1.20949	3.08082	-4.20943	1425.9519	1429.9989	1433.4532
C	-1.00826	3.58636	-1.59791	1438.0908	1440.8885	1442.1528
H	-0.33339	4.19537	-0.98251	1448.1144	1449.7310	1451.7948
H	-1.69212	4.26142	-2.12875	1453.7433	1454.6880	1459.3110
H	-1.60339	2.95405	-0.92558	1461.5526	1464.9501	1465.6195
C	-2.36896	1.86725	2.64264	1466.5161	1469.5299	1475.4991
H	-2.62130	0.80969	2.77394	1479.2905	1481.0535	1484.3384
H	-2.90815	2.45184	3.39878	1486.8832	1491.1976	1494.6937
H	-2.73171	2.18273	1.65659	1496.8157	1501.0543	1503.1884
C	-0.53830	3.57842	2.57509	1511.8604	1513.7926	1519.6419
H	-1.05981	4.18378	3.32714	1545.0109	1566.1353	1599.8686
H	0.53716	3.76123	2.66132	1650.9887	1687.4395	1787.8690
H	-0.85981	3.92010	1.58351	1825.3801	2848.5341	3020.2126
C	-0.40201	1.65802	4.17718	3026.9825	3028.5127	3035.1514
H	0.67562	1.82201	4.29943	3036.8989	3038.5747	3039.2708
H	-0.92719	2.23415	4.94926	3040.9582	3042.4049	3043.3484
H	-0.61373	0.59358	4.33856	3043.5353	3109.8182	3111.0099
Ir	1.25413	-0.25968	0.21714	3111.9849	3115.7957	3116.2790
C	-3.23819	0.11283	-0.48328	3121.5303	3121.9202	3123.0103
C	-4.49068	0.17590	0.09250	3126.1227	3126.7213	3127.0504
C	-5.26835	-0.94983	0.34684	3129.0746	3130.7328	3131.1909
C	-3.45478	-2.30451	-0.56757	3143.5937	3145.1509	3145.8388
C	-4.72959	-2.17444	0.00286	3147.4601	3147.8663	3149.5617
H	-5.30070	-3.08424	0.18709	3161.8592	3172.3310	3175.2193
H	-1.05528	-0.35950	-1.44296	3208.4013	3221.3745	3458.6200
H	-2.66672	1.02239	-0.65349			
C	-2.98388	-3.66292	-0.82774			
H	-3.78199	-4.42584	-0.64330			
O	-1.87800	-4.02464	-1.18049			
H	-6.24976	-0.84211	0.79652			
F	-4.97536	1.37496	0.41935			

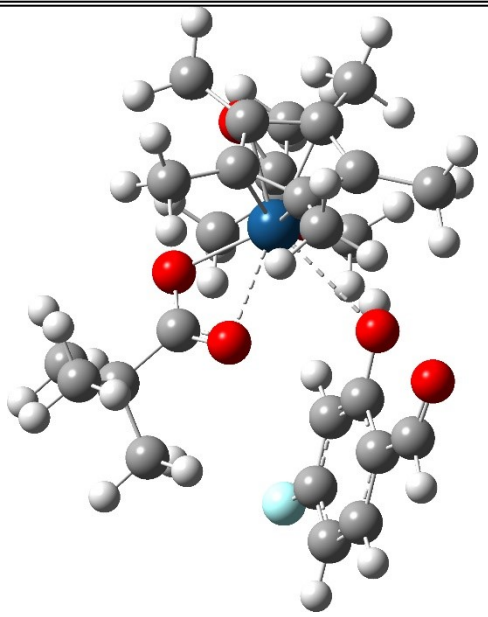
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.605623 Electronic Energy = -1706.72566793
Internal Energy (E)= -1706.08056593 Enthalpy (H)= -1706.07962193
Gibbs Free Energy (G)=-1706.18803993 Gibbs Free Energy of Solvation=-1706.24032032

St.Pt.	General Structure	Ball & Stick model

TS_4-1





Cartesian co-ordinate

Atoms	X	Y	Z
C	2.90397	-1.01002	-0.83539
C	3.02675	-0.93142	0.60827
C	2.12541	-1.92203	1.18744
C	1.45027	-2.58138	0.11298
C	1.91517	-2.01415	-1.14366
C	-2.32025	-0.68318	-1.38580
C	-1.71373	0.74636	2.97085
C	-0.79915	0.23824	1.86179
O	0.32116	0.81631	1.68122
O	-1.12318	-0.77744	1.20622
C	1.92177	-2.15293	2.64335
H	1.90322	-1.20471	3.19296
H	0.96960	-2.65947	2.82853
H	2.72530	-2.77225	3.06114
C	0.40394	-3.62648	0.23981
H	-0.37066	-3.51245	-0.52578
H	0.85337	-4.62167	0.12479
H	-0.08475	-3.57914	1.21688
C	1.51062	-2.47810	-2.49926
H	0.46824	-2.81369	-2.51349
H	1.61658	-1.67630	-3.23888
H	2.14655	-3.31241	-2.82322
C	3.66847	-0.19963	-1.81917
H	3.06549	-0.00111	-2.71172
H	3.94663	0.76692	-1.39040
H	4.57370	-0.73489	-2.13353
C	3.93130	-0.02295	1.35609
H	3.64859	0.03070	2.41180
H	4.96779	-0.37965	1.29503
H	3.86805	0.98647	0.93635
C	1.45729	2.38568	-0.76105
O	0.69211	1.35413	-0.98879
O	2.55778	2.34837	-0.22564
C	0.81465	3.71465	-1.18064

Frequencies

-85.0344	-22.7958	38.0770
46.2777	49.0289	56.0270
69.0575	73.5297	78.4773
79.5363	94.3708	96.2680
103.9030	115.5395	124.0498
133.2229	152.2522	155.2466
157.4153	165.0842	172.6106
183.0667	185.5028	190.1434
192.0235	198.5897	202.4005
208.1420	211.9129	222.1322
228.4797	244.4046	262.4851
263.9967	272.1574	278.4481
285.3263	291.5941	299.6256
306.8048	311.0455	324.0523
331.3402	332.3614	339.1421
340.8999	343.7121	347.1608
353.5056	358.1425	376.0276
379.5117	388.0772	393.2517
409.0144	418.7872	427.3006
441.9850	453.1450	468.0225
472.1878	492.9563	532.2269
538.5180	545.2124	548.2575
549.6283	568.0606	582.0537
589.4830	602.6209	616.1149
622.6871	629.1182	633.8347
652.9510	716.1272	764.1998
786.0199	793.0149	804.1128
808.1085	810.2808	811.7654
820.0295	826.3426	845.0172
908.5120	927.0886	938.5055
939.7841	947.9072	949.2041
951.8716	955.2094	963.5342
968.6778	983.8356	1013.0490
1029.2412	1029.5284	1030.3747
1035.6739	1039.4353	1042.4380
1042.9420	1046.5715	1050.2958
1052.1580	1098.6623	1101.3399
1111.2545	1114.3444	1184.6800

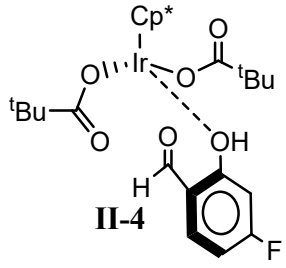
O	-1.06689	-1.10607	-1.63964	1188.9913	1191.9305	1230.9227
C	0.16329	3.60846	-2.55803	1236.7905	1238.8140	1242.2056
H	-0.63162	2.85603	-2.58003	1244.7639	1258.6673	1263.6247
H	-0.27637	4.57481	-2.83784	1271.0632	1323.6456	1351.2958
H	0.90104	3.34361	-3.32653	1358.5488	1372.4191	1373.0817
C	1.86866	4.81545	-1.19529	1375.2102	1381.9464	1383.4951
H	1.40488	5.77620	-1.45498	1389.1168	1395.7292	1407.2664
H	2.35245	4.91036	-0.21845	1408.0698	1409.1507	1413.7361
H	2.65272	4.60285	-1.93185	1414.3330	1417.5181	1424.2997
C	-0.24515	4.03675	-0.12003	1440.4188	1441.3735	1446.8187
H	0.21744	4.12434	0.87162	1447.1571	1452.0983	1453.6874
H	-0.73618	4.99061	-0.35421	1457.3308	1458.2654	1461.1072
H	-1.01750	3.25751	-0.06629	1461.6317	1467.1505	1470.4973
C	-3.13908	0.86886	2.43618	1471.1846	1473.7510	1477.2580
H	-3.47471	-0.06871	1.97824	1479.2178	1481.3169	1481.6589
H	-3.82411	1.12652	3.25444	1487.7491	1488.4204	1492.5692
H	-3.20779	1.66455	1.68306	1498.4280	1499.5150	1502.2737
C	-1.24214	2.08873	3.51478	1506.5627	1514.2760	1526.1353
H	-1.91390	2.42074	4.31724	1531.9638	1562.2906	1657.1857
H	-0.22553	2.02348	3.91637	1667.2873	1686.5092	1774.7119
H	-1.24049	2.85479	2.73040	1829.8658	2843.4837	3022.2999
C	-1.66494	-0.31361	4.07714	3023.5900	3029.3440	3033.7486
H	-0.64238	-0.43351	4.46133	3033.8686	3035.1182	3036.8209
H	-2.30663	-0.01391	4.91566	3037.8215	3038.9011	3041.2447
H	-2.00898	-1.28404	3.70199	3042.4245	3107.9139	3108.3667
Ir	1.03955	-0.44990	0.05390	3108.6090	3113.2344	3113.7510
C	-2.57331	0.67176	-1.18874	3116.6357	3120.2733	3122.5824
C	-3.86597	1.07578	-0.92155	3122.9795	3124.4373	3124.5037
C	-4.93406	0.18776	-0.83851	3126.9713	3130.8956	3138.0808
C	-3.36770	-1.62222	-1.31440	3139.2713	3140.6486	3143.3159
C	-4.66022	-1.15279	-1.03806	3145.8192	3147.1708	3152.0446
H	-5.46883	-1.88149	-0.98752	3156.4222	3162.5826	3176.0464
H	-0.52722	-0.32958	-1.87189	3189.8566	3228.7444	3709.4326
H	-1.74849	1.38389	-1.18967			
C	-3.19838	-3.05526	-1.55419			
H	-4.16404	-3.61479	-1.47233			
O	-2.17439	-3.64764	-1.82920			
H	-5.93074	0.55790	-0.62183			
F	-4.08930	2.37203	-0.70669			

Statistical Thermodynamic Analysis

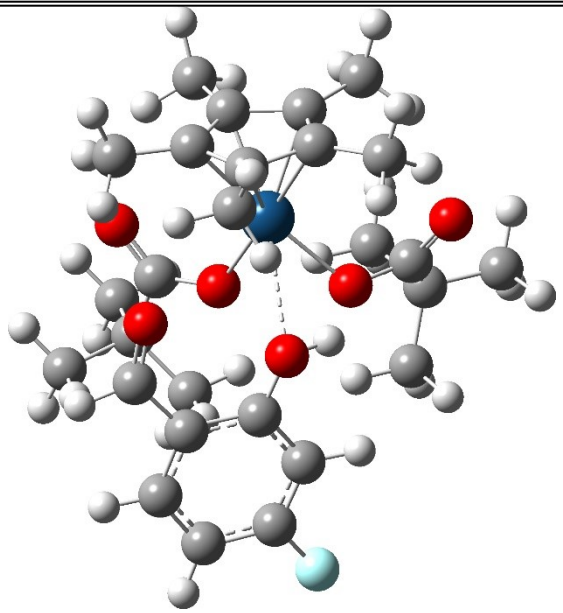
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.604499 Electronic Energy = -1706.70078335
Internal Energy (E)= -1706.05814735 Enthalpy (H)= -1706.05720435
Gibbs Free Energy (G)=-1706.16201035 Gibbs Free Energy of Solvation=-1706.22207577

St.Pt.	General Structure	Ball & Stick model

II-4



II-4



Cartesian co-ordinate

Atoms	X	Y	Z
C	2.97042	-0.26634	-1.32359
C	3.27193	-0.02630	0.05602
C	2.81974	-1.18226	0.83153
C	2.23858	-2.12810	-0.07620
C	2.30706	-1.54148	-1.40099
Ir	1.14254	-0.24544	-0.11915
O	-0.57654	-0.33596	0.95491
O	0.21952	1.61216	-0.50026
O	-0.92493	-2.78864	-1.60079
C	-2.11699	-2.60868	-1.45605
H	-2.79065	-3.47001	-1.21814
C	-2.84403	-1.34140	-1.53005
C	-2.23526	-0.09326	-1.79200
C	-4.21924	-1.37439	-1.25597
C	-3.00111	1.07220	-1.72907
C	-4.99419	-0.23066	-1.21316
H	-4.67758	-2.34339	-1.05752
C	-4.35132	0.98096	-1.44393
H	-2.55137	2.04406	-1.91631
O	-0.94090	-0.03708	-2.12818
H	-0.57625	0.83858	-1.86689
C	-0.82730	-1.18747	1.91561
C	-2.19065	-0.99162	2.59609
C	0.85018	2.75625	-0.33674
C	0.17073	3.66494	0.69130
O	1.89890	3.06572	-0.88354
O	-0.07330	-2.07226	2.29805
C	1.82164	-2.15936	-2.66299
H	1.30669	-3.10315	-2.47749
H	1.10988	-1.50526	-3.17840
H	2.67466	-2.33603	-3.33102
C	3.26417	0.64049	-2.46559
H	3.09702	1.68396	-2.17839
H	4.30225	0.51566	-2.80069

Frequencies

17.7050	35.9384	39.9187
47.4089	53.0252	61.8742
67.0179	76.5687	83.2409
86.2525	93.5491	101.4174
111.4867	120.4341	127.5867
129.0822	131.0286	145.2178
147.1136	163.9693	172.3494
179.3856	189.0384	196.0466
200.7834	212.0284	215.1807
223.2148	229.1078	233.3785
243.4203	246.7562	253.9508
258.1878	262.6039	282.4961
285.3696	292.5435	300.5643
307.1296	310.5786	311.8594
316.7187	318.5432	319.1878
328.2658	337.7225	352.0806
357.5326	359.5437	378.4700
384.9066	396.8855	398.5081
399.7698	416.9835	434.2143
443.6106	458.2107	466.6539
479.8306	491.4171	534.8742
540.4344	543.8089	547.5828
568.0238	572.4091	575.8387
582.4897	600.3800	602.1881
631.9443	642.4862	649.3915
724.1353	750.3826	768.7450
796.5216	801.5404	807.6915
809.4544	811.8405	815.2671
817.1412	821.9912	877.5146
904.7765	917.2173	941.0492
944.7135	945.6260	949.4312
949.9116	953.7618	962.3586
966.5794	975.9186	1009.4914
1029.9255	1034.4330	1035.5106
1036.8088	1037.2967	1040.9311
1043.9156	1044.9293	1045.8774
1052.7415	1096.8468	1102.6004
1115.9724	1117.6049	1187.9326

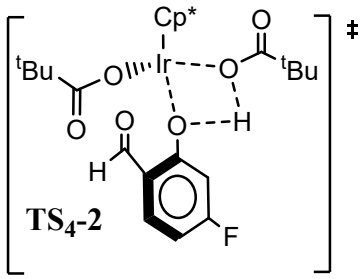
H	2.60924	0.41738	-3.31467	1193.3511	1194.6934	1225.5439
C	3.97339	1.16857	0.58892	1233.9742	1238.4068	1238.8232
H	3.83056	1.26869	1.66913	1239.2375	1250.1124	1267.2705
H	5.05158	1.08027	0.40023	1268.8018	1333.8587	1345.1818
H	3.61199	2.08263	0.10242	1356.8528	1359.9514	1367.6827
C	2.97655	-1.34140	2.29914	1368.7624	1376.7713	1380.1172
H	2.16715	-1.95078	2.70867	1382.0691	1385.3311	1393.1548
H	3.94278	-1.80881	2.53035	1397.8756	1401.9239	1406.9479
H	2.94300	-0.36752	2.80047	1412.6186	1415.5526	1421.4126
C	1.72216	-3.48449	0.24148	1423.3016	1434.8206	1436.9422
H	2.50430	-4.23476	0.06408	1440.6207	1448.8546	1450.4646
H	1.38957	-3.53955	1.27961	1451.3779	1455.9840	1459.9120
H	0.85942	-3.72331	-0.38763	1461.5971	1463.9409	1464.2489
C	-2.96048	0.20711	2.05611	1471.9938	1472.9651	1475.2310
H	-3.14790	0.11392	0.98048	1475.4858	1477.0942	1481.2957
H	-3.92849	0.28690	2.56941	1484.1839	1486.7757	1493.3674
H	-2.41139	1.14326	2.21765	1494.2965	1495.9323	1496.2761
C	-1.92493	-0.80528	4.09191	1507.4757	1513.0265	1514.3556
H	-2.87478	-0.70345	4.63291	1537.1449	1560.7099	1649.5135
H	-1.37697	-1.66067	4.49960	1684.4838	1772.7290	1777.1487
H	-1.33393	0.10142	4.27793	1830.9799	2842.9989	3013.9633
C	-3.00234	-2.27182	2.38494	3020.9040	3025.9735	3029.0811
H	-2.44301	-3.14791	2.72991	3035.2027	3037.1998	3038.7633
H	-3.94658	-2.21498	2.94252	3039.2086	3039.9357	3045.6890
H	-3.25108	-2.41307	1.32389	3046.7143	3098.2594	3101.3733
C	0.77179	5.06246	0.64306	3106.5462	3108.5383	3114.2453
H	0.61448	5.52842	-0.33686	3117.2462	3119.4988	3121.4710
H	0.30662	5.69957	1.40626	3122.7236	3127.3447	3130.0062
H	1.85162	5.03293	0.82170	3132.6671	3137.6927	3138.6686
C	-1.33794	3.71999	0.45996	3144.4518	3151.7868	3161.3038
H	-1.77816	2.71683	0.50182	3162.3588	3168.6548	3170.7520
H	-1.81152	4.34266	1.23029	3181.7599	3189.1786	3203.6929
H	-1.57517	4.16604	-0.51576	3210.6996	3228.2350	3521.5537
C	0.44775	3.01949	2.05678			
H	1.52932	2.93625	2.23855			
H	0.01905	3.63574	2.85797			
H	0.00691	2.01581	2.10940			
H	-6.05746	-0.24748	-0.99808			
F	-5.06615	2.10199	-1.40261			

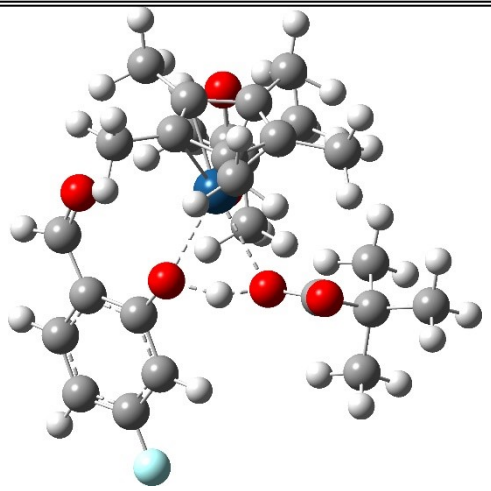
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.604877 Electronic Energy = -1706.70885636
Internal Energy (E)= -1706.06422336 Enthalpy (H)= -1706.06327936
Gibbs Free Energy (G)=-1706.17336936 Gibbs Free Energy of Solvation=-1706.23244823

St.Pt.	General Structure	Ball & Stick model

TS_4-2





Cartesian co-ordinate

Atoms	X	Y	Z
C	2.80381	-0.39916	-1.34236
C	3.04960	0.01851	0.01202
C	2.67426	-1.05578	0.90987
C	2.19473	-2.15362	0.09241
C	2.28978	-1.73632	-1.29699
Ir	0.94750	-0.45299	-0.18565
O	-0.73051	-0.44962	0.93955
O	-0.00004	1.79844	-0.44977
O	-0.70531	-2.79762	-1.30449
C	-1.90392	-2.58292	-1.30355
H	-2.61805	-3.42432	-1.12372
C	-2.58023	-1.31132	-1.50741
C	-1.92041	-0.07137	-1.71369
C	-3.98325	-1.33770	-1.45093
C	-2.70338	1.08670	-1.83305
C	-4.75579	-0.20159	-1.58383
H	-4.46709	-2.30084	-1.28747
C	-4.07948	1.00050	-1.77208
H	-2.23451	2.05621	-1.97852
O	-0.59687	0.04284	-1.82659
H	-0.28467	1.12633	-1.38449
C	-0.94354	-1.11409	2.04262
C	-2.27624	-0.77210	2.72247
C	0.76272	2.87531	-0.46624
C	0.52800	3.76651	0.75247
O	1.53865	3.15634	-1.36539
O	-0.18807	-1.94341	2.53397
C	1.93510	-2.53558	-2.49792
H	1.47448	-3.48750	-2.23180
H	1.22667	-1.99256	-3.13232
H	2.84389	-2.72752	-3.08288
C	3.00292	0.43129	-2.56110
H	2.65287	1.45776	-2.39311
H	4.06290	0.46381	-2.84464
H	2.43919	0.02085	-3.40478
C	3.64729	1.32174	0.39564
H	3.40253	1.59692	1.42639
H	4.74079	1.24569	0.32568

Frequencies

-134.9090	23.1266	38.8290
40.1413	51.1506	64.0879
72.3491	78.3004	84.0290
93.0332	99.8048	106.9517
109.3687	116.9799	119.0700
125.3528	141.5703	158.6423
166.4998	172.3959	176.9374
186.7359	191.1593	194.5632
199.4469	206.5409	214.9425
221.0736	222.4472	227.1079
236.5500	243.8476	250.0462
252.9036	262.0478	273.2618
279.7808	280.0120	296.5927
301.1397	309.5499	314.9518
317.8950	320.5211	328.4181
331.8648	345.9181	357.8735
362.1879	374.0880	385.0343
388.4114	392.3474	396.0117
402.9306	443.6245	450.2565
457.4875	463.9091	474.2821
484.1107	513.6751	532.5719
540.0525	545.6024	550.9541
579.8633	583.0631	586.2839
593.8969	604.3738	612.3644
648.4536	649.3539	666.9773
730.7911	746.3890	785.8987
792.5659	801.8802	806.9580
810.7502	813.4680	817.6902
820.2579	828.3805	857.6743
923.7963	925.8308	946.4790
947.1545	950.4965	953.3598
955.6069	958.0318	963.7193
971.3569	982.8930	1020.1625
1027.3137	1032.4118	1036.7868
1039.3041	1040.2989	1042.5503
1045.1048	1045.5760	1049.1230
1054.6919	1101.6643	1105.3682
1114.5884	1116.7237	1190.3646
1194.5059	1220.0796	1231.8285
1235.8200	1241.7753	1245.3887
1247.8927	1264.1293	1267.7479
1270.0550	1344.9119	1358.9667

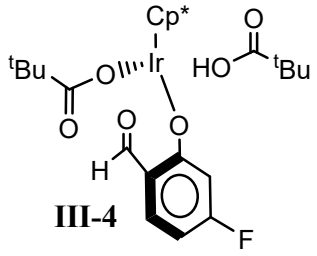
H	3.32426	2.12877	-0.27217	1367.0219	1375.9194	1380.4444
C	2.83975	-1.07023	2.38677	1381.0360	1382.7705	1385.7630
H	1.99612	-1.58503	2.85653	1392.8958	1394.9656	1396.7474
H	3.77398	-1.57663	2.66290	1400.3362	1410.6424	1417.0724
H	2.87717	-0.05214	2.78921	1417.3568	1420.5746	1429.4611
C	1.77807	-3.49177	0.57997	1436.4647	1440.7460	1441.7951
H	2.64303	-4.16837	0.60144	1443.6366	1446.6756	1448.2271
H	1.35248	-3.41047	1.58301	1454.6158	1455.9422	1459.7548
H	1.00830	-3.91677	-0.07064	1463.1462	1464.6312	1466.2416
C	-3.04556	0.32103	1.99082	1468.9894	1473.6591	1477.0086
H	-3.34979	-0.00921	0.99104	1477.9688	1479.8434	1481.3628
H	-3.95064	0.57890	2.55711	1487.9948	1493.4634	1499.0209
H	-2.44240	1.22954	1.86524	1499.7838	1502.5631	1503.9780
C	-1.95683	-0.32494	4.15027	1505.4648	1511.1676	1516.8421
H	-2.88613	-0.13327	4.70249	1527.7572	1555.0992	1626.7068
H	-1.38514	-1.09451	4.67894	1646.4984	1685.9594	1769.6003
H	-1.36874	0.60276	4.15199	1808.1979	1814.5707	2849.7594
C	-3.10829	-2.05515	2.76161	3016.2229	3024.2978	3026.3478
H	-2.56548	-2.85628	3.27416	3031.1979	3034.4782	3034.5779
H	-4.05575	-1.87653	3.28666	3034.6330	3035.4699	3040.6170
H	-3.34876	-2.39778	1.74529	3045.7352	3047.0368	3094.2959
C	1.60655	4.83778	0.83174	3105.7575	3108.4811	3110.7652
H	1.62607	5.44690	-0.07776	3113.8188	3116.9819	3120.0336
H	1.42304	5.49427	1.69161	3120.9676	3123.7642	3130.8207
H	2.60156	4.38988	0.94869	3132.1098	3135.4151	3138.4319
C	-0.84580	4.41876	0.54414	3138.6241	3141.5387	3146.9105
H	-1.63722	3.66140	0.49424	3148.0523	3155.8976	3158.4657
H	-1.06729	5.09720	1.37790	3161.4783	3166.4799	3189.7540
H	-0.86598	5.00582	-0.38309	3203.5210	3209.1681	3229.0465
C	0.49766	2.93437	2.03616			
H	1.48223	2.49963	2.25816			
H	0.22544	3.57414	2.88572			
H	-0.22657	2.11439	1.96338			
H	-5.83971	-0.21631	-1.54189			
F	-4.79203	2.11845	-1.90117			

Statistical Thermodynamic Analysis

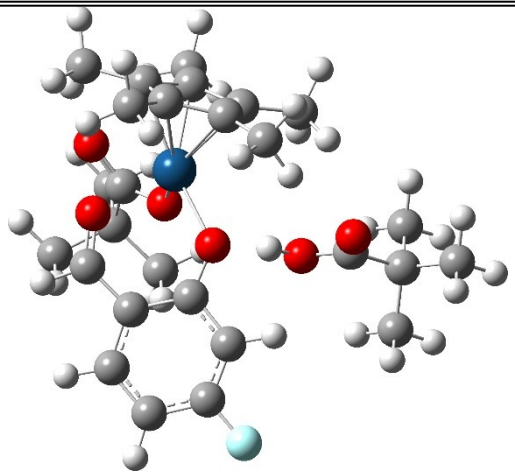
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.601832 Electronic Energy = -1706.69864937
Internal Energy (E)= -1706.05816537 Enthalpy (H)= -1706.05722137
Gibbs Free Energy (G)=-1706.16399337 Gibbs Free Energy of Solvation=-1706.21849461

St.Pt.	General Structure	Ball & Stick model

III-4



III-4



Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.38822	-2.45646	-1.12424
C	-1.11134	-2.47020	0.30326
C	-2.23544	-1.84669	0.97428
C	-3.15641	-1.38908	-0.02389
C	-2.63579	-1.78547	-1.33126
Ir	-1.26281	-0.43842	-0.33824
O	-0.37956	0.84780	1.04872
O	2.35337	-0.72715	0.58492
O	-2.03331	1.43527	-1.13144
C	-1.32383	2.39900	-1.46942
H	-1.86640	3.32947	-1.72203
C	0.09172	2.47154	-1.59825
C	0.95331	1.32745	-1.52573
C	0.63531	3.74504	-1.88658
C	2.33057	1.53879	-1.76772
C	1.97917	3.94012	-2.07811
H	-0.04817	4.59211	-1.94238
C	2.80077	2.80506	-2.01626
H	3.01015	0.69144	-1.74655
O	0.55582	0.11384	-1.29608
H	1.62423	-0.50808	-0.04754
C	-1.10353	1.56693	1.85152
C	-0.31484	2.67928	2.56326
C	3.05575	-1.74286	0.09142
C	4.27191	-2.07106	0.94408
O	2.74593	-2.33719	-0.92450
O	-2.31256	1.45040	2.03703
C	-3.30031	-1.50744	-2.63326
H	-3.71851	-0.49508	-2.65016
H	-2.59372	-1.58812	-3.46469
H	-4.11976	-2.21452	-2.81391
C	-0.44618	-2.95486	-2.16111
H	0.58559	-2.67161	-1.91428
H	-0.49426	-4.04887	-2.23111
H	-0.68077	-2.53901	-3.14566
C	0.03398	-3.14081	0.97657
H	0.40365	-2.53303	1.81019
H	-0.27351	-4.11559	1.37821

Frequencies

20.1192	27.8856	32.9845
44.4698	46.9156	66.9217
69.3110	77.4717	84.2718
85.9685	88.8787	96.5650
109.4945	111.6214	122.3453
135.7137	146.2199	153.9469
170.5069	178.0493	182.6029
185.3743	195.9445	200.1458
205.3179	213.3563	217.4966
223.6153	235.2377	238.9480
247.6689	255.6085	260.2131
265.6828	275.4661	291.1685
299.5946	302.5679	307.9223
311.1395	317.1946	320.1642
327.7801	338.1824	341.7600
342.9989	362.1193	380.7446
383.1190	385.0404	388.5065
393.4671	405.8047	419.2303
428.0988	439.1280	443.8244
446.6266	454.0582	467.1206
468.7512	532.4191	537.3977
543.5710	549.2003	565.5115
571.8708	580.2046	589.1072
591.1014	595.7153	606.2346
640.1005	646.1940	660.8200
714.6494	759.0243	766.4546
784.9133	793.0483	796.6038
809.2716	814.3197	817.2367
819.5270	834.1933	888.4011
915.7680	916.6472	939.4942
949.4795	950.3072	955.0956
957.3453	957.5598	961.1999
961.3752	989.0534	1006.9184
1009.8918	1038.7891	1042.2933
1044.3946	1045.3306	1047.3535
1048.2686	1051.2509	1052.5354
1054.5948	1097.1082	1102.2921
1119.2753	1126.9457	1187.0623
1187.6031	1192.7029	1220.3406
1242.1322	1242.6569	1250.3546
1250.5103	1255.1198	1270.8503
1283.8645	1295.6353	1353.8350
1372.9468	1378.9250	1380.7738

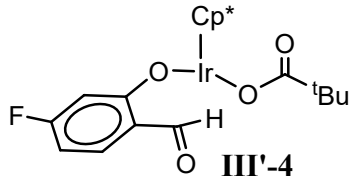
H	0.86415	-3.30340	0.28093	1381.4514	1383.1617	1384.0753
C	-2.37941	-1.68765	2.44473	1386.9766	1398.0570	1402.5057
H	-2.93913	-0.78104	2.68746	1404.0475	1408.8277	1413.4647
H	-2.89268	-2.56117	2.86783	1421.7729	1431.8077	1433.0024
H	-1.39877	-1.60618	2.92574	1435.5587	1438.8200	1441.0516
C	-4.40625	-0.62775	0.24265	1450.7363	1451.8791	1455.1367
H	-5.20152	-1.28783	0.61116	1456.4064	1459.9912	1463.5038
H	-4.20784	0.14899	0.98962	1466.4168	1467.6007	1469.2901
H	-4.76830	-0.13186	-0.66323	1470.5682	1476.2361	1476.5798
C	1.18770	2.58113	2.32338	1477.4443	1480.9574	1485.5233
H	1.43445	2.65939	1.25677	1487.2333	1489.4295	1495.5869
H	1.70264	3.39218	2.85674	1497.9514	1500.8221	1507.0631
H	1.58802	1.62500	2.67992	1516.4816	1520.9438	1530.5811
C	-0.61747	2.60124	4.05834	1534.8696	1537.2748	1593.0792
H	-0.13435	3.43231	4.58908	1687.7067	1715.3333	1760.2003
H	-1.69661	2.64754	4.23575	1832.6391	2988.6152	3017.2266
H	-0.24005	1.66429	4.48881	3023.4948	3024.2665	3028.4423
C	-0.84025	4.00692	2.00794	3030.5466	3034.3222	3035.4757
H	-1.92266	4.08781	2.15580	3037.8889	3039.1258	3040.8738
H	-0.35068	4.84935	2.51471	3041.8566	3096.4103	3102.1938
H	-0.62751	4.09779	0.93225	3104.5713	3106.9838	3114.7709
C	5.02576	-3.23748	0.32044	3116.6347	3117.2546	3120.6376
H	5.36231	-2.99497	-0.69328	3122.7627	3123.9071	3126.4684
H	5.90398	-3.48398	0.93012	3130.7015	3134.8445	3137.8876
H	4.39026	-4.12721	0.25052	3138.6449	3139.8103	3142.9447
C	5.17282	-0.83456	1.01284	3143.4618	3143.5486	3146.1700
H	4.65644	0.01184	1.47706	3154.2135	3169.7123	3171.4834
H	6.06797	-1.06320	1.60514	3218.9282	3231.4120	3441.0225
H	5.50303	-0.52892	0.01170			
C	3.79742	-2.44336	2.35161			
H	3.14852	-3.32899	2.32840			
H	4.66349	-2.68121	2.98218			
H	3.24427	-1.62073	2.81725			
H	2.41391	4.91247	-2.28274			
F	4.10506	2.97407	-2.21711			

Statistical Thermodynamic Analysis

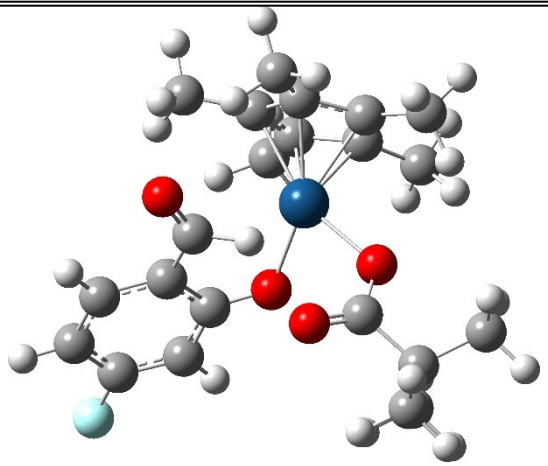
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.606382 Electronic Energy = -1706.73164957
Internal Energy (E)= -1706.08613157 Enthalpy (H)= -1706.08518857
Gibbs Free Energy (G)=-1706.19438257 Gibbs Free Energy of Solvation=-1706.24521039

St.Pt.	General Structure	Ball & Stick model

III'-4



III'-4



Cartesian co-ordinate

Atoms	X	Y	Z
C	1.38566	-2.36662	-0.79553
C	2.33215	-1.74515	0.07563
C	1.71535	-1.63422	1.39082
C	0.40647	-2.27567	1.32103
C	0.19659	-2.71214	-0.02292
C	-2.45934	0.05607	-0.86902
Ir	0.52886	-0.53657	0.03711
C	-3.78817	-0.01946	-1.32716
C	-4.83040	0.45520	-0.56661
C	-2.16250	0.59339	0.41810
C	-4.51630	1.02008	0.67871
C	-3.24010	1.10064	1.18015
H	-3.05290	1.53073	2.15926
H	-5.86418	0.42178	-0.89463
H	-0.36852	0.19417	-1.52340
O	1.56018	1.24617	0.07110
C	1.13112	2.28447	-0.59970
C	1.78100	3.59566	-0.14557
O	0.26410	2.25988	-1.46162
H	-3.95946	-0.44914	-2.31186
C	-1.38569	-0.35057	-1.73930
O	-1.44445	-1.02940	-2.74661
O	-0.96574	0.61025	0.92790
C	1.61187	4.65580	-1.22641
H	0.55618	4.78570	-1.48246
H	2.01498	5.61597	-0.87853
H	2.14204	4.37380	-2.14417
C	1.01787	4.01296	1.11712
H	1.11238	3.25109	1.90007
H	1.41151	4.96322	1.50213
H	-0.04920	4.14530	0.89832
C	3.26028	3.40856	0.18182
H	3.82118	3.06063	-0.69562
H	3.69654	4.36493	0.49977
H	3.40318	2.68088	0.98781
C	3.66932	-1.19225	-0.26997
H	3.72397	-0.12979	-0.00053
H	4.46222	-1.72784	0.26638

Frequencies

26.1954	32.0876	41.3155
55.6186	62.1571	75.8515
86.7805	99.0436	119.5210
128.4693	138.7583	150.6246
157.7838	166.5165	175.0266
178.8790	183.1961	191.5034
194.9460	207.4196	212.3500
217.3969	226.4137	228.3246
238.1455	245.8835	255.1667
282.9550	289.8880	294.0032
304.8474	307.6274	310.4161
317.7485	326.4322	349.5844
370.6759	390.0678	393.0282
421.5374	432.5443	443.2791
447.9730	451.6215	470.1474
526.9118	535.8348	540.7560
543.7955	564.5022	577.0301
585.6936	592.4096	597.5543
606.1962	644.4952	654.4167
675.7005	721.6110	756.9795
791.7124	801.6873	803.2963
810.0455	818.0087	829.6732
843.1356	917.1484	948.7611
950.9544	952.9616	955.3054
959.5645	960.4730	997.8955
1038.1724	1039.3547	1041.7225
1043.2146	1044.5128	1047.4840
1050.3668	1070.0290	1090.2305
1092.8756	1104.2736	1105.0057
1175.4438	1181.3473	1186.3335
1236.7458	1243.9593	1247.1931
1256.0838	1265.9124	1338.8053
1357.3065	1375.6132	1379.0787
1380.6830	1387.5271	1394.9798
1396.3453	1400.0346	1403.7629
1414.9976	1435.7239	1438.2406
1439.6145	1440.8879	1445.2496
1449.2286	1452.5236	1456.3675
1457.4714	1459.2533	1464.1889
1466.7354	1469.5784	1470.0565
1477.6346	1480.5176	1484.3333
1486.2875	1494.9236	1505.9113
1515.3777	1522.6877	1536.0214

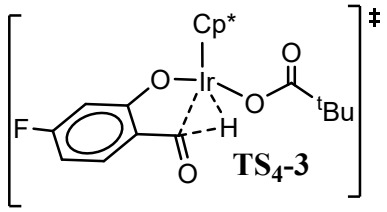
H	3.86952	-1.27226	-1.34205	1543.1466	1611.6777	1683.1322
C	1.52931	-2.62269	-2.25286	1785.8376	1806.5752	2291.1127
H	2.39798	-2.10360	-2.66723	3024.4280	3026.8238	3034.5042
H	1.64737	-3.69718	-2.44242	3037.2694	3037.9220	3039.8200
H	0.63939	-2.27781	-2.79431	3041.2041	3043.8228	3104.9960
C	-0.98447	-3.44987	-0.54757	3114.8748	3116.3416	3116.9866
H	-1.17114	-3.20277	-1.59712	3121.7129	3122.0675	3122.7379
H	-0.82650	-4.53336	-0.47106	3127.5172	3131.0304	3136.4646
H	-1.89090	-3.19987	0.01340	3146.3890	3147.2588	3148.6912
C	-0.56833	-2.38215	2.43807	3149.1024	3150.4392	3155.9080
H	-1.59798	-2.32546	2.06944	3192.0279	3222.0352	3223.1918
H	-0.44670	-3.33452	2.96894			
H	-0.43690	-1.56924	3.15857			
C	2.36836	-1.04599	2.59012			
H	1.62920	-0.72694	3.33117			
H	3.04265	-1.76938	3.06694			
H	2.95448	-0.16376	2.30988			
F	-5.52396	1.48877	1.41734			
H	-1.92266	4.08781	2.15580			
H	-0.35068	4.84935	2.51471			
H	-0.62751	4.09779	0.93225			
C	5.02576	-3.23748	0.32044			
H	5.36231	-2.99497	-0.69328			
H	5.90398	-3.48398	0.93012			
H	4.39026	-4.12721	0.25052			
C	5.17282	-0.83456	1.01284			
H	4.65644	0.01184	1.47706			
H	6.06797	-1.06320	1.60514			
H	5.50303	-0.52892	0.01170			
C	3.79742	-2.44336	2.35161			
H	3.14852	-3.32899	2.32840			
H	4.66349	-2.68121	2.98218			
H	3.24427	-1.62073	2.81725			
H	2.41391	4.91247	-2.28274			
F	4.10506	2.97407	-2.21711			

Statistical Thermodynamic Analysis

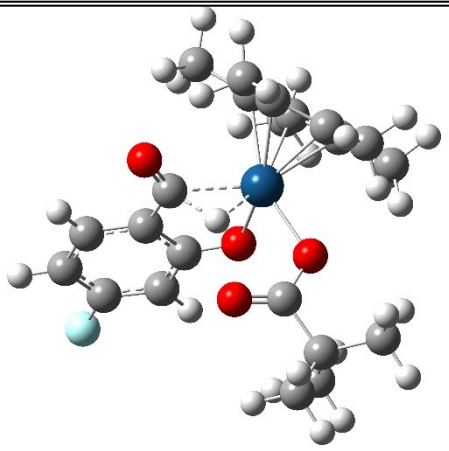
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.454630 Electronic Energy = -1359.86176235
Internal Energy (E)= -1359.37658535 Enthalpy (H)= -1359.37564135
Gibbs Free Energy (G)=-1359.46682335 Gibbs Free Energy of Solvation=-1359.51311674

St.Pt.	General Structure	Ball & Stick model

TS_4-3



TS_4-3



Cartesian co-ordinate

Atoms	X	Y	Z
C	2.12845	-1.81042	-0.78222
C	2.76883	-0.78031	-0.02697
C	2.28493	-0.85240	1.34716
C	1.36095	-1.93927	1.42637
C	1.21820	-2.50743	0.10994
C	-2.25549	-0.80760	-0.73928
Ir	0.60636	-0.38007	-0.02434
C	-3.47038	-1.21999	-1.31018
C	-4.65984	-0.97731	-0.66105
C	-2.21785	-0.15146	0.51436
C	-4.60543	-0.30989	0.57160
C	-3.43886	0.10552	1.17111
H	-3.45411	0.61370	2.13010
H	-5.62259	-1.27204	-1.06571
H	-0.18855	0.21008	-1.38359
O	0.94280	1.66711	0.12510
C	0.21402	2.47204	-0.59710
C	0.33338	3.93939	-0.17407
O	-0.55453	2.12443	-1.48726
H	-3.44406	-1.72174	-2.27466
C	-0.99035	-1.01992	-1.40947
O	-0.78784	-1.66652	-2.41359
O	-1.08099	0.18479	1.05385
C	-0.11717	4.84180	-1.31620
H	-1.13442	4.59269	-1.63212
H	-0.09095	5.89168	-0.99668
H	0.53698	4.73337	-2.18971
C	-0.61763	4.09476	1.01871
H	-0.31566	3.44561	1.84893
H	-0.61684	5.13561	1.36818
H	-1.64255	3.82730	0.73241
C	1.75756	4.29246	0.24519
H	2.46684	4.13068	-0.57715
H	1.80995	5.35185	0.52881
H	2.08465	3.69231	1.10072
C	3.75850	0.22038	-0.50747
H	3.44179	1.23263	-0.22809
H	4.74440	0.03398	-0.06298
H	3.86163	0.19190	-1.59580

Frequencies

-155.2980	16.0571	27.3960
41.3068	50.8811	67.1910
82.3049	86.0598	119.5701
135.9067	142.0901	147.0184
158.9948	160.9656	168.5332
170.7113	179.3829	183.0943
187.9584	199.0986	202.3271
217.7831	223.2790	229.7268
237.2811	259.1031	267.9263
272.7039	281.7885	293.5228
294.6589	297.5563	313.8593
315.9507	321.5767	330.9957
356.1661	375.3335	390.5072
403.2622	413.4068	433.1381
441.5219	448.8755	454.5742
498.7434	538.2871	540.3606
545.3075	559.7065	570.9063
587.3514	590.0446	598.3024
609.2604	642.0276	650.4577
674.8519	711.1391	753.4181
775.8989	792.1948	802.0483
809.7276	812.3154	822.6759
826.8677	850.3299	910.9509
926.6153	946.2858	947.3566
949.2111	950.7515	953.8615
957.7535	991.3066	1037.0417
1037.7349	1040.0204	1041.2497
1041.8130	1043.8565	1049.4722
1085.8072	1089.3305	1104.9535
1106.4344	1176.2708	1182.3356
1187.8501	1236.2068	1244.4302
1248.1946	1254.2350	1264.0086
1340.9859	1357.0843	1372.8091
1374.3266	1377.3044	1386.4586
1392.0484	1394.3380	1396.8219
1411.8024	1415.1253	1433.3011
1440.6462	1443.1397	1444.3732
1447.8400	1449.5884	1453.4845
1457.6767	1460.9274	1461.2936
1462.5472	1467.0313	1467.8760
1469.3130	1474.4095	1479.8496
1485.6991	1502.8294	1503.2790
1515.5117	1519.6760	1528.9708

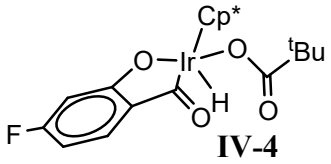
C	2.35337	-2.15545	-2.21095	1543.0694	1621.6056	1675.8865
H	3.00854	-1.42792	-2.69816	1738.7809	1788.6621	1878.9386
H	2.82167	-3.14442	-2.29381	3024.1728	3027.3503	3035.5494
H	1.40356	-2.17703	-2.75514	3036.0716	3037.1351	3040.3475
C	0.41459	-3.70927	-0.24702	3042.2195	3045.2718	3104.9482
H	0.08823	-3.66676	-1.29052	3114.3414	3114.7043	3116.7681
H	1.00578	-4.62355	-0.10734	3119.2352	3122.0574	3122.1664
H	-0.48232	-3.78957	0.37673	3128.7597	3132.0252	3135.5807
C	0.57344	-2.33795	2.62250	3143.4291	3150.8538	3150.8771
H	-0.42764	-2.67988	2.33928	3150.9402	3151.6931	3157.5781
H	1.07065	-3.15546	3.15934	3201.2829	3226.1295	3226.3536
H	0.44710	-1.49914	3.31307			
C	2.72429	0.05222	2.44445			
H	2.08507	-0.04741	3.32642			
H	3.75605	-0.16834	2.74733			
H	2.68055	1.09902	2.12269			
F	-5.76044	-0.07347	1.19674			
H	-1.92266	4.08781	2.15580			
H	-0.35068	4.84935	2.51471			
H	-0.62751	4.09779	0.93225			
C	5.02576	-3.23748	0.32044			
H	5.36231	-2.99497	-0.69328			
H	5.90398	-3.48398	0.93012			
H	4.39026	-4.12721	0.25052			
C	5.17282	-0.83456	1.01284			
H	4.65644	0.01184	1.47706			
H	6.06797	-1.06320	1.60514			
H	5.50303	-0.52892	0.01170			
C	3.79742	-2.44336	2.35161			
H	3.14852	-3.32899	2.32840			
H	4.66349	-2.68121	2.98218			
H	3.24427	-1.62073	2.81725			
H	2.41391	4.91247	-2.28274			
F	4.10506	2.97407	-2.21711			

Statistical Thermodynamic Analysis

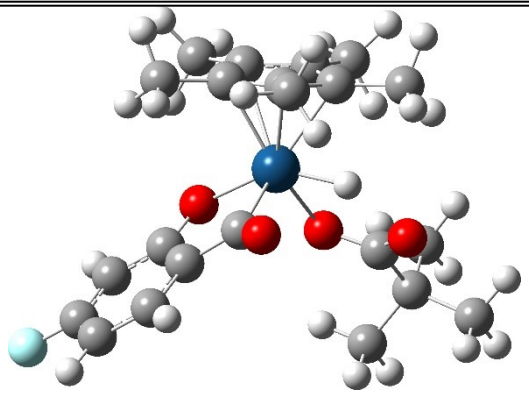
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.450763 Electronic Energy = -1359.85668246
Internal Energy (E)= -1359.37573346 Enthalpy (H)= -1359.37479046
Gibbs Free Energy (G)=-1359.46550346 Gibbs Free Energy of Solvation=-1359.50488209

St.Pt.	General Structure	Ball & Stick model

IV-4



IV-4



Cartesian co-ordinate

Atoms	X	Y	Z
C	0.61543	-2.49372	-0.84991
C	1.85887	-1.95603	-0.33271
C	1.78922	-1.94164	1.12186
C	0.49625	-2.31800	1.49287
C	-0.27613	-2.59192	0.27161
C	-2.38203	0.55123	-0.84369
Ir	0.22461	-0.49525	-0.08431
C	-3.51580	0.96823	-1.55199
C	-4.61285	1.46130	-0.87406
C	-2.33403	0.61789	0.56312
C	-4.54518	1.51822	0.52239
C	-3.45059	1.11386	1.25801
H	-3.44945	1.18549	2.34101
H	-5.51117	1.80317	-1.37815
H	1.04364	-0.00698	-1.36751
O	1.03582	1.35868	0.39516
C	1.92266	1.88471	-0.39858
C	2.52800	3.18156	0.14987
O	2.28962	1.40230	-1.46976
H	-3.50445	0.89589	-2.63695
C	-1.19825	-0.00539	-1.50048
O	-1.09528	-0.22174	-2.68588
O	-1.25682	0.20772	1.18863
C	-1.67490	-3.10565	0.27139
H	-2.13726	-3.00879	-0.71615
H	-1.70659	-4.16379	0.56217
H	-2.29469	-2.54283	0.97854
C	0.36598	-2.90258	-2.25923
H	1.02272	-3.73841	-2.52989
H	-0.66901	-3.22477	-2.40347
H	0.53793	-2.07346	-2.95385
C	3.10774	-1.73125	-1.11241
H	3.78938	-2.58339	-0.99005
H	2.89392	-1.60781	-2.17803
H	3.62323	-0.82344	-0.78180
C	2.88860	-1.44461	1.99219
H	3.81902	-1.99562	1.80799
H	3.09111	-0.38302	1.79266
H	2.64063	-1.53882	3.05300
C	-0.11001	-2.31139	2.84703
H	0.63395	-2.13440	3.62845

Frequencies

19.2833	21.3594	39.6048
47.1158	57.6332	76.0175
90.2701	116.1247	125.6418
133.7266	143.8481	153.2972
161.7401	165.4168	171.0259
186.0772	191.2909	194.6623
196.9974	200.3867	207.3742
216.1848	225.3578	228.7183
243.4282	259.4701	266.4034
276.8750	284.8182	289.7591
295.0982	300.2497	304.0723
308.2301	319.7258	330.1546
364.1186	369.4235	390.6187
410.6035	418.5088	437.5418
446.3499	456.0196	457.8024
532.4039	534.1255	549.5517
563.1986	570.0902	587.3243
596.0217	613.2741	618.3574
633.2007	644.8509	651.6422
684.8093	730.1563	756.9224
783.8920	794.4537	805.5992
807.5576	811.4260	823.1864
837.4340	888.3940	905.2934
945.9420	946.5404	949.8618
950.0521	953.5105	957.1226
967.4172	993.3029	1023.9032
1035.2243	1036.3842	1045.0425
1046.2144	1047.2270	1052.4993
1083.1533	1089.1150	1103.8232
1106.2238	1173.2789	1176.6191
1187.6603	1234.6941	1242.3498
1247.1988	1252.8616	1265.8798
1344.3666	1358.6944	1363.7644
1371.7411	1376.3622	1384.9840
1389.7390	1398.5759	1400.8836
1402.6509	1411.5022	1427.7491
1432.0665	1434.8900	1444.3711
1447.7998	1449.1688	1450.9570
1454.2069	1456.3890	1457.4555
1460.4323	1461.7220	1466.2204
1473.0854	1473.6226	1476.3454
1479.9511	1488.5113	1501.7130
1510.0216	1515.2179	1525.0004
1586.8324	1634.6488	1672.1049
1726.5224	1813.1067	2060.2292

H	-0.86569	-1.51501	2.90595	3016.6760	3030.7609	3032.0150
H	-0.61285	-3.26342	3.05617	3033.4437	3036.3121	3038.1453
C	3.34267	2.81351	1.39322	3040.0017	3043.2434	3099.1892
H	3.82525	3.70912	1.80530	3102.5107	3109.9435	3112.4367
H	2.70284	2.37634	2.16808	3118.4006	3125.3049	3126.5645
H	4.13427	2.09253	1.14327	3128.9669	3130.5933	3140.7590
C	3.43713	3.81155	-0.89699	3141.0834	3144.7014	3146.0731
H	2.87849	4.06499	-1.80468	3149.9482	3151.4540	3155.3763
H	3.88303	4.73137	-0.49685	3200.4865	3225.0798	3225.3311
H	4.24219	3.12835	-1.18721			
C	1.41076	4.15227	0.53140			
H	1.84338	5.07873	0.93126			
H	0.80283	4.41682	-0.34270			
H	0.74840	3.71899	1.28682			
F	-5.60757	1.99199	1.17820			
H	-1.92266	4.08781	2.15580			
H	-0.35068	4.84935	2.51471			
H	-0.62751	4.09779	0.93225			
C	5.02576	-3.23748	0.32044			
H	5.36231	-2.99497	-0.69328			
H	5.90398	-3.48398	0.93012			
H	4.39026	-4.12721	0.25052			
C	5.17282	-0.83456	1.01284			
H	4.65644	0.01184	1.47706			
H	6.06797	-1.06320	1.60514			
H	5.50303	-0.52892	0.01170			
C	3.79742	-2.44336	2.35161			
H	3.14852	-3.32899	2.32840			
H	4.66349	-2.68121	2.98218			
H	3.24427	-1.62073	2.81725			
H	2.41391	4.91247	-2.28274			
F	4.10506	2.97407	-2.21711			

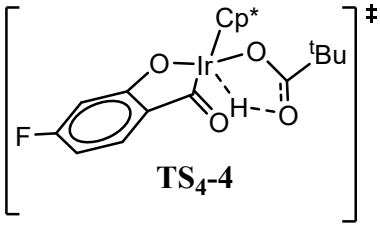
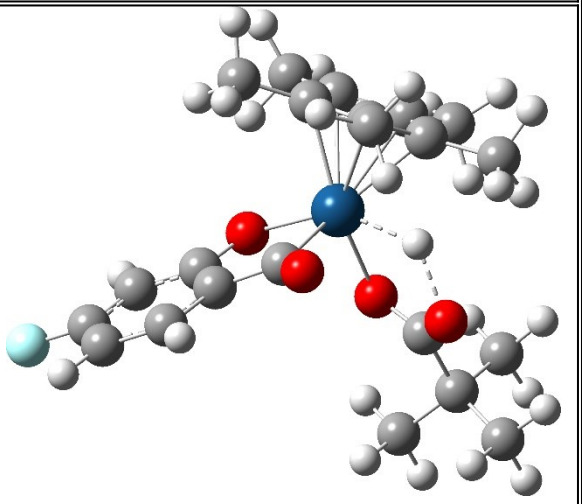
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm

Zero-point correction= 0.452041 Electronic Energy = -1359.86384848

Internal Energy (E)= -1359.38114948 Enthalpy (H)= -1359.38020648

Gibbs Free Energy (G)=-1359.47218048 Gibbs Free Energy of Solvation=-1359.51297699

St.Pt.	General Structure	Ball & Stick model
TS_4-4	 **TS_4-4**	

Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.82625	-2.37049	0.99730
C	-2.00443	-1.79216	0.39270
C	-1.89875	-1.93082	-1.05673
C	-0.63318	-2.44456	-1.34754
C	0.08466	-2.65098	-0.08032
C	2.36006	0.50616	0.81990
Ir	-0.25093	-0.50776	0.02753
C	3.47498	0.94622	1.54325
C	4.62055	1.33977	0.87978
C	2.37985	0.44769	-0.58829
C	4.61934	1.27418	-0.51796
C	3.54497	0.84382	-1.26818
H	3.59709	0.81702	-2.35198
H	5.50714	1.69425	1.39587
H	-1.10230	0.25083	1.23709
O	-0.94549	1.38767	-0.58031
C	-1.67294	2.00926	0.28005
C	-2.28089	3.32116	-0.20649
O	-1.92410	1.56582	1.41648
H	3.41006	0.97161	2.62859
C	1.12111	0.05881	1.45961
O	0.95425	-0.03103	2.65623
O	1.31774	0.02035	-1.22688
C	1.43695	-3.26951	0.02254
H	1.87580	-3.10601	1.01217
H	1.39261	-4.35175	-0.15700
H	2.12164	-2.83318	-0.71366
C	-0.64254	-2.63933	2.44968
H	-1.37655	-3.37929	2.79167
H	0.35709	-3.03019	2.65950
H	-0.75291	-1.72332	3.04088
C	-3.24810	-1.40098	1.11406
H	-3.95425	-2.24156	1.14101
H	-3.03212	-1.09676	2.14235
H	-3.74618	-0.55671	0.62460

Frequencies

-464.8881	19.9817	31.2007
38.4585	48.9260	75.0030
82.8930	98.2077	120.6181
132.0980	141.6977	153.4464
155.6279	171.5961	189.0650
192.9355	198.7153	204.1258
208.6585	214.1531	218.1995
227.4833	232.0630	234.1568
246.3996	260.0636	266.0522
273.4445	279.8068	290.1380
295.9545	299.1982	306.0821
313.9204	327.0558	329.2363
350.3327	371.6597	389.5684
409.6686	415.6497	436.0085
444.1349	456.0582	458.5081
476.8532	533.8770	537.7601
552.3826	568.9589	584.4926
595.1128	597.1433	620.0201
622.9549	637.6530	644.8502
652.3401	685.0774	733.7664
767.1740	788.5635	802.4663
810.1240	813.1710	833.3597
835.1673	862.0555	904.1608
942.6680	947.2598	948.3212
953.3354	954.9733	955.3455
961.7165	992.5893	1032.4326
1035.2981	1043.1196	1045.7534
1046.7797	1053.1966	1058.2961
1084.4000	1091.3962	1103.6644
1106.9557	1174.0311	1177.2335
1187.6465	1235.3795	1239.7426
1253.7190	1253.7490	1267.9449
1344.8011	1367.2205	1373.9243
1377.2643	1378.3235	1389.2026
1399.0771	1400.8885	1401.2389
1402.1185	1421.9653	1427.1082
1439.2020	1441.1958	1448.1045
1450.2885	1455.5086	1457.8394
1459.9138	1460.7717	1462.3559
1465.3691	1467.3596	1467.8766

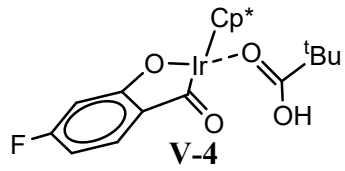
C	-2.93273	-1.43067	-2.00296	1472.7911	1474.5851	1481.4636
H	-3.89133	-1.94308	-1.85241	1485.1941	1500.8165	1504.5216
H	-3.10747	-0.35658	-1.84901	1511.0690	1515.9689	1523.2267
H	-2.63339	-1.57029	-3.04534	1559.2360	1589.1340	1633.7025
C	0.01286	-2.60430	-2.67545	1671.8211	1754.5780	1812.9107
H	-0.69119	-2.44085	-3.49585	3016.8834	3025.7124	3031.0998
H	0.82922	-1.87420	-2.77519	3033.0009	3034.9298	3037.9134
H	0.44520	-3.60615	-2.78604	3040.0549	3041.9446	3098.3773
C	-3.36753	2.94215	-1.21982	3099.3820	3112.2920	3113.8635
H	-3.86797	3.84708	-1.58702	3118.0561	3119.8341	3125.8047
H	-2.93636	2.41247	-2.07725	3126.6247	3134.5286	3134.9410
H	-4.13035	2.30046	-0.75741	3143.4604	3143.9534	3148.4113
C	-2.89939	4.08427	0.95791	3149.3442	3150.4161	3153.4250
H	-2.14547	4.33432	1.71258	3198.7189	3224.2157	3225.0635
H	-3.34361	5.01856	0.59191			
H	-3.67927	3.49621	1.45236			
C	-1.21040	4.17134	-0.88854			
H	-1.65788	5.10469	-1.25362			
H	-0.40933	4.43422	-0.18720			
H	-0.76013	3.64366	-1.73440			
F	5.72838	1.65258	-1.15981			
H	-1.92266	4.08781	2.15580			
H	-0.35068	4.84935	2.51471			
H	-0.62751	4.09779	0.93225			
C	5.02576	-3.23748	0.32044			
H	5.36231	-2.99497	-0.69328			
H	5.90398	-3.48398	0.93012			
H	4.39026	-4.12721	0.25052			
C	5.17282	-0.83456	1.01284			
H	4.65644	0.01184	1.47706			
H	6.06797	-1.06320	1.60514			
H	5.50303	-0.52892	0.01170			
C	3.79742	-2.44336	2.35161			
H	3.14852	-3.32899	2.32840			
H	4.66349	-2.68121	2.98218			
H	3.24427	-1.62073	2.81725			
H	2.41391	4.91247	-2.28274			
F	4.10506	2.97407	-2.21711			

Statistical Thermodynamic Analysis

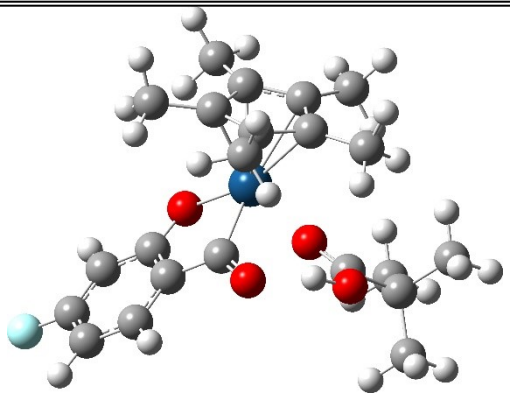
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.450728 Electronic Energy = -1359.86317078
Internal Energy (E)= -1359.38258578 Enthalpy (H)= -1359.38164178
Gibbs Free Energy (G)=-1359.47113178 Gibbs Free Energy of Solvation=-1359.51105117

St.Pt.	General Structure	Ball & Stick model

V-4



V-4



Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.44306	-2.22640	1.28354
C	-1.70210	-1.80336	0.74510
C	-1.73188	-2.17084	-0.67849
C	-0.48565	-2.69314	-1.02877
C	0.37644	-2.64701	0.16276
C	2.27114	0.90243	0.70475
Ir	-0.08017	-0.59326	-0.07669
C	3.25234	1.58367	1.43758
C	4.44281	1.94277	0.83966
C	2.45599	0.59651	-0.66985
C	4.61125	1.62462	-0.51518
C	3.66767	0.97796	-1.28232
H	3.85163	0.77153	-2.33219
H	5.23787	2.46020	1.36737
H	-1.01692	1.39531	1.77111
O	-1.14354	1.26216	-0.65557
C	-1.85772	1.93198	0.10109
C	-2.93525	2.84649	-0.45178
O	-1.80691	1.89992	1.40508
H	3.04998	1.81469	2.48157
C	0.96098	0.53925	1.21193
O	0.49850	0.93614	2.29523
O	1.50274	-0.00182	-1.32832
C	1.76666	-3.18047	0.21819
H	2.30894	-2.77297	1.07827
H	1.78009	-4.27613	0.29037
H	2.32380	-2.88952	-0.67933
C	-0.05415	-2.19441	2.71949
H	-0.49687	-3.04106	3.25916
H	1.03293	-2.24768	2.83658
H	-0.38084	-1.26339	3.19540
C	-2.87878	-1.33446	1.53137
H	-3.48600	-2.17893	1.88571
H	-2.56536	-0.75425	2.40633
H	-3.53327	-0.69493	0.92646
C	-2.88828	-1.87996	-1.56955
H	-3.77220	-2.46147	-1.27602
H	-3.16561	-0.81748	-1.51652
H	-2.66418	-2.10831	-2.61565
C	0.01167	-3.08196	-2.37582
H	-0.74963	-2.93974	-3.14855

Frequencies

24.9403	25.3652	55.0794
59.5982	79.2564	82.3862
102.5449	114.4475	125.9820
139.0556	143.9701	155.0625
161.0188	171.4069	175.2905
186.0022	192.7373	207.7940
211.4022	221.2567	229.4830
234.0108	241.4356	250.6716
259.2102	265.7205	269.0144
271.8307	290.0496	299.4067
307.4878	309.8240	315.7762
333.7373	342.6430	363.9239
387.6103	394.7902	408.2696
414.1049	415.2009	442.4989
452.5609	466.5276	470.1161
532.0626	537.8318	549.7636
555.3047	574.0454	575.9609
592.3490	605.5205	612.0093
624.1569	656.4670	657.1068
697.6935	738.5794	764.5916
783.4208	787.2211	805.8991
806.9359	809.0611	834.0670
886.1760	906.6068	920.5788
948.7284	950.6353	953.2621
954.1282	961.4386	965.8125
990.6678	1031.6150	1041.3592
1044.0065	1047.6076	1048.6410
1049.0794	1060.6673	1085.5499
1087.7556	1105.6633	1105.9276
1175.5425	1180.8647	1182.6648
1237.0494	1243.6109	1248.4347
1263.2021	1266.2563	1336.0472
1344.3502	1365.7295	1373.1826
1383.0812	1388.9079	1389.7057
1396.1424	1397.1228	1400.5055
1414.3495	1427.6439	1432.8558
1442.5073	1450.3832	1451.1371
1452.2057	1455.8755	1456.6028
1460.2018	1462.4775	1463.9236
1465.2756	1468.2004	1469.1223
1479.9064	1485.6277	1487.8467
1499.7734	1509.2012	1512.6998
1514.3682	1530.2002	1537.8299
1591.9446	1618.9824	1654.7956
1676.0476	1741.1400	3018.7929

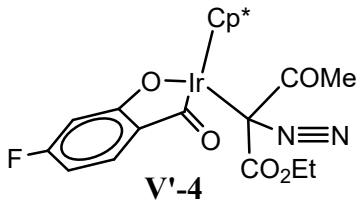
H	0.88328	-2.47342	-2.64897	3025.9478	3030.2820	3032.6838
H	0.32119	-4.13501	-2.39373	3032.8081	3039.2415	3040.5918
C	-4.28664	2.23296	-0.05892	3044.6146	3086.2779	3090.1229
H	-5.09745	2.86390	-0.44274	3103.0540	3105.9197	3115.9721
H	-4.41149	1.23116	-0.49382	3116.3525	3123.2944	3125.8121
H	-4.39283	2.15601	1.02851	3131.1027	3133.2933	3136.9146
C	-2.79892	4.23749	0.17004	3138.0386	3139.4578	3140.7145
H	-1.82892	4.68752	-0.07258	3141.0107	3143.5384	3151.4861
H	-3.58221	4.89231	-0.23038	3193.2758	3217.4422	3222.4658
H	-2.89906	4.20265	1.25891			
C	-2.82743	2.93040	-1.96914			
H	-3.61926	3.58365	-2.35480			
H	-1.86053	3.34017	-2.28020			
H	-2.93428	1.94449	-2.43451			
F	5.76351	1.97924	-1.09398			
H	-1.92266	4.08781	2.15580			
H	-0.35068	4.84935	2.51471			
H	-0.62751	4.09779	0.93225			
C	5.02576	-3.23748	0.32044			
H	5.36231	-2.99497	-0.69328			
H	5.90398	-3.48398	0.93012			
H	4.39026	-4.12721	0.25052			
C	5.17282	-0.83456	1.01284			
H	4.65644	0.01184	1.47706			
H	6.06797	-1.06320	1.60514			
H	5.50303	-0.52892	0.01170			
C	3.79742	-2.44336	2.35161			
H	3.14852	-3.32899	2.32840			
H	4.66349	-2.68121	2.98218			
H	3.24427	-1.62073	2.81725			
H	2.41391	4.91247	-2.28274			
F	4.10506	2.97407	-2.21711			

Statistical Thermodynamic Analysis

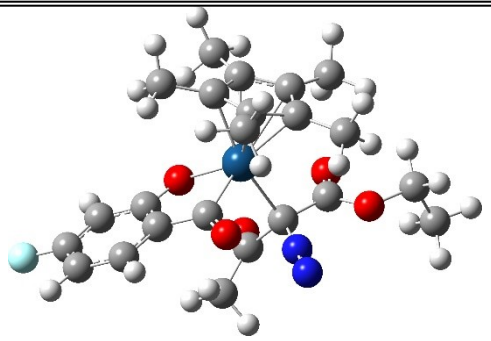
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.456824 Electronic Energy = -1359.89809940
Internal Energy (E)= -1359.4113384 Enthalpy (H)= -1359.4103954
Gibbs Free Energy (G)=-1359.4997344 Gibbs Free Energy of Solvation=-1359.5362575

St.Pt.	General Structure	Ball & Stick model

V'-4



V'-4



Cartesian co-ordinate

Atoms	X	Y	Z
C	0.35828	2.50968	0.87304
C	1.65053	1.94025	0.61776
C	1.85718	1.91813	-0.83418
C	0.65352	2.28122	-1.44426
C	-0.32160	2.60026	-0.39696
C	-2.60495	-0.30640	0.79700
Ir	0.06810	0.51771	0.00119
C	-2.55644	-0.49325	-0.60502
C	-3.72756	-0.90387	-1.27218
C	-3.78420	-0.53039	1.51788
C	-4.86985	-1.09539	-0.52409
C	-4.93725	-0.91954	0.86331
H	-3.76404	-0.39170	2.59696
H	-5.87726	-1.09544	1.37699
H	-3.72847	-1.06904	-2.34514
C	1.00550	-1.51897	0.07802
C	2.41645	-1.46511	-0.44266
C	0.09033	-2.54301	-0.62976
O	0.27411	-2.79218	-1.79025
N	1.00021	-1.66206	1.45853
N	0.95974	-1.73973	2.57892
C	3.12721	1.58036	-1.53594
H	3.01238	0.74057	-2.23039
H	3.48467	2.44728	-2.10605
H	3.91715	1.31790	-0.82339
C	2.68574	1.69833	1.66346
H	3.41433	0.94513	1.34368
H	3.23507	2.61704	1.91124
H	2.21662	1.32877	2.58366
C	-0.14852	2.92004	2.20970
H	-0.00479	2.12277	2.94742
H	0.37658	3.82097	2.55219
H	-1.22030	3.13978	2.18315
C	-1.68454	3.14368	-0.65734
H	-2.32486	3.05560	0.22634
H	-1.64478	4.20211	-0.94780
H	-2.17367	2.59033	-1.46754
C	0.34059	2.27613	-2.89826
H	0.07966	3.28186	-3.25324
H	1.18753	1.91264	-3.48778
H	-0.51454	1.61814	-3.09990
C	-1.32133	0.04617	1.41090

Frequencies

21.5480	29.4085	33.8615
42.7578	75.3449	85.5968
88.6723	102.5198	115.7827
116.6826	124.5376	129.3626
137.3665	143.7250	155.2622
155.8351	162.3883	182.8539
193.8450	200.1255	207.3377
213.3711	221.2255	223.6162
232.7067	242.6286	245.1363
247.3580	268.2525	273.0783
278.3089	287.1491	297.3622
301.8060	306.3550	312.5168
318.2496	324.1435	325.7022
359.3876	362.9072	369.4185
389.0202	406.1594	407.9619
446.7447	452.0562	460.7075
465.2565	491.9416	505.2142
534.2469	537.7199	540.1132
552.2673	573.0518	575.8209
587.7005	595.9423	602.0271
609.2781	623.3857	653.4739
657.0281	685.2188	735.0338
765.3604	767.9658	778.0118
799.8283	805.3714	820.1408
823.7625	830.3169	877.4208
885.0951	946.9805	949.3849
966.0227	971.1296	983.7110
988.3087	1030.7858	1034.1242
1040.6346	1047.5000	1049.8556
1058.9292	1063.5527	1086.7753
1097.4030	1098.3115	1099.7537
1109.9589	1123.3251	1170.5493
1179.8820	1183.6560	1186.6874
1197.6014	1233.8727	1249.1035
1261.9812	1318.7758	1344.7573
1374.9874	1378.2050	1378.9600
1382.2785	1394.3540	1395.8996
1399.5898	1401.8237	1411.6799
1429.4213	1437.2442	1442.4426
1446.3278	1448.7661	1454.5061
1461.4772	1465.4680	1466.5754
1469.3247	1471.2563	1474.9452
1477.7668	1483.7191	1489.6330
1498.1225	1506.8869	1508.7890
1510.7003	1514.0422	1521.6327
1578.4449	1624.9684	1667.7458
1746.9395	1855.7488	1901.2933

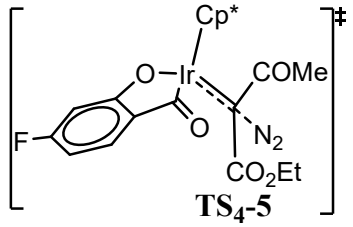
O	-1.42332	-0.32744	-1.23419	2268.8205	3029.3175	3031.7633
O	-1.12468	0.06781	2.61851	3032.6023	3037.8780	3038.9867
O	2.70539	-1.44583	-1.60920	3043.4046	3053.5912	3071.4009
C	4.69665	-1.43479	0.18585	3104.9973	3107.8777	3108.4901
H	5.21083	-0.97805	1.03780	3117.4995	3123.1819	3129.7772
H	4.81748	-0.79114	-0.69273	3133.8524	3136.1215	3140.9320
O	3.30692	-1.44309	0.56772	3143.6781	3145.0509	3146.5029
C	5.18463	-2.83495	-0.08756	3159.0008	3161.0410	3177.1189
H	4.66605	-3.25867	-0.95293	3194.8935	3219.1818	3225.1642
H	6.25765	-2.82472	-0.30448			
H	5.01615	-3.48171	0.77945			
C	-0.94986	-3.23234	0.20704			
H	-1.69187	-3.66584	-0.46690			
H	-0.47322	-4.04452	0.77203			
H	-1.45230	-2.57021	0.91897			
F	-5.98399	-1.47921	-1.15564			
H	-0.62751	4.09779	0.93225			
C	5.02576	-3.23748	0.32044			
H	5.36231	-2.99497	-0.69328			
H	5.90398	-3.48398	0.93012			
H	4.39026	-4.12721	0.25052			
C	5.17282	-0.83456	1.01284			
H	4.65644	0.01184	1.47706			
H	6.06797	-1.06320	1.60514			
H	5.50303	-0.52892	0.01170			
C	3.79742	-2.44336	2.35161			
H	3.14852	-3.32899	2.32840			
H	4.66349	-2.68121	2.98218			
H	3.24427	-1.62073	2.81725			
H	2.41391	4.91247	-2.28274			
F	4.10506	2.97407	-2.21711			

Statistical Thermodynamic Analysis

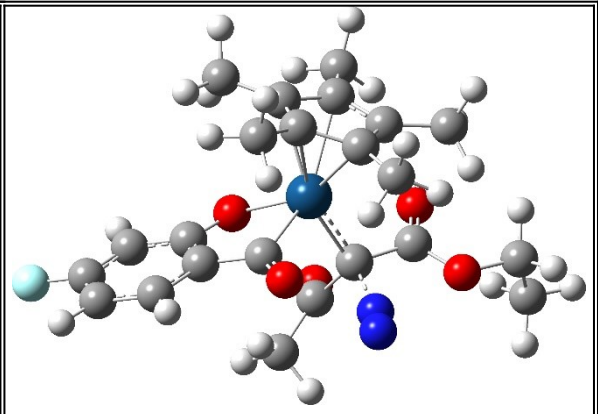
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.453318 Electronic Energy = -1581.32521491
Internal Energy (E)= -1580.83852991 Enthalpy (H)= -1580.83758591
Gibbs Free Energy (G)=-1580.93446891 Gibbs Free Energy of Solvation=-1580.97578702

St.Pt.	General Structure	Ball & Stick model

TS_4-5



TS_4-5



Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.38191	2.65016	0.48707
C	0.93775	2.28436	0.94008
C	1.75442	2.06142	-0.23968
C	0.93855	2.18993	-1.39454
C	-0.40048	2.50979	-0.93656
C	-2.54821	-0.47285	0.76788
Ir	0.06568	0.49950	-0.04342
C	-2.47947	-0.70143	-0.62815
C	-3.63463	-1.16216	-1.29119
C	-3.72903	-0.70247	1.48601
C	-4.77922	-1.35566	-0.54759
C	-4.86549	-1.13737	0.83342
H	-3.72379	-0.52711	2.55993
H	-5.80741	-1.31582	1.34262
H	-3.62274	-1.36058	-2.35837
C	1.12364	-1.26269	0.06496
C	2.56365	-1.20147	-0.38177
C	0.42283	-2.49295	-0.54105
O	0.68974	-2.80770	-1.67433
N	1.22631	-1.59345	1.67784
N	1.02193	-1.42995	2.76510
C	3.22942	1.86626	-0.21921
H	3.59006	1.40889	-1.14479
H	3.72721	2.83759	-0.10047
H	3.54581	1.23667	0.62132
C	1.40088	2.31440	2.35640
H	2.37729	1.82826	2.46367
H	1.49737	3.34256	2.72995
H	0.69425	1.77850	3.00268
C	-1.50372	3.07886	1.36889
H	-1.48326	2.54081	2.32269
H	-1.43408	4.15339	1.58238
H	-2.47863	2.89059	0.90708
C	-1.57371	2.69294	-1.83448
H	-2.50881	2.74749	-1.26836
H	-1.47695	3.61410	-2.42292
H	-1.65971	1.85005	-2.53008
C	1.35168	2.04004	-2.81779
H	1.70124	2.99233	-3.24030
H	2.15130	1.30098	-2.92633

Frequencies

-399.6859	29.3678	31.7695
41.0886	45.5756	80.0371
87.5678	94.7758	103.4499
110.3658	118.9296	128.6182
137.8683	143.5439	151.8324
152.8139	156.6670	160.9099
172.2980	180.5373	188.7591
193.9612	207.8350	222.1979
223.8838	229.6830	236.5283
244.4017	249.3416	254.7238
259.5667	272.6351	281.6659
290.7929	300.2141	303.7562
305.8917	318.7532	325.0949
329.7237	347.1991	361.4210
393.5136	401.2938	404.3706
416.8853	419.9136	433.0016
447.6572	454.6889	465.5379
506.5519	534.1524	539.8426
553.7403	564.8031	571.2733
575.7555	592.5973	598.9030
603.4080	609.9420	653.8424
657.4045	684.9646	707.7916
736.9218	752.4266	764.9878
799.4432	806.2953	816.8382
820.0185	832.6681	877.4648
887.0445	900.9224	946.2872
949.3659	953.4103	980.7180
988.4936	1004.6542	1033.8715
1041.2485	1043.3497	1045.7022
1049.4379	1050.8410	1087.4365
1093.6818	1096.0960	1098.9011
1117.2649	1122.6827	1173.0347
1179.9825	1184.3727	1188.9887
1202.8819	1235.9047	1250.4585
1277.7532	1334.0572	1343.8502
1377.2314	1384.3176	1385.8833
1391.0503	1393.9631	1397.8376
1400.0953	1417.0075	1423.7442
1438.8972	1442.5372	1451.6024
1455.7775	1455.9616	1458.4644
1458.8946	1461.3647	1464.4581
1465.1626	1467.1934	1473.3214
1479.9719	1482.1471	1483.0074
1498.3239	1501.2910	1507.9656
1509.2066	1521.6482	1522.8108

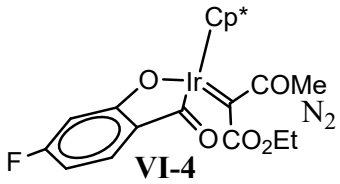
H	0.51174	1.69451	-3.42998	1550.5641	1622.1399	1667.8070
C	-1.28621	-0.05388	1.37538	1731.2348	1838.4995	1879.3333
O	-1.35006	-0.51431	-1.25649	2269.7512	3027.6534	3030.0089
O	-1.09556	0.03075	2.58249	3034.8870	3037.5437	3039.6376
O	2.86814	-0.93736	-1.51671	3046.7975	3052.4330	3071.8055
C	4.83073	-1.49133	0.21348	3102.2843	3107.5843	3113.4071
H	5.37596	-1.25971	1.13328	3118.0501	3119.6105	3127.4620
H	5.00874	-0.69686	-0.51909	3131.6206	3137.0607	3144.6836
O	3.44180	-1.46421	0.60065	3144.9581	3145.5876	3155.2808
C	5.19828	-2.84393	-0.34264	3158.0820	3163.3613	3178.7862
H	4.63733	-3.04529	-1.26048	3195.4201	3219.7037	3225.2864
H	6.26633	-2.87597	-0.58119			
H	4.98518	-3.63498	0.38342			
C	-0.54560	-3.27040	0.30610			
H	-1.18491	-3.85086	-0.36298			
H	0.01315	-3.96975	0.94182			
H	-1.16620	-2.64464	0.95460			
F	-5.87879	-1.78089	-1.17693			
H	-0.62751	4.09779	0.93225			
C	5.02576	-3.23748	0.32044			
H	5.36231	-2.99497	-0.69328			
H	5.90398	-3.48398	0.93012			
H	4.39026	-4.12721	0.25052			
C	5.17282	-0.83456	1.01284			
H	4.65644	0.01184	1.47706			
H	6.06797	-1.06320	1.60514			
H	5.50303	-0.52892	0.01170			
C	3.79742	-2.44336	2.35161			
H	3.14852	-3.32899	2.32840			
H	4.66349	-2.68121	2.98218			
H	3.24427	-1.62073	2.81725			
H	2.41391	4.91247	-2.28274			
F	4.10506	2.97407	-2.21711			

Statistical Thermodynamic Analysis

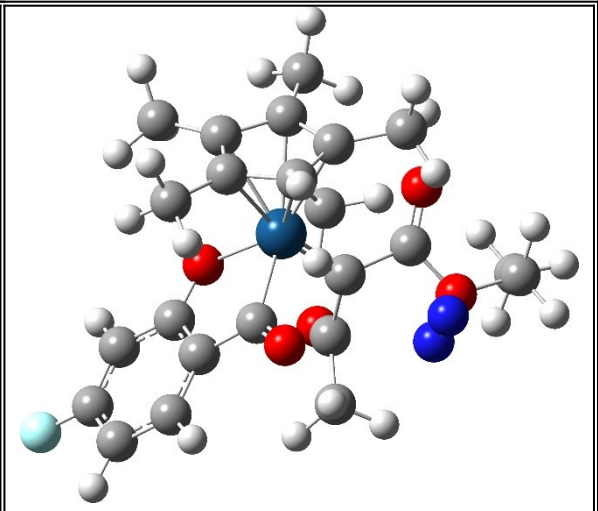
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.451298 Electronic Energy = -1581.31711518
Internal Energy (E)= -1580.83246418 Enthalpy (H)= -1580.83152118
Gibbs Free Energy (G)=-1580.92786118 Gibbs Free Energy of Solvation=-1580.96570517

St.Pt.	General Structure	Ball & Stick model

VI-4



VI-4



Cartesian co-ordinate

Atoms	X	Y	Z
C	0.58594	-2.73745	0.25082
C	-0.61198	-2.44452	0.99124
C	-1.66937	-2.18185	0.03979
C	-1.12915	-2.34706	-1.28162
C	0.26108	-2.66058	-1.14289
C	2.42604	0.63883	0.77914
Ir	-0.07132	-0.57570	-0.14421
C	2.49156	0.62884	-0.62915
C	3.64685	1.12807	-1.26050
C	3.47577	1.15572	1.55276
C	4.65770	1.61776	-0.46320
C	4.60636	1.65007	0.93792
H	3.37339	1.15315	2.63563
H	5.44750	2.05619	1.49062
H	3.72926	1.14392	-2.34238
C	-1.00234	1.07660	-0.27065
C	-2.47042	1.23475	-0.48618
C	-0.31881	2.40618	-0.42636
O	-0.26473	2.86958	-1.54892
N	-1.84171	1.20410	2.90535
N	-2.22480	0.34948	3.49183
C	-3.10915	-2.03415	0.38756
H	-3.68092	-1.61693	-0.44337
H	-3.53390	-3.01213	0.65063
H	-3.24626	-1.37189	1.24862
C	-0.77146	-2.56783	2.46705
H	-1.81961	-2.46166	2.76263
H	-0.42998	-3.55583	2.80018
H	-0.18911	-1.80660	2.99874
C	1.90332	-3.11411	0.84018
H	2.00115	-2.72867	1.86043
H	2.02470	-4.20455	0.87939
H	2.73768	-2.70666	0.25828
C	1.21640	-2.83691	-2.26980
H	2.25213	-2.72473	-1.93590
H	1.10833	-3.83302	-2.71736
H	1.04570	-2.09098	-3.05315

Frequencies

-50.6266	-17.2306	-6.3063
24.0734	27.9718	33.7635
44.9399	53.5428	60.8512
75.1975	87.0241	90.6664
93.9138	106.5724	115.4852
128.5525	132.8232	141.9881
147.2442	154.3104	158.2098
163.0663	168.7669	177.7662
193.0099	209.0226	220.8374
226.3399	227.1785	233.6490
234.5241	243.9679	258.5793
265.1089	271.7375	278.2513
284.2420	305.5220	309.5856
312.1232	317.8467	326.2629
329.5286	352.4564	360.3217
404.2002	409.5677	422.0401
455.1784	456.0648	458.8415
531.7516	539.0105	543.5669
548.1149	558.2583	569.0753
583.0581	588.5151	601.5292
603.4109	625.0996	644.8832
649.3993	685.6241	729.9484
756.2085	763.8188	771.2782
797.0256	813.8268	815.6610
816.9219	837.4386	868.8900
882.1910	942.1288	951.5676
953.4000	962.5020	981.4040
990.4101	1005.9729	1021.4997
1032.9491	1038.2868	1041.5291
1043.9110	1054.1453	1084.6349
1089.7871	1103.3873	1107.9207
1115.8934	1125.7428	1178.5577
1179.6270	1187.6176	1190.4030
1235.9468	1245.9980	1250.6458
1266.0793	1311.8828	1339.3297
1364.6450	1378.4202	1379.5671
1382.8892	1389.6334	1392.2373
1402.6258	1408.9797	1411.3833
1430.6106	1437.5794	1439.4175
1446.4084	1447.9477	1453.9835
1457.6994	1464.9297	1467.0915
1469.0379	1469.7352	1470.1302

C	-1.88386	-2.23503	-2.55920	1473.6783	1479.9880	1482.1835
H	-2.42668	-3.16559	-2.77420	1487.4701	1497.0242	1503.7262
H	-2.60890	-1.41757	-2.51160	1511.8341	1521.0342	1525.2029
H	-1.21270	-2.04136	-3.40163	1530.6725	1626.4723	1669.6736
C	1.19381	0.10917	1.35373	1788.4289	1802.6575	1821.9045
O	1.47920	0.17073	-1.31751	2465.3046	3034.2517	3039.5565
O	0.95415	0.04283	2.54113	3039.9059	3042.0412	3042.4006
O	-3.17245	0.53936	-1.18795	3048.2428	3051.3648	3071.4103
C	-4.27609	2.71240	-0.06927	3112.3870	3120.0252	3122.6536
H	-4.56106	3.29348	0.81267	3123.3782	3125.1279	3129.6283
H	-4.90785	1.81978	-0.12896	3133.5503	3135.4605	3144.8246
O	-2.91760	2.31182	0.18270	3146.4838	3150.8632	3154.8874
C	-4.34044	3.53134	-1.33555	3177.4153	3181.2977	3183.8060
H	-4.07454	2.91783	-2.20188	3197.6994	3223.9173	3228.5574
H	-5.35075	3.92503	-1.48785			
H	-3.64271	4.37342	-1.28162			
C	0.20818	3.13010	0.77877			
H	1.13500	3.65146	0.51770			
H	-0.54311	3.88194	1.05197			
H	0.35969	2.48010	1.64404			
F	5.75585	2.09542	-1.05228			
H	-0.62751	4.09779	0.93225			
C	5.02576	-3.23748	0.32044			
H	5.36231	-2.99497	-0.69328			
H	5.90398	-3.48398	0.93012			
H	4.39026	-4.12721	0.25052			
C	5.17282	-0.83456	1.01284			
H	4.65644	0.01184	1.47706			
H	6.06797	-1.06320	1.60514			
H	5.50303	-0.52892	0.01170			
C	3.79742	-2.44336	2.35161			
H	3.14852	-3.32899	2.32840			
H	4.66349	-2.68121	2.98218			
H	3.24427	-1.62073	2.81725			
H	2.41391	4.91247	-2.28274			
F	4.10506	2.97407	-2.21711			

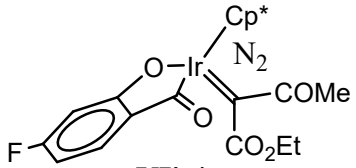
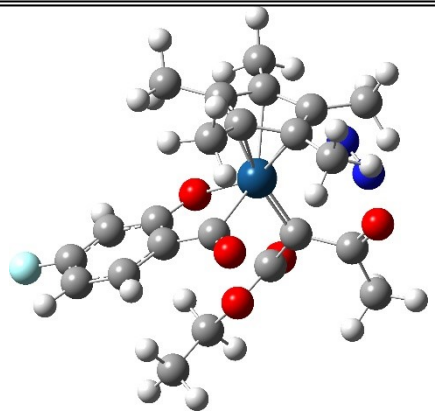
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm

Zero-point correction= 0.448853 Electronic Energy = -1581.36573682

Internal Energy (E)= -1580.88330082 Enthalpy (H)= -1580.88235782

Gibbs Free Energy (G)=-1580.98149082 Gibbs Free Energy of Solvation=-1581.01462837

St.Pt.	General Structure	Ball & Stick model
VI'-4	 **VI'-4**	

Cartesian co-ordinate

Atoms	X	Y	Z
C	1.30164	-2.50396	-0.55045
C	2.31318	-1.53142	-0.92499
C	2.80802	-0.93544	0.28471
C	2.01616	-1.44926	1.38106
C	1.11160	-2.43724	0.85091
C	-2.14034	-0.81309	-0.69740
Ir	0.66160	-0.31154	-0.00215
C	-2.13193	-0.41958	0.66051
C	-3.34248	-0.47008	1.38065
C	-3.32112	-1.22370	-1.33149
C	-4.47646	-0.89954	0.72528
C	-4.50472	-1.28038	-0.62344
H	-3.27670	-1.49874	-2.38285
H	-5.43982	-1.61051	-1.06454
H	-3.37790	-0.17948	2.42631
C	0.59911	1.53386	-0.45150
C	1.61876	2.28295	-1.25035
C	-0.50777	2.36950	0.09904
C	-2.78989	2.90373	0.02402
H	-2.92389	2.50804	1.04019
H	-2.56522	3.97350	0.11355
C	-3.97806	2.63013	-0.85734
H	-4.87319	3.10493	-0.44303
H	-3.81511	3.02332	-1.86619
H	-4.16240	1.55275	-0.93480
O	-1.65910	2.23592	-0.56369
O	-0.34540	3.10746	1.04713
C	3.99343	-0.04611	0.40142
H	4.09239	0.36049	1.41239
H	4.90663	-0.61368	0.18005
H	3.93419	0.78546	-0.30695
C	2.85977	-1.36679	-2.29930
H	3.50105	-0.48588	-2.36061
H	3.43652	-2.25314	-2.59679
H	2.04587	-1.22956	-3.02056
C	0.64150	-3.43827	-1.50006
H	0.46699	-2.96040	-2.46851
H	1.28199	-4.31511	-1.66203

Frequencies

23.6842	34.6738	41.4382
53.7881	64.6380	65.8692
71.5324	76.1178	82.1391
90.6560	98.1041	105.1912
113.7425	123.3154	129.9240
136.6605	138.0878	144.4736
153.3076	156.9463	165.0236
172.8186	176.2921	185.3183
202.3792	203.1922	209.4609
210.9590	223.1164	230.2706
234.8063	246.0654	260.1591
270.6992	274.9689	278.3535
287.6940	292.1439	300.8276
307.7209	313.9633	323.8854
330.6337	363.0375	376.1322
394.7572	403.8181	405.1198
413.4327	447.3854	459.3363
479.8410	532.4145	538.7716
551.4126	559.9602	576.9436
579.8032	586.6186	597.2707
603.6423	622.0593	652.7431
667.3149	680.7525	729.3797
739.4801	761.6433	798.0875
800.6212	806.4389	809.2174
819.6527	841.9814	851.2672
890.1375	936.2067	950.5461
955.5189	960.9388	991.2803
1024.0727	1026.9010	1031.3477
1032.1965	1036.8103	1041.5744
1055.2969	1060.5373	1084.8061
1089.8517	1103.3513	1107.6526
1109.5830	1140.4582	1171.3805
1175.1403	1180.6555	1184.9950
1230.3213	1238.3875	1254.6367
1273.1948	1316.0307	1341.2445
1369.1107	1377.2650	1382.2286
1384.0259	1388.1909	1393.2218
1400.5513	1406.6477	1421.0145
1431.4313	1439.0263	1442.4195
1444.3842	1446.3368	1449.7399
1456.0644	1459.0262	1461.6734
1463.3857	1467.5360	1473.9222
1476.2645	1476.6711	1479.5239

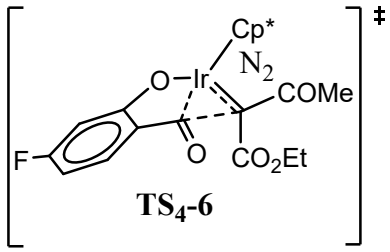
H	-0.32444	-3.79060	-1.12232	1491.6693	1501.6908	1503.9386
C	0.11483	-3.18598	1.66553	1510.9029	1514.3445	1522.4897
H	-0.58881	-3.73883	1.03584	1552.4274	1625.7299	1669.2146
H	0.61035	-3.90410	2.33111	1774.5843	1823.6182	1828.8064
H	-0.46706	-2.49842	2.29062	2467.3050	3037.5986	3037.9668
C	2.15583	-1.13166	2.82910	3038.9400	3039.0829	3039.6746
H	2.72780	-1.91042	3.35157	3043.3855	3046.7282	3051.1019
H	2.66229	-0.17566	2.98839	3100.4408	3115.9265	3117.7693
H	1.17211	-1.06095	3.30668	3120.2696	3120.6795	3124.2905
C	-0.86805	-0.71925	-1.39759	3128.6230	3143.5798	3146.4188
O	-1.02465	-0.00989	1.21951	3146.7160	3152.1803	3158.9935
O	-0.66352	-0.90199	-2.57075	3170.7506	3175.9965	3178.7842
N	2.66709	3.01569	1.75389	3195.9752	3218.3578	3221.4438
N	2.52711	2.45171	2.69375			
C	1.38281	3.75081	-1.49252			
H	1.35297	4.29989	-0.54527			
H	2.17593	4.14291	-2.13177			
H	0.41021	3.90229	-1.97882			
O	2.59014	1.72025	-1.73310			
F	-5.62001	-0.96008	1.41033			
H	-0.62751	4.09779	0.93225			
C	5.02576	-3.23748	0.32044			
H	5.36231	-2.99497	-0.69328			
H	5.90398	-3.48398	0.93012			
H	4.39026	-4.12721	0.25052			
C	5.17282	-0.83456	1.01284			
H	4.65644	0.01184	1.47706			
H	6.06797	-1.06320	1.60514			
H	5.50303	-0.52892	0.01170			
C	3.79742	-2.44336	2.35161			
H	3.14852	-3.32899	2.32840			
H	4.66349	-2.68121	2.98218			
H	3.24427	-1.62073	2.81725			
H	2.41391	4.91247	-2.28274			
F	4.10506	2.97407	-2.21711			

Statistical Thermodynamic Analysis

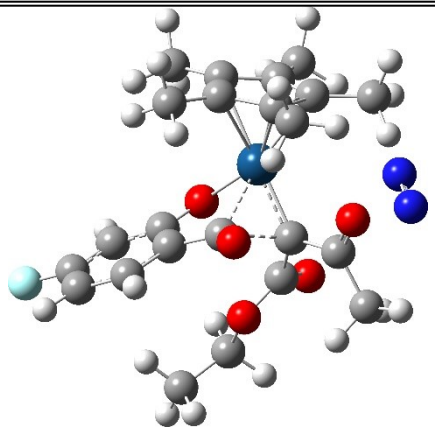
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.449479 Electronic Energy = -1581.37201414
Internal Energy (E)= -1580.88683014 Enthalpy (H)= -1580.88588714
Gibbs Free Energy (G)=-1580.98892414 Gibbs Free Energy of Solvation=-1581.02141606

St.Pt.	General Structure	Ball & Stick model

TS_4-6



TS_4-6



Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.39560	-2.38073	0.56218
C	-2.26965	-1.35255	1.12438
C	-2.93464	-0.70349	0.04251
C	-2.43272	-1.29439	-1.19339
C	-1.53584	-2.36811	-0.84848
C	2.00761	-0.57062	0.84815
Ir	-0.77912	-0.33227	-0.15210
C	2.03696	-0.67526	-0.56916
C	3.22890	-1.12435	-1.17378
C	3.11650	-0.93414	1.62537
C	4.29238	-1.47449	-0.36940
C	4.27261	-1.39472	1.02879
H	3.04313	-0.83673	2.70619
H	5.14903	-1.69163	1.59562
H	3.29559	-1.21041	-2.25398
C	-0.17184	1.43232	0.40319
C	-0.89914	2.24889	1.41827
C	0.81015	2.18761	-0.44271
C	3.05749	2.71811	-0.87246
H	2.94238	2.24065	-1.85516
H	2.86393	3.78986	-1.00308
C	4.40207	2.43704	-0.25799
H	5.20095	2.83299	-0.89291
H	4.48560	2.89931	0.73108
H	4.55071	1.35671	-0.14629
O	2.06824	2.16687	0.01104
O	0.46251	2.82109	-1.41494
C	-3.99520	0.33195	0.16959
H	-4.19418	0.82301	-0.78787
H	-4.93442	-0.12276	0.51075
H	-3.69939	1.09626	0.89741
C	-2.51175	-1.15173	2.57890
H	-3.21400	-0.33418	2.75305
H	-2.92288	-2.07265	3.01353
H	-1.58758	-0.89752	3.10957
C	-0.53176	-3.28527	1.37043
H	-0.25039	-2.81575	2.31833
H	-1.05968	-4.21915	1.60440
H	0.39125	-3.54359	0.84048

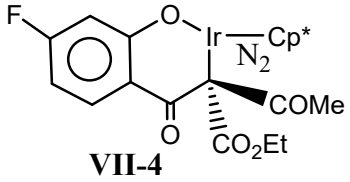
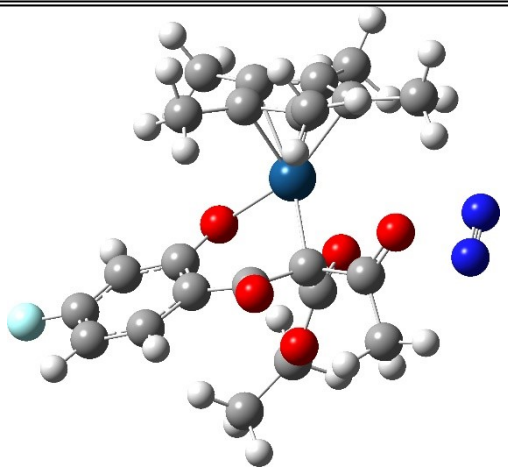
Frequencies

-252.4895	27.7002	35.6787
43.5358	49.3150	73.5566
82.0739	86.6274	92.5578
96.8771	101.2410	106.3930
114.1396	123.2456	128.3484
136.6589	139.4771	147.3120
156.7446	164.0514	173.9272
177.8099	192.1655	200.8956
203.2290	207.0185	215.2447
222.5923	229.4539	233.1942
235.5370	263.3382	275.1071
282.3661	290.3215	296.6148
301.6366	310.1064	318.5947
322.8380	332.4357	335.2543
366.9857	381.7040	392.5410
397.1241	404.2369	416.7945
425.3515	442.2950	449.2182
476.2114	525.3394	537.5238
543.3685	546.0841	551.6136
575.6333	579.2527	590.4521
601.1233	608.8805	657.0595
667.2464	678.6147	724.4261
736.9018	757.1719	802.1364
811.1301	811.7703	816.0880
820.9970	827.8082	841.7687
890.3195	930.1610	957.9030
962.4849	970.4997	994.4061
1021.3497	1029.3497	1034.7657
1037.3058	1040.6718	1046.9138
1048.3687	1050.4563	1091.3423
1097.1237	1105.8423	1108.7019
1112.9286	1139.2642	1172.0068
1179.8046	1183.6445	1188.6890
1231.6543	1240.0126	1255.4485
1300.0994	1315.9523	1339.8566
1373.9350	1376.3029	1379.7126
1383.1745	1395.5500	1400.5978
1400.6750	1405.3353	1427.2452
1434.4023	1441.7478	1442.9661
1447.4367	1453.1546	1455.0737
1457.7401	1460.9105	1466.3506
1467.4196	1470.5898	1474.9257
1476.6703	1482.9536	1497.3079
1498.2983	1512.0281	1515.3551

C	-0.76152	-3.18195	-1.82509	1524.7502	1527.4914	1533.4211
H	0.11502	-3.64095	-1.35597	1553.8378	1616.3253	1670.6555
H	-1.37700	-3.98447	-2.25043	1783.1474	1827.7910	1841.3641
H	-0.39917	-2.55856	-2.65002	2462.7854	3035.9516	3036.7692
C	-2.86517	-0.93702	-2.57159	3038.2950	3039.7125	3040.1162
H	-3.75079	-1.51634	-2.86648	3042.7571	3044.1176	3049.2176
H	-3.11609	0.12587	-2.65024	3097.2966	3117.3410	3120.3655
H	-2.07305	-1.13967	-3.29951	3121.5522	3121.9500	3123.1449
C	0.81131	-0.03803	1.47935	3129.1492	3141.7277	3143.5191
O	1.00231	-0.34874	-1.29196	3146.0814	3146.8950	3155.7569
O	0.56197	0.03100	2.65289	3161.2036	3168.1637	3176.1786
N	-2.53283	3.26223	-1.24733	3195.7185	3219.6861	3222.2090
N	-2.75535	2.69502	-2.16908			
C	-0.47131	3.68080	1.60591			
H	-0.54131	4.23792	0.66466			
H	-1.09921	4.15151	2.36477			
H	0.57920	3.71317	1.92255			
O	-1.79614	1.76483	2.08880			
F	5.40681	-1.92210	-0.95088			
H	-0.62751	4.09779	0.93225			
C	5.02576	-3.23748	0.32044			
H	5.36231	-2.99497	-0.69328			
H	5.90398	-3.48398	0.93012			
H	4.39026	-4.12721	0.25052			
C	5.17282	-0.83456	1.01284			
H	4.65644	0.01184	1.47706			
H	6.06797	-1.06320	1.60514			
H	5.50303	-0.52892	0.01170			
C	3.79742	-2.44336	2.35161			
H	3.14852	-3.32899	2.32840			
H	4.66349	-2.68121	2.98218			
H	3.24427	-1.62073	2.81725			
H	2.41391	4.91247	-2.28274			
F	4.10506	2.97407	-2.21711			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.450489 Electronic Energy = -1581.35484988
Internal Energy (E)= -1580.86996988 Enthalpy (H)= -1580.86902588
Gibbs Free Energy (G)=-1580.96831088 Gibbs Free Energy of Solvation=-1581.00479493

St.Pt.	General Structure	Ball & Stick model
VII-4	 **VII-4**	

Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.12416	-2.28455	0.70493
C	-2.07540	-1.34022	1.25788
C	-2.90230	-0.87714	0.18178
C	-2.51579	-1.61370	-1.02058
C	-1.46048	-2.50143	-0.69866
C	2.34179	-0.01193	1.00636
Ir	-0.79363	-0.42680	-0.22551
C	2.25078	-0.63343	-0.26936
C	3.41146	-1.24120	-0.79212
C	3.54126	-0.07280	1.72658
C	4.57560	-1.24426	-0.05293
C	4.67598	-0.67413	1.21462
H	3.55247	0.39124	2.71039
H	5.61660	-0.71140	1.75458
H	3.37092	-1.72603	-1.76358
C	0.12186	1.23418	0.74647
C	-0.80082	2.17755	1.52725
C	0.43039	1.77117	-0.60280
C	2.01278	2.59193	-2.15569
H	1.69386	1.71448	-2.72878
H	1.52112	3.47626	-2.57767
C	3.50963	2.72687	-2.08745
H	3.92640	2.83526	-3.09357
H	3.80121	3.60044	-1.49609
H	3.94454	1.83419	-1.62415
O	1.55244	2.42419	-0.79356
O	-0.38343	1.50932	-1.50595
C	-4.07073	0.03740	0.29866
H	-4.35750	0.44335	-0.67683
H	-4.94059	-0.49927	0.70082
H	-3.84283	0.87709	0.96192
C	-2.14896	-0.96733	2.69728
H	-2.85860	-0.15481	2.86227
H	-2.45524	-1.83933	3.29013
H	-1.17596	-0.62528	3.07204
C	-0.09296	-3.02866	1.47758

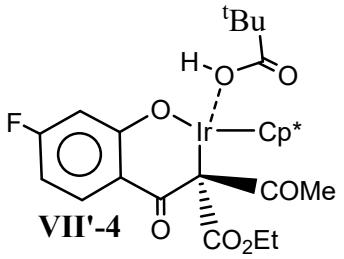
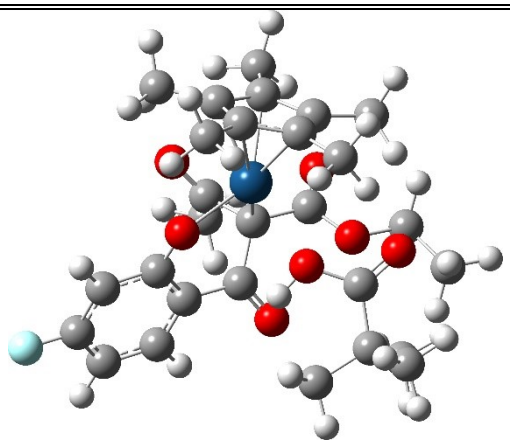
Frequencies

28.7857	43.2480	51.2459
66.7977	71.3459	77.1793
85.2814	90.1170	98.6505
105.1198	108.8382	117.0227
120.1826	125.9230	131.0566
139.6227	152.0452	156.0270
174.9712	178.6562	182.0628
187.9744	206.1312	214.8585
219.3785	225.5045	230.6563
231.1520	237.6192	254.1711
258.2433	268.4130	274.1651
276.3477	288.5819	293.1183
301.6307	305.9532	312.7262
322.8466	329.2047	355.9339
383.8158	390.2697	403.1976
406.1294	425.6360	427.4738
464.6248	472.5462	492.7776
526.5168	538.9541	539.2548
549.3066	556.2512	573.4827
587.8362	593.9421	597.2177
607.7173	650.9870	654.0486
675.2963	717.7925	737.3041
765.2881	785.6334	794.4759
806.1477	814.1024	823.8868
834.9658	846.4753	868.6800
897.4275	949.7289	958.4012
968.2766	993.5994	1002.7451
1020.8606	1037.1066	1039.9706
1041.9993	1049.1059	1050.3964
1054.4226	1080.6786	1088.8648
1093.0350	1105.8847	1111.2711
1132.3117	1155.1730	1172.2458
1180.8595	1185.3784	1187.5377
1213.7958	1255.2707	1292.9923
1300.6821	1338.8094	1371.7884
1374.7627	1375.8351	1378.0355
1386.2071	1391.0951	1393.1514
1401.2062	1406.2566	1434.6815
1436.5728	1443.6314	1446.8312
1449.0267	1450.4338	1453.5054
1459.8455	1461.6506	1463.6232

H	0.30330	-2.41417	2.29336	1464.0968	1469.7484	1472.1431
H	-0.51899	-3.94159	1.91557	1473.4761	1483.7861	1489.0599
H	0.74904	-3.32210	0.84139	1492.0966	1496.9400	1503.1520
C	-0.67489	-3.37564	-1.61078	1505.4229	1520.2748	1525.7693
H	0.38107	-3.07102	-1.60674	1552.9703	1623.5064	1670.3522
H	-0.73001	-4.42484	-1.29502	1681.2563	1730.9164	1845.7365
H	-1.03492	-3.31331	-2.64176	2468.7334	3027.0170	3032.7595
C	-3.11579	-1.38270	-2.36309	3037.4267	3038.5743	3039.2463
H	-4.10632	-1.84979	-2.43671	3050.3610	3051.0238	3063.6804
H	-3.23977	-0.30961	-2.55215	3103.4283	3112.8146	3114.5915
H	-2.48640	-1.78734	-3.16091	3117.3944	3120.6535	3124.9590
C	1.22094	0.72276	1.61917	3138.7766	3140.0863	3141.5855
O	1.15314	-0.69121	-0.98829	3147.0236	3148.4378	3149.3439
O	1.14156	0.88760	2.83695	3158.1152	3176.2601	3179.9097
N	-2.52198	3.38721	-0.79737	3200.4316	3213.0197	3221.2943
N	-3.26078	2.81321	-1.38503			
C	-0.19743	3.50731	1.88067			
H	0.11588	4.03357	0.97009			
H	-0.92630	4.11237	2.42423			
H	0.69494	3.34648	2.49481			
O	-1.93873	1.89375	1.82981			
F	5.65716	-1.83590	-0.57139			
H	-0.62751	4.09779	0.93225			
C	5.02576	-3.23748	0.32044			
H	5.36231	-2.99497	-0.69328			
H	5.90398	-3.48398	0.93012			
H	4.39026	-4.12721	0.25052			
C	5.17282	-0.83456	1.01284			
H	4.65644	0.01184	1.47706			
H	6.06797	-1.06320	1.60514			
H	5.50303	-0.52892	0.01170			
C	3.79742	-2.44336	2.35161			
H	3.14852	-3.32899	2.32840			
H	4.66349	-2.68121	2.98218			
H	3.24427	-1.62073	2.81725			
H	2.41391	4.91247	-2.28274			
F	4.10506	2.97407	-2.21711			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.452593 Electronic Energy = -1581.39303549
Internal Energy (E)= -1580.90612649 Enthalpy (H)= -1580.90518349
Gibbs Free Energy (G)=-1581.00378049 Gibbs Free Energy of Solvation=-1581.0402139

St.Pt.	General Structure	Ball & Stick model
VII'-4		

VII'-4

Cartesian co-ordinate

Atoms	X	Y	Z
C	1.61486	-2.02379	-2.01089
C	2.40914	-0.87268	-1.73186
C	2.81752	-0.89828	-0.33592
C	2.27331	-2.09036	0.25151
C	1.47044	-2.75277	-0.76753
O	-0.17391	1.34050	-1.35566
C	0.20473	2.64694	-1.30259
O	1.37993	2.90763	-1.27434
C	-0.89537	3.70554	-1.32954
C	-2.42165	-0.91065	-0.39700
H	-1.13537	1.21999	-1.42298
C	2.76078	0.22173	-2.67204
H	2.63274	1.19843	-2.19161
H	3.80908	0.12544	-2.98437
H	2.13485	0.20431	-3.56947
C	3.73697	0.07711	0.31027
H	4.78460	-0.14540	0.06796
H	3.51763	1.09865	-0.02616
H	3.62370	0.04787	1.40046
C	0.70100	-4.00919	-0.58106
H	-0.04855	-4.12727	-1.36952
H	1.36948	-4.87981	-0.60517
H	0.17832	-3.98738	0.37974
C	0.93595	-2.37574	-3.28792
H	1.06612	-1.58992	-4.03798
H	1.33441	-3.30866	-3.70583
H	-0.14106	-2.50632	-3.12898
C	2.55475	-2.62133	1.60946
H	3.52342	-3.13882	1.60020
H	2.59552	-1.82200	2.35631
H	1.78356	-3.32976	1.92211
Ir	0.64696	-0.83230	-0.39742
C	-0.64501	4.56492	-2.57266
H	-0.78724	3.98997	-3.49676

Frequencies

16.1471	30.5849	43.9447
47.6004	64.5301	71.5377
76.9393	80.6540	87.3243
88.1842	89.3945	99.8347
103.3979	113.5606	116.4294
122.3018	128.4243	137.5614
141.3816	145.0980	150.0320
157.7086	162.8107	174.7496
186.7095	192.3975	198.3151
202.0105	212.6617	233.7002
235.5326	241.7531	245.6532
249.7908	253.6667	259.5114
272.7077	276.0946	288.5017
296.7671	308.6423	312.3605
315.1283	325.0179	332.3799
336.4426	338.5006	362.8250
369.6165	373.6802	388.3911
393.6815	394.2268	406.2977
412.4825	421.6399	426.0665
442.5443	450.7810	458.1224
491.6974	507.8391	532.7831
534.0268	542.5795	546.9024
551.7010	571.4126	574.4761
584.4887	587.8473	599.7605
604.6733	606.1562	648.8654
656.6623	678.4824	717.2160
755.5140	763.8932	767.1290
773.4237	784.0350	784.5602
806.2658	813.9014	817.2785
833.9736	875.7406	882.0230
893.2206	909.0363	941.6725
951.2624	952.9067	965.2117
965.3603	991.5954	1000.3643
1004.6862	1008.6544	1021.2029
1035.3577	1037.6629	1038.2017
1043.2646	1047.7786	1049.3886
1065.7856	1090.1353	1097.0028
1104.3926	1105.7884	1115.4332

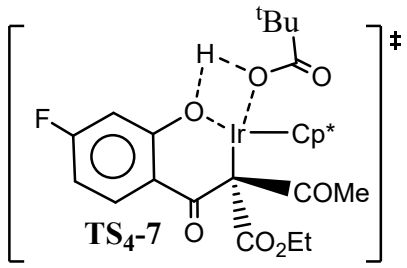
H	-1.35124	5.40385	-2.58624	1120.3162	1130.0295	1145.9655
H	0.37344	4.96579	-2.56866	1169.1476	1177.1529	1187.4531
C	-2.30898	3.13090	-1.36606	1190.2512	1193.0426	1213.9000
H	-2.54717	2.57768	-0.44855	1238.4034	1253.3515	1266.8887
H	-3.02799	3.95506	-1.43612	1275.2737	1277.9928	1304.3471
H	-2.48611	2.49416	-2.24583	1326.4777	1335.0597	1371.8565
C	-0.72337	4.55217	-0.06456	1377.1924	1378.7714	1380.2307
H	-0.83907	3.93388	0.83495	1381.6980	1386.9502	1390.6112
H	0.26600	5.02153	-0.04972	1396.3062	1404.8636	1410.6126
H	-1.48602	5.34054	-0.05052	1417.2074	1418.4672	1435.7477
O	-1.30475	-1.15097	-1.04232	1441.2890	1442.2207	1444.9896
C	-2.54084	0.02663	0.66447	1451.3846	1453.3269	1454.4908
C	-3.81136	0.34123	1.17321	1455.6433	1459.9348	1460.3061
C	-3.59710	-1.53879	-0.85922	1465.1966	1467.5694	1470.2180
C	-4.95941	-0.27471	0.71681	1476.2045	1477.6905	1478.8745
C	-4.81339	-1.21952	-0.29875	1489.8810	1492.0938	1493.3795
C	-1.38684	0.71198	1.28484	1497.6015	1498.4905	1502.3753
O	-1.50943	1.85579	1.71145	1507.9034	1517.5738	1523.4612
H	-3.53381	-2.25874	-1.66965	1523.6476	1534.2983	1544.9020
H	-5.94286	-0.06047	1.12272	1618.6288	1673.0772	1748.9002
H	-3.86097	1.08715	1.96418	1778.7741	1832.1938	1881.2821
C	-0.14098	-0.11916	1.49509	3019.9774	3031.6780	3034.4334
C	-0.57863	-1.30228	2.39072	3035.7779	3036.2088	3039.4174
C	0.98409	0.60034	2.16232	3044.5715	3044.8160	3045.7198
C	2.25789	2.55793	2.35674	3049.0313	3052.5071	3097.6222
H	3.21338	2.02741	2.25671	3110.3394	3110.6010	3116.3764
H	2.01857	2.58159	3.42683	3118.6376	3121.2817	3123.3292
C	2.32317	3.93629	1.75680	3134.9483	3135.7299	3139.7512
H	3.13656	4.50477	2.21993	3140.2900	3142.2015	3142.4045
H	2.49606	3.88395	0.67595	3145.1159	3147.5872	3148.5160
H	1.38646	4.47721	1.92643	3148.6958	3148.9098	3159.3148
O	1.23320	1.82204	1.67193	3172.0879	3178.8745	3191.3123
O	1.67101	0.11043	3.04690	3219.7941	3224.1313	3768.7803
O	-0.53999	-2.46218	2.03709			
C	-1.08545	-0.93714	3.76265			
H	-1.67129	-1.76512	4.16784			
H	-0.21549	-0.76180	4.40506			
H	-1.67523	-0.01370	3.75986			
F	-5.90846	-1.83413	-0.75509			

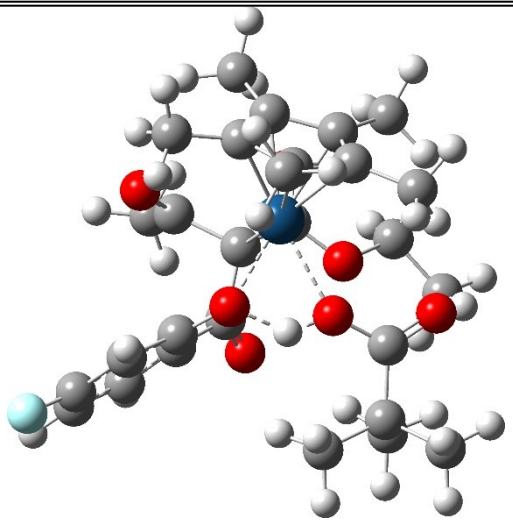
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.593986 Electronic Energy = -1818.76130652
Internal Energy (E)= -1818.12682452 Enthalpy (H)= -1818.12588052
Gibbs Free Energy (G)=-1818.23765152 Gibbs Free Energy of Solvation=-1818.28830392

St.Pt.	General Structure	Ball & Stick model

TS_4-7





Cartesian co-ordinate

Atoms	X	Y	Z
C	0.87686	-2.31534	-2.04459
C	2.07246	-1.64420	-1.69069
C	2.32701	-1.86674	-0.26975
C	1.30456	-2.75749	0.22753
C	0.35873	-2.96234	-0.84361
O	0.43544	1.24526	-1.13496
C	1.17813	2.35099	-1.23083
O	2.38376	2.28952	-1.13201
C	0.42121	3.66274	-1.41957
C	-2.53755	0.17797	-0.54659
H	-0.60058	0.99121	-1.37546
C	2.91254	-0.76867	-2.55026
H	3.04761	0.21648	-2.08595
H	3.90399	-1.21777	-2.69345
H	2.46255	-0.61730	-3.53593
C	3.53907	-1.40077	0.45646
H	4.39032	-2.06850	0.26691
H	3.81808	-0.39281	0.12510
H	3.36145	-1.36620	1.53664
C	-0.87526	-3.78872	-0.80675
H	-1.63381	-3.37797	-1.48311
H	-0.65825	-4.81715	-1.12524
H	-1.30369	-3.80330	0.19636
C	0.17283	-2.30113	-3.35583
H	0.69554	-1.67594	-4.08548
H	0.09473	-3.31351	-3.77152
H	-0.84262	-1.90223	-3.24265
C	1.29356	-3.40536	1.56397
H	1.97982	-4.26244	1.55374
H	1.62354	-2.71039	2.34290
H	0.29552	-3.76351	1.82703
Ir	0.43615	-0.87480	-0.39842
C	1.09744	4.44293	-2.54628
H	0.97210	3.94150	-3.51452
H	0.65144	5.44203	-2.62478
H	2.16903	4.55211	-2.35303
C	-1.06038	3.46754	-1.72534

Frequencies

-882.2387	26.8797	36.3413
49.1653	55.0823	66.3039
74.5490	84.3620	88.0610
97.6056	107.5142	114.3682
115.5705	118.0719	124.8797
127.3445	141.7566	144.5439
155.9605	162.5945	164.2919
165.1265	180.1900	182.1865
188.7275	194.6472	199.6044
209.3604	213.8168	218.9391
226.7431	228.0272	236.7082
239.5104	247.9680	257.8619
269.3829	272.5097	285.7889
290.3665	298.0078	312.8549
313.0885	315.9443	320.2287
330.8957	332.6091	364.0753
367.7941	371.1093	380.0814
385.5960	389.7659	408.1532
411.9744	421.2142	427.4189
439.9360	445.7428	451.9524
456.8358	492.7789	530.6739
534.9849	539.1841	543.9122
551.5818	556.0569	572.7469
588.4887	593.2598	603.5564
605.0077	631.6971	641.4836
650.5454	680.4178	725.6116
756.2512	764.0204	772.0765
788.4293	808.1425	809.8323
812.0777	819.9494	833.0657
850.9508	883.0229	889.1065
905.5132	937.4368	944.0390
946.1454	951.0358	958.5993
966.7062	976.1251	989.5283
1001.2986	1012.0216	1025.8146
1032.7996	1037.5653	1041.8998
1043.4453	1044.4741	1047.9805
1051.2172	1090.0397	1096.3870
1103.2218	1104.0538	1112.5663
1130.0959	1145.8496	1174.5832
1176.9267	1185.3421	1189.5545
1192.9797	1202.4760	1219.8743

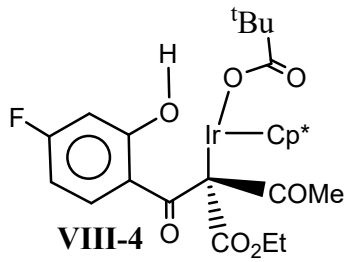
H	-1.59088	2.99366	-0.88897	1235.9194	1255.3920	1266.2022
H	-1.52719	4.44603	-1.88927	1273.9927	1284.8898	1311.8795
H	-1.22312	2.87149	-2.63336	1334.5924	1343.4310	1370.4363
C	0.57000	4.42458	-0.09575	1375.5202	1377.5705	1378.6882
H	0.16004	3.84883	0.74500	1382.0111	1382.9521	1383.6749
H	1.62508	4.63725	0.10936	1390.3542	1403.3569	1411.9212
H	0.02874	5.37698	-0.16210	1412.7729	1419.5034	1430.4610
O	-1.43498	-0.06615	-1.26877	1440.5172	1444.1960	1446.0458
C	-2.46630	0.83282	0.69806	1450.0493	1452.5136	1454.6082
C	-3.64696	1.21999	1.33946	1456.5711	1457.7127	1461.8886
C	-3.78585	-0.13027	-1.09236	1463.6728	1465.7058	1467.9796
C	-4.89024	0.91840	0.80753	1469.7287	1471.1401	1479.6846
C	-4.92739	0.23547	-0.40231	1482.0376	1484.2431	1485.1245
C	-1.18329	1.09718	1.39715	1487.5108	1492.3117	1495.6832
O	-1.01528	2.14924	1.99425	1507.3882	1509.8886	1527.0141
H	-3.85355	-0.62478	-2.05695	1533.7691	1537.7611	1557.3974
H	-5.81742	1.18882	1.30289	1638.7586	1673.1161	1769.3907
H	-3.56277	1.74994	2.28620	1780.4990	1825.7248	1832.8227
C	-0.22463	-0.08001	1.51465	2093.3986	3025.5841	3026.8701
C	-1.03658	-1.11772	2.31758	3030.2387	3032.2690	3033.8662
C	1.05487	0.24254	2.21935	3035.2329	3036.4701	3039.1419
C	2.85783	1.72636	2.46156	3047.0115	3048.0108	3050.7797
H	3.61952	1.00238	2.14189	3092.3098	3108.5522	3111.4341
H	2.74725	1.61945	3.54722	3112.7384	3112.9287	3113.3363
C	3.21353	3.13039	2.05495	3114.4260	3116.4364	3121.5675
H	4.17056	3.41949	2.50180	3138.4353	3139.2664	3139.2966
H	3.29532	3.20211	0.96534	3142.0831	3142.6499	3148.1372
H	2.44658	3.83529	2.39398	3148.3732	3148.7172	3149.1397
O	1.61102	1.39493	1.83517	3169.2044	3190.2498	3193.2605
O	1.59357	-0.50347	3.02419	3207.0568	3214.7484	3225.9127
O	-1.53591	-2.10281	1.81290			
C	-1.26388	-0.80869	3.77517			
H	-2.15072	-1.34352	4.12312			
H	-0.38921	-1.14823	4.33989			
H	-1.36237	0.26760	3.95820			
F	-6.11570	-0.06496	-0.93188			

Statistical Thermodynamic Analysis

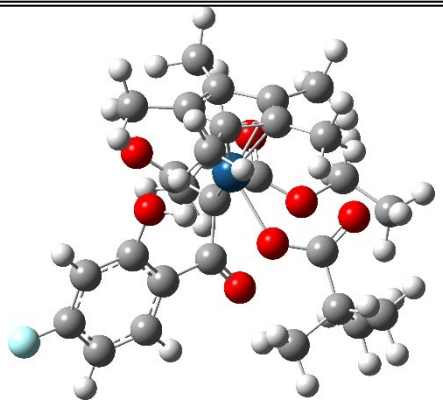
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.590277 Electronic Energy = -1818.75281512
Internal Energy (E)= -1818.12303612 Enthalpy (H)= -1818.12209212
Gibbs Free Energy (G)=-1818.23014312 Gibbs Free Energy of Solvation=-1818.27662307

St.Pt.	General Structure	Ball & Stick model

VIII-4



VIII-4



Cartesian co-ordinate

Atoms	X	Y	Z
C	0.62328	-2.55227	-1.79066
C	1.88554	-2.05559	-1.38376
C	1.95748	-2.15416	0.07209
C	0.75949	-2.84412	0.53326
C	-0.09069	-3.01444	-0.60198
O	0.62831	1.03580	-1.13260
C	1.73828	1.72421	-1.12796
O	2.81985	1.29696	-0.74698
C	1.58659	3.16357	-1.63989
C	-2.65278	0.58609	-0.77582
H	-0.96528	0.72485	-1.70691
C	2.94308	-1.48115	-2.25607
H	3.47153	-0.67053	-1.74718
H	3.66386	-2.26087	-2.53561
H	2.51931	-1.06695	-3.17730
C	3.14143	-1.78330	0.89032
H	3.92732	-2.54596	0.80774
H	3.54385	-0.82229	0.54493
H	2.86277	-1.68649	1.94509
C	-1.44562	-3.62736	-0.61980
H	-2.05292	-3.20290	-1.42714
H	-1.37448	-4.71036	-0.78717
H	-1.97438	-3.44071	0.31806
C	0.06402	-2.57452	-3.16940
H	0.68522	-1.99836	-3.86145
H	-0.00152	-3.60247	-3.54869
H	-0.94487	-2.14637	-3.18904
C	0.50877	-3.33194	1.91517
H	1.04978	-4.27437	2.07270
H	0.84590	-2.60934	2.66689
H	-0.55643	-3.51451	2.08239
Ir	0.30735	-0.89737	-0.34424
C	2.60568	3.37369	-2.75935
H	2.37841	2.74410	-3.63036
H	2.59393	4.42048	-3.08959
H	3.61411	3.12647	-2.41221
C	0.17946	3.46649	-2.14443
H	-0.56023	3.36642	-1.33982
H	0.13580	4.49988	-2.51263
H	-0.10668	2.80740	-2.97474

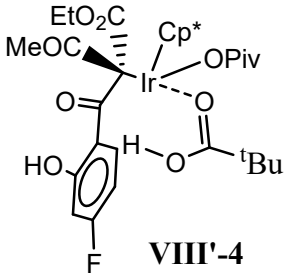
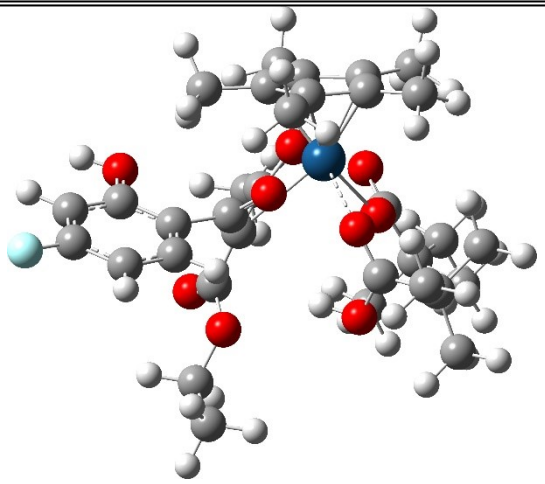
Frequencies

29.8360	33.8661	42.4379
63.6093	68.9076	71.7637
76.2106	83.1945	97.5633
104.3611	111.6179	117.3642
131.6022	133.7888	137.1076
139.2724	144.6130	149.5012
153.3342	161.4365	170.2646
175.0053	183.0228	185.2615
195.5804	199.4240	208.0939
217.4169	223.4330	232.0366
237.6493	245.8208	251.7334
259.9719	267.4874	273.6016
282.5161	287.2335	293.2800
304.0536	314.6692	321.8168
323.1163	325.5391	340.0185
357.1888	359.7405	364.4893
368.5078	373.2226	386.4986
386.8080	388.7043	401.0712
410.8767	422.9908	434.5224
439.3925	447.3441	477.0899
484.3788	509.2142	531.2684
536.2997	541.9870	554.3657
557.0550	564.2687	577.3227
586.8136	601.6241	605.4790
614.8326	629.6076	641.7057
668.9906	710.7798	750.0440
755.6005	785.6043	791.3818
804.5338	806.2430	812.8215
815.3279	830.9738	835.1358
861.1573	877.1393	892.4029
909.9069	925.2549	947.7224
948.2159	954.6286	964.4455
974.5558	984.3593	989.8644
995.2066	1013.0139	1020.5657
1021.9198	1037.9265	1039.0104
1045.4385	1056.3053	1057.3732
1058.7277	1091.8467	1099.1620
1104.3813	1106.6876	1119.4859
1134.2282	1150.6358	1160.4935
1169.7751	1188.8476	1192.5929
1201.6471	1232.4146	1239.6850
1246.3838	1266.5428	1267.5393
1297.9355	1315.6141	1327.5526
1343.1417	1366.9147	1367.9989
1369.4806	1375.3818	1379.3438

C	1.90585	4.09334	-0.46626	1383.8319	1383.9351	1386.6504
H	1.23179	3.90065	0.37903	1397.6720	1402.9079	1408.8297
H	2.93847	3.95210	-0.12981	1416.3531	1429.7413	1430.7014
H	1.78332	5.13887	-0.77892	1438.7688	1441.5970	1446.0331
O	-1.61788	0.01506	-1.48575	1450.6600	1455.3028	1456.6317
C	-2.39682	1.38089	0.34431	1458.4614	1459.4574	1459.7669
C	-3.47335	2.03513	0.94818	1466.3422	1468.1330	1469.2025
C	-3.94245	0.38405	-1.24296	1475.5824	1480.1240	1486.0780
C	-4.77524	1.85152	0.50344	1486.4860	1487.6156	1490.3683
C	-4.98536	1.01016	-0.57872	1495.3874	1500.9184	1503.1803
C	-1.05446	1.50883	1.00887	1508.4173	1518.9071	1527.6551
O	-0.64637	2.61323	1.31528	1532.7548	1542.9836	1557.3155
H	-4.12589	-0.22578	-2.12198	1652.5058	1685.5332	1768.0349
H	-5.62190	2.33729	0.97847	1774.0340	1792.4148	1826.3676
H	-3.26732	2.68060	1.79946	3022.0491	3026.3362	3035.2729
C	-0.41420	0.19747	1.41619	3037.9225	3038.5326	3039.8697
C	-1.51135	-0.59668	2.14199	3040.2091	3040.7718	3041.9892
C	0.78938	0.30855	2.29744	3050.3088	3060.5994	3102.5664
C	2.82735	1.35478	2.77791	3106.5092	3116.8436	3117.9084
H	3.35216	0.39315	2.71343	3122.1961	3123.6876	3123.9802
H	2.54543	1.49677	3.82888	3125.3991	3125.8366	3126.9765
C	3.66858	2.48247	2.24641	3138.0642	3140.7018	3141.3374
H	4.60096	2.55300	2.81663	3144.2643	3148.3879	3151.5111
H	3.90319	2.30777	1.19060	3156.1020	3160.0664	3167.5691
H	3.13805	3.43665	2.33187	3169.6669	3176.9015	3193.8700
O	1.63293	1.28803	1.98529	3220.9061	3225.1282	3423.9961
O	1.01262	-0.47996	3.20689			
O	-2.10740	-1.52477	1.63246			
C	-1.89181	-0.11745	3.52099			
H	-2.93778	-0.36912	3.71436			
H	-1.25773	-0.63092	4.25091			
H	-1.72273	0.95843	3.64879			
F	-6.22865	0.81633	-1.01856			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.595901 Electronic Energy = -1818.76417520
Internal Energy (E)= -1818.1287682 Enthalpy (H)= -1818.1278242
Gibbs Free Energy (G)=-1818.2357842 Gibbs Free Energy of Solvation=-1818.28488305

St.Pt.	General Structure	Ball & Stick model
VIII'-4	 **VIII'-4**	

Cartesian co-ordinate

Atoms	X	Y	Z
H	0.93641	1.35635	0.23531
C	-2.01487	-2.69233	-1.18126
C	-1.65250	-2.93349	0.17748
C	-2.61356	-2.25140	1.03789
C	-3.57905	-1.59748	0.19344
C	-3.18642	-1.82304	-1.18819
C	-2.74927	1.96822	-0.18856
O	-1.87396	1.20395	0.39515
O	-3.59933	1.60145	-0.99432
C	-2.59852	3.45744	0.16670
O	0.04393	-0.42374	1.45445
C	0.47990	0.63031	1.91913
O	0.94455	1.61430	1.19149
C	0.54006	0.85267	3.41865
C	-4.76092	-0.82011	0.64581
H	-5.62184	-1.48817	0.77970
H	-4.56314	-0.32271	1.60184
H	-5.01074	-0.04451	-0.08173
C	-3.90345	-1.31907	-2.38796
H	-4.83449	-1.87857	-2.54729
H	-4.13523	-0.25651	-2.25714
H	-3.28442	-1.42218	-3.28405
C	-2.64416	-2.32563	2.52160
H	-1.63315	-2.27858	2.94026
H	-3.22248	-1.50029	2.94916
H	-3.10174	-3.26658	2.85433
C	-0.47207	-3.70005	0.65734
H	-0.19232	-3.38336	1.66778
H	-0.69389	-4.77442	0.68492
H	0.39210	-3.51885	0.01106
C	-1.30506	-3.16060	-2.39955
H	-0.32063	-3.56595	-2.15736
H	-1.89416	-3.93397	-2.90872
H	-1.15158	-2.32789	-3.09374
C	-0.89856	0.75902	3.93568
H	-0.91670	0.94595	5.01631

Frequencies

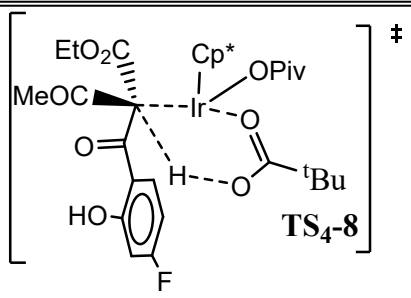
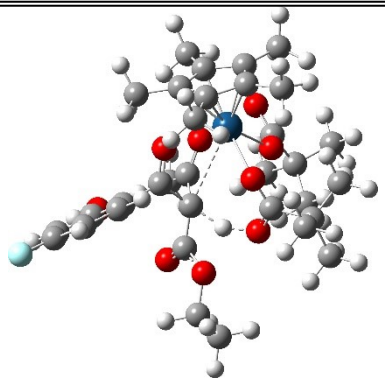
19.8883	31.5225	44.4612
50.2860	57.6369	61.9665
68.2313	70.3331	77.8089
81.8433	86.4585	94.2757
100.0498	100.3000	104.0829
109.1484	112.2813	120.9122
127.9279	135.9881	138.7736
149.2562	153.3237	158.6773
159.5339	167.7547	170.6169
177.6228	182.1851	184.9276
197.7166	204.5160	210.2943
214.3415	219.3264	219.3813
222.4526	231.1359	236.2966
238.6436	242.6683	249.2121
253.3073	258.1539	267.1717
268.4382	275.4825	291.0037
298.8438	303.9071	309.3948
311.2411	314.5889	316.6379
319.1898	322.0301	324.3818
328.9160	334.3145	335.6475
342.0848	343.8243	356.1052
370.7175	386.3850	390.4205
392.5573	396.7760	402.3169
421.0126	423.0439	435.0465
444.7470	452.6398	453.5351
475.1596	492.6726	506.8799
527.4674	536.4618	539.1881
541.3946	546.3503	549.7768
572.4038	580.2011	591.5738
593.6530	602.6461	603.4206
623.9867	629.5445	636.2003
645.7341	720.0462	731.6306
757.3580	767.2604	775.4380
793.8936	795.4094	805.2502
806.2452	810.5682	811.0764
819.3086	827.1736	832.9192
836.1386	881.1798	895.7907
903.3819	915.4338	947.9317
949.2520	952.8799	960.5014
962.4067	964.3291	969.4612

H	-1.54274	1.49564	3.44036	979.7818	1007.2463	1013.9624
H	-1.31603	-0.23461	3.74376	1027.7933	1032.2623	1033.7601
C	1.14269	2.20397	3.78395	1035.4884	1038.4387	1044.3049
H	1.17347	2.30369	4.87593	1045.5541	1046.9541	1047.5470
H	2.16355	2.30813	3.40133	1048.7254	1056.7166	1057.3870
H	0.54704	3.03193	3.38312	1093.3754	1096.5341	1101.1463
C	1.38566	-0.27868	4.01219	1108.6279	1124.3735	1143.0715
H	0.96115	-1.25856	3.76364	1158.7044	1173.4793	1183.0237
H	2.41630	-0.24405	3.63427	1186.0064	1189.9258	1222.5703
H	1.41996	-0.18091	5.10402	1236.7844	1237.9413	1240.2235
C	-3.91458	4.18213	-0.08991	1248.1215	1267.8234	1272.9165
H	-4.70996	3.79870	0.56126	1284.9445	1290.1647	1296.3219
H	-3.79891	5.25572	0.10913	1305.7573	1320.4699	1346.2026
H	-4.24114	4.04707	-1.12504	1366.8236	1371.4918	1372.3429
C	-1.51558	4.01483	-0.76309	1376.2187	1376.6725	1377.5608
H	-1.37174	5.08782	-0.57866	1381.4143	1384.2080	1385.4466
H	-0.55286	3.51143	-0.59669	1385.9214	1387.1145	1389.5078
H	-1.80052	3.88451	-1.81481	1397.3785	1408.5771	1417.9487
C	-2.16917	3.65777	1.61700	1422.0066	1423.9872	1427.3560
H	-2.10591	4.73047	1.84403	1435.0361	1435.6212	1441.2127
H	-2.89245	3.21125	2.31309	1443.0555	1447.1406	1449.2395
H	-1.18658	3.20958	1.80195	1450.5781	1452.5382	1453.7126
Ir	-1.63913	-0.79944	-0.19629	1454.8309	1460.4942	1462.1120
C	1.45557	0.65806	-1.62208	1464.1589	1466.7809	1467.9313
C	1.78085	-0.65328	-1.08481	1470.1404	1472.5965	1473.6196
O	0.96816	-1.58470	-1.04179	1475.9397	1476.2529	1477.3909
C	3.14666	-0.96692	-0.53092	1478.4319	1480.1469	1484.8074
C	4.34177	-0.83832	-1.24992	1486.4700	1487.8164	1494.6035
C	3.20136	-1.50788	0.75065	1496.7165	1503.6563	1507.2068
C	5.55765	-1.20718	-0.67931	1513.9729	1515.8761	1538.2345
C	4.40457	-1.86344	1.35285	1562.3233	1577.3389	1667.6099
H	2.26139	-1.63866	1.28633	1677.8548	1708.5050	1758.3730
C	5.56482	-1.70525	0.61582	1764.5004	1834.7358	3022.8304
H	6.49469	-1.12295	-1.22642	3025.0238	3030.4922	3034.7320
O	4.26490	-0.35340	-2.51265	3037.6285	3038.4993	3039.6399
H	5.14530	-0.29650	-2.89870	3040.8717	3042.6624	3043.4278
C	0.18016	0.86267	-2.23507	3044.1461	3046.4859	3047.7521
C	2.49227	1.69517	-1.79644	3054.9987	3089.3850	3100.0773
C	4.42536	2.60981	-0.79225	3111.1293	3114.7192	3117.2188
H	4.10337	3.64655	-0.95309	3119.6715	3120.8208	3123.5858
H	5.01375	2.32004	-1.67524	3126.2146	3127.0874	3130.1942
C	5.19839	2.43588	0.48987	3133.7770	3133.8938	3134.6080
H	6.10784	3.04535	0.48218	3135.4771	3142.7773	3144.1231
H	4.58916	2.73462	1.34942	3144.3493	3147.0064	3150.8586
H	5.48176	1.38460	0.62396	3151.3480	3151.6705	3157.2141
O	3.28198	1.76507	-0.69802	3158.1746	3165.3363	3175.3937
O	2.63743	2.45421	-2.73228	3177.6999	3183.5608	3189.8468
C	-0.02853	1.91518	-3.28764	3216.7066	3410.8733	3897.2290
H	-1.09412	1.94815	-3.52995			
H	0.31777	2.89592	-2.94866			
H	0.56709	1.69073	-4.17842			
O	-0.85925	0.20120	-1.95591			
H	4.45240	-2.26791	2.35944			
F	6.73797	-2.05129	1.15428			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm

Zero-point correction= 0.743621	Electronic Energy = -2165.58762226
Internal Energy (E)= -2164.79474226	Enthalpy (H)= -2164.79379826
Gibbs Free Energy (G)=-2164.92198326	Gibbs Free Energy of Solvation=-2164.98932705

St.Pt.	General Structure	Ball & Stick model
TS_4-8		

Cartesian co-ordinate

Atoms	X	Y	Z
H	1.10596	1.21182	-0.09305
C	-1.93597	-2.61823	-1.28380
C	-1.52089	-2.94783	0.03890
C	-2.49578	-2.38673	0.96983
C	-3.52866	-1.73798	0.19710
C	-3.15616	-1.82408	-1.19941
C	-2.93464	1.88752	-0.08655
O	-2.07537	1.14588	0.54746
O	-3.77315	1.49066	-0.89058
C	-2.75277	3.38923	0.18512
O	-0.00221	-0.44307	1.35594
C	0.43417	0.66431	1.76263
O	0.86424	1.59395	1.00686
C	0.50938	0.88967	3.26925
C	-4.72721	-1.04863	0.74131
H	-5.57832	-1.74081	0.77490
H	-4.54188	-0.68514	1.75785
H	-4.98291	-0.18245	0.12389
C	-3.91560	-1.30312	-2.36538
H	-4.56811	-2.07952	-2.78659
H	-4.50956	-0.43153	-2.08186
H	-3.22162	-0.97518	-3.14672
C	-2.44400	-2.54751	2.44684
H	-1.43338	-2.33807	2.81627
H	-3.13084	-1.85784	2.94756

Frequencies

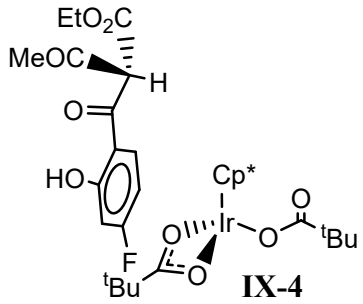
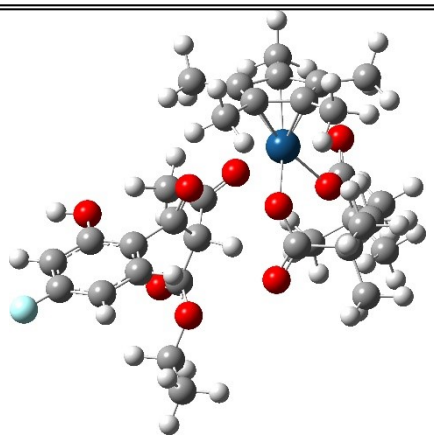
-509.3778	20.7033	24.1658
32.0854	46.4801	54.7152
56.3364	63.9797	64.6636
73.7149	83.3402	85.0926
86.8270	91.5360	94.5550
100.7655	108.4293	110.5169
116.2407	121.4446	129.1986
133.4183	137.7926	149.0218
151.2047	154.7882	161.0039
171.9598	175.4210	181.9480
192.2379	193.8463	195.9562
199.7688	215.2026	218.2580
222.3454	224.9932	229.6714
233.5144	239.3626	245.9548
248.9949	250.6312	261.6994
265.8157	275.6821	281.5106
283.5659	297.4302	300.1060
304.2013	307.0460	310.5137
325.2628	328.6894	335.8574
336.7631	337.2588	340.1715
344.5477	349.7788	364.7300
370.7439	374.5245	391.6646
395.7391	403.1944	407.3264
415.0305	426.2356	429.8511
433.4266	440.7029	449.3671
460.5808	462.2433	491.1324
517.6272	522.8433	535.6130
537.9202	545.4943	549.8122
565.8126	569.7893	579.7917
590.1694	601.1436	602.6176

H	-2.71129	-3.57066	2.74077	610.4002	632.2115	634.2493
C	-0.29492	-3.69084	0.43643	642.3986	699.1164	725.9184
H	0.04035	-3.37342	1.43067	750.1751	762.5606	789.7277
H	-0.48866	-4.77051	0.47416	793.9663	802.3427	804.6878
H	0.52389	-3.49160	-0.26141	805.8777	806.8638	812.5090
C	-1.27514	-2.99467	-2.56000	815.2718	822.5993	828.8737
H	-0.28214	-3.41544	-2.39503	858.0525	892.8769	902.6948
H	-1.89413	-3.73303	-3.08660	909.8201	921.4534	941.9620
H	-1.15920	-2.12457	-3.21377	948.1487	950.1163	953.2691
C	-0.90376	0.76159	3.84159	956.3646	961.2481	966.3252
H	-0.87442	0.89529	4.93049	967.8333	982.5998	1003.1028
H	-1.57392	1.51810	3.41742	1011.4574	1030.4456	1033.0947
H	-1.32913	-0.22357	3.62169	1036.7323	1037.5057	1041.1470
C	1.09193	2.25755	3.60265	1041.4686	1043.1965	1043.9632
H	1.15744	2.37408	4.69193	1045.3712	1051.2746	1053.3706
H	2.09511	2.37693	3.17970	1089.5712	1095.4417	1100.4541
H	0.46788	3.06735	3.20911	1107.0020	1110.0380	1141.5179
C	1.40730	-0.20629	3.85439	1153.5900	1166.8781	1171.6628
H	1.01021	-1.20510	3.63672	1185.3253	1188.4726	1213.5875
H	2.42566	-0.14316	3.44752	1223.9985	1235.6790	1240.4891
H	1.47090	-0.08961	4.94351	1247.9105	1251.6241	1258.6955
C	-4.04992	4.13352	-0.10448	1268.6348	1270.0160	1272.6384
H	-4.84748	3.81793	0.57979	1284.0448	1313.4027	1346.9063
H	-3.90178	5.21416	0.02219	1357.6332	1360.4925	1371.8151
H	-4.39294	3.94034	-1.12510	1372.8299	1373.5910	1376.5320
C	-1.66007	3.84662	-0.78908	1378.3041	1379.1968	1380.5525
H	-1.46992	4.92168	-0.67008	1383.2912	1387.9221	1391.8766
H	-0.72084	3.30878	-0.59445	1395.4766	1405.2684	1405.8558
H	-1.96480	3.66416	-1.82801	1408.4028	1411.3325	1422.0215
C	-2.29255	3.66461	1.61260	1423.5759	1426.9309	1429.2860
H	-2.19909	4.74705	1.77373	1437.8558	1441.9888	1442.2158
H	-3.00934	3.27562	2.34819	1448.7199	1450.2218	1450.9304
H	-1.31752	3.20144	1.79936	1456.4173	1457.0960	1461.3309
Ir	-1.63932	-0.78754	-0.13365	1461.3900	1464.2798	1467.9111
C	1.44446	0.80742	-1.40834	1468.8580	1470.5240	1472.4338
C	1.82300	-0.60520	-1.15954	1473.9691	1476.9811	1477.6656
O	1.07652	-1.54363	-1.40973	1480.1347	1480.9547	1486.0049
C	3.14331	-0.94321	-0.52254	1486.9113	1489.3204	1490.2943
C	4.35985	-0.81451	-1.19954	1498.0245	1500.1063	1509.4376
C	3.13628	-1.51340	0.74561	1515.2370	1527.7669	1534.2035
C	5.55004	-1.21586	-0.60111	1545.3642	1560.4788	1664.6892
C	4.31546	-1.90367	1.37522	1669.8320	1681.9353	1712.8704
H	2.17646	-1.63913	1.24667	1759.7629	1775.6132	1848.1588
C	5.50211	-1.74683	0.68093	3014.7167	3023.3991	3025.2642
H	6.50719	-1.13075	-1.11183	3032.1938	3035.9949	3036.6793
O	4.31564	-0.28842	-2.44832	3038.0474	3039.2509	3039.4326
H	5.20216	-0.24330	-2.82187	3043.5602	3046.6947	3046.8914
C	0.18880	1.00140	-2.13172	3049.7114	3059.2163	3097.3877
C	2.54072	1.79442	-1.64940	3101.7733	3104.0604	3108.6751
C	4.53397	2.64385	-0.72071	3111.0717	3112.1386	3115.5973
H	4.22525	3.68769	-0.85772	3119.0160	3122.3465	3123.6311
H	5.07963	2.35092	-1.62880	3125.6923	3126.8398	3130.2379
C	5.35159	2.43990	0.52830	3132.2036	3139.2212	3140.6749
H	6.28085	3.01666	0.48118	3141.0023	3144.2131	3146.1143
H	4.79218	2.75888	1.41351	3147.0662	3149.1690	3150.9934
H	5.60310	1.37918	0.64960	3156.6773	3158.8749	3161.3218
O	3.37411	1.82209	-0.59215	3163.4013	3173.5161	3183.2323
O	2.67666	2.53525	-2.59859	3188.6131	3218.6300	3898.1596
C	0.06966	1.93690	-3.29427			
H	-0.95638	1.89947	-3.66810			
H	0.32600	2.95790	-2.99380			

H	0.79054	1.67652	-4.07497
O	-0.86263	0.42170	-1.79836
H	4.32352	-2.33335	2.37242
F	6.64983	-2.12651	1.24923

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.737074 Electronic Energy = -2165.57547338
Internal Energy (E)= -2164.78915938 Enthalpy (H)= -2164.78821638
Gibbs Free Energy (G)=-2164.91751838 Gibbs Free Energy of Solvation=-2164.98251904

St.Pt.	General Structure	Ball & Stick model
IX-4	 **IX-4**	

Cartesian co-ordinate

Atoms	X	Y	Z
H	1.18592	1.04742	-0.27275
C	-2.06577	-2.14052	-1.74814
C	-1.63682	-2.79865	-0.55728
C	-2.58212	-2.45391	0.49646
C	-3.61248	-1.60742	-0.08430
C	-3.27570	-1.38354	-1.46374
C	-2.85658	2.02551	0.27416
O	-2.04341	1.14152	0.77416
O	-3.77705	1.79651	-0.50514
C	-2.49063	3.45745	0.68865
O	0.00671	-0.65858	1.12372
C	0.39866	0.32380	1.88778
O	0.81405	1.40860	1.48477
C	0.34002	0.02987	3.39405
C	-4.77202	-1.02598	0.64113
H	-5.65247	-1.67370	0.54208
H	-4.54719	-0.91304	1.70751
H	-4.99932	-0.03121	0.24623

Frequencies

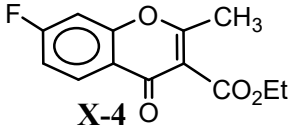
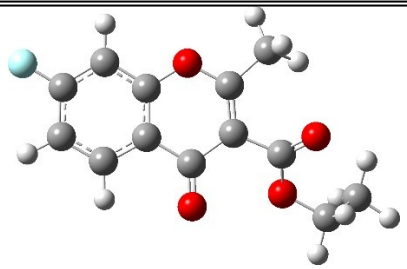
15.6994	37.7217	43.9019
49.3157	55.4174	62.4324
65.2949	70.9483	75.2105
81.2002	83.1615	87.9764
94.7244	102.9196	107.2143
111.4077	118.0936	121.0226
124.9561	129.7164	134.4514
146.5312	149.8886	158.9543
165.5984	167.7756	170.9433
181.9076	189.3280	192.1969
197.4299	202.3768	206.8733
210.0523	219.4873	220.4219
224.8416	228.3197	228.7347
234.8450	247.6583	253.8692
257.2596	260.4623	271.4559
283.2331	288.9801	295.9393
299.7098	304.3200	311.2052
312.8242	315.0010	322.1348
326.1193	330.8699	335.9364
342.0895	346.0967	348.6609
352.5028	353.5770	356.2883
372.4060	389.3861	390.3934
396.1816	409.1776	420.9372

C	-4.06272	-0.61285	-2.46155	425.8253	432.5710	441.6579
H	-4.81870	-1.25454	-2.93384	447.5992	451.3353	455.8292
H	-4.54816	0.24486	-1.99006	481.4650	486.1061	506.6326
H	-3.41299	-0.22122	-3.25124	526.2887	536.5383	537.8475
C	-2.55465	-3.00657	1.87610	542.7733	546.9386	557.5296
H	-1.54663	-2.95196	2.30273	577.1850	587.3296	591.3026
H	-3.23017	-2.46074	2.54167	596.3214	602.6615	608.8795
H	-2.86385	-4.06008	1.87055	618.8781	633.8565	642.4811
C	-0.42061	-3.63719	-0.37750	667.5326	687.5688	737.6948
H	-0.04178	-3.54189	0.64657	762.2407	793.0417	799.3478
H	-0.63811	-4.69735	-0.56054	803.2724	806.5635	809.4730
H	0.38306	-3.31829	-1.05026	811.8893	812.9446	814.2152
C	-1.42396	-2.19983	-3.08703	817.1911	832.3414	862.1381
H	-0.42333	-2.63175	-3.04041	863.7057	903.4181	908.7481
H	-2.04497	-2.80708	-3.75871	914.9308	947.0415	950.9971
H	-1.33871	-1.19990	-3.52692	953.3569	957.5187	961.2670
C	-1.13847	-0.00479	3.79433	964.9223	970.9872	978.1624
H	-1.22990	-0.18624	4.87388	998.0567	1004.6058	1015.1850
H	-1.63568	0.94349	3.55577	1023.3083	1034.9789	1037.5776
H	-1.67165	-0.80009	3.26086	1040.3258	1041.7195	1042.1325
C	1.05734	1.12364	4.17514	1043.7078	1047.7681	1049.8325
H	1.01611	0.90569	5.25079	1051.0687	1053.4506	1071.4552
H	2.10966	1.19545	3.87668	1096.1274	1099.4193	1108.1652
H	0.59916	2.10273	4.00100	1109.5528	1111.8511	1143.2089
C	0.98874	-1.32101	3.69474	1161.0673	1173.5296	1186.8005
H	0.50493	-2.13120	3.13694	1189.0651	1217.2440	1235.5701
H	2.05549	-1.31259	3.43123	1236.0399	1242.0252	1246.4252
H	0.91366	-1.54582	4.76690	1251.4446	1263.0819	1273.5526
C	-3.64998	4.39880	0.39286	1274.8009	1278.0240	1282.3701
H	-4.53219	4.13819	0.99062	1294.0250	1302.5997	1349.1206
H	-3.36748	5.43267	0.63206	1358.8105	1366.7830	1369.4614
H	-3.94025	4.34628	-0.66112	1372.1103	1373.7222	1375.9922
C	-1.26975	3.83346	-0.16256	1378.0405	1384.1822	1385.2310
H	-0.94771	4.85639	0.07455	1388.2791	1392.9764	1398.1406
H	-0.43793	3.14707	0.04537	1400.5070	1409.9805	1411.6640
H	-1.51243	3.79312	-1.23353	1413.9193	1417.5568	1429.9735
C	-2.10554	3.53376	2.16428	1431.9503	1433.2453	1437.2722
H	-1.89062	4.57597	2.43691	1441.3562	1446.0322	1448.4076
H	-2.92024	3.18063	2.81102	1449.9942	1453.4228	1454.4356
H	-1.21085	2.93437	2.36386	1457.1302	1459.2630	1463.4282
Ir	-1.69466	-0.66582	-0.17072	1464.1148	1466.1413	1468.0927
C	1.53439	0.93901	-1.33197	1471.0616	1471.8871	1473.5556
C	2.00195	-0.50900	-1.40527	1476.0275	1478.7693	1480.8659
O	1.33843	-1.32774	-2.01190	1482.2518	1485.5397	1490.6231
C	3.20381	-0.93590	-0.62791	1491.5287	1495.8049	1499.3422
C	4.49404	-0.67257	-1.09457	1500.0754	1500.7646	1512.1402
C	3.03181	-1.68865	0.52967	1518.0783	1538.3088	1543.9107
C	5.60391	-1.14123	-0.39995	1561.7418	1668.2839	1682.5511
C	4.12876	-2.15729	1.24601	1732.9404	1760.6029	1771.1438
H	2.01551	-1.87530	0.87843	1809.4444	1865.8329	2834.6181
C	5.39407	-1.87264	0.76147	3017.4296	3018.1303	3021.4151
H	6.61915	-0.95850	-0.74605	3029.9420	3031.8694	3033.5211
O	4.59501	0.04217	-2.24402	3035.7145	3037.4547	3037.8271
H	5.51953	0.14463	-2.49427	3040.6466	3045.7351	3046.6518
C	0.31695	1.07448	-2.21391	3050.7813	3054.3113	3095.7753
C	2.61130	1.99103	-1.48504	3098.9503	3102.5721	3104.8452
C	4.53518	2.83578	-0.43165	3111.2962	3113.4257	3116.5715
H	4.18477	3.87389	-0.47696	3117.8492	3122.3621	3123.4072
H	5.10567	2.64327	-1.35033	3124.5947	3127.1533	3130.1483
C	5.32964	2.54290	0.81336	3130.6127	3130.9307	3140.0883
H	6.22520	3.17091	0.85401	3140.7260	3140.9010	3142.6731

H	4.72848	2.73508	1.70722	3143.6449	3149.9025	3151.3971
H	5.63799	1.49063	0.83185	3154.3756	3155.3473	3183.2675
O	3.40098	1.96109	-0.41178	3184.6704	3186.4120	3193.6101
O	2.73933	2.76963	-2.40078	3201.0500	3218.3803	3899.8338
C	0.45943	1.47405	-3.64058			
H	-0.50869	1.40630	-4.14219			
H	0.87891	2.48130	-3.71473			
H	1.19038	0.80618	-4.11595			
O	-0.79011	0.78592	-1.77051			
H	4.01762	-2.73539	2.15839			
F	6.46279	-2.31752	1.42418			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.744073 Electronic Energy = -2165.58395376
Internal Energy (E)= -2164.79091176 Enthalpy (H)= -2164.78996776
Gibbs Free Energy (G)=-2164.91785576 Gibbs Free Energy of Solvation=-2164.98566426

St.Pt.	General Structure	Ball & Stick model
X-4	 **X-4**	

Cartesian co-ordinate

Atoms	X	Y	Z
C	1.83359	0.63393	0.05264
C	1.37278	-0.66697	-0.12302
C	-0.06344	-0.93769	-0.30979
C	-0.35592	1.50190	-0.07698
O	0.97379	1.69297	0.06327
C	2.30456	-1.71087	-0.13004
C	3.18342	0.92529	0.22226
C	3.65084	-1.45960	0.03898
C	4.06371	-0.13831	0.21103
H	1.92006	-2.71735	-0.27427
H	3.52791	1.94532	0.35600
O	-0.47398	-2.06336	-0.54223
C	-0.90961	0.26493	-0.22675
C	-1.06315	2.80957	-0.04016
H	-1.24711	3.16388	-1.06016

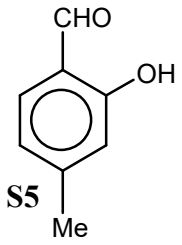
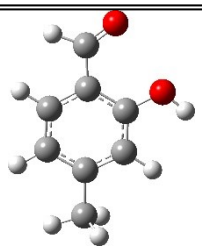
Frequencies

33.2908	48.2620	75.0606
101.8999	104.7664	124.9877
143.5874	189.7469	208.8927
236.5086	243.0440	276.6258
290.7717	303.6739	345.9667
366.3870	393.4940	403.1828
458.1939	463.3749	480.2305
515.3755	563.9079	577.8605
610.7013	628.4072	670.0885
697.9812	741.6942	768.5498
788.0329	804.8970	830.2451
836.7430	842.5184	894.5051
920.2644	965.7416	982.4978
1019.5617	1033.6636	1048.8835
1104.5951	1115.8657	1128.8690
1156.0498	1181.8470	1205.3313
1231.0668	1263.7919	1312.9431
1326.7614	1340.9967	1382.8385
1390.3655	1402.9993	1411.2570

H	-2.04027	2.72894	0.43727	1423.3614	1453.1396	1461.5522
H	-0.44071	3.54164	0.48008	1469.2682	1474.0848	1489.4741
C	-2.38615	0.17243	-0.37122	1490.3496	1547.6980	1636.7676
C	-4.28348	-1.15232	0.05769	1678.1503	1691.4428	1805.9621
H	-4.40190	-2.23792	0.11784	1830.4115	3048.4413	3064.9944
H	-4.61035	-0.81124	-0.93037	3072.1324	3129.8962	3140.6277
C	-5.03464	-0.44448	1.15860	3147.9346	3153.6570	3185.2413
H	-6.10084	-0.68886	1.10885	3205.1694	3223.3752	3231.5705
H	-4.65876	-0.74981	2.14051			
H	-4.92753	0.63984	1.05986			
O	-3.07430	1.02024	-0.90249			
O	-2.86936	-0.93962	0.18256			
H	4.39456	-2.25021	0.03954			
F	5.36230	0.10746	0.37073			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.218805 Electronic Energy = -902.243247336
Internal Energy (E)= -902.008625336 Enthalpy (H)= -902.007681336
Gibbs Free Energy (G)=-902.068220336 Gibbs Free Energy of Solvation=-902.086616732

St.Pt.	General Structure	Ball & Stick model
S5		

Cartesian co-ordinate

Atoms	X	Y	Z
C	0.37955	0.81808	-0.00002
O	1.24757	1.84470	-0.00001
C	-0.99761	1.02822	-0.00003
C	-1.89879	-0.03558	-0.00002
C	0.88187	-0.50015	-0.00002
C	-1.40287	-1.34074	-0.00001
C	-0.03483	-1.55400	-0.00002
H	0.35840	-2.57070	-0.00004
H	-2.09466	-2.18010	-0.00001
C	2.31249	-0.83884	-0.00002
H	2.47933	-1.94687	-0.00013
O	3.24760	-0.07292	0.00009
H	-1.37779	2.05206	-0.00005
H	0.75340	2.67295	-0.00012

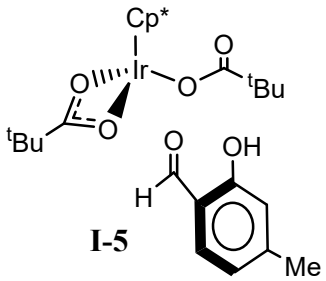
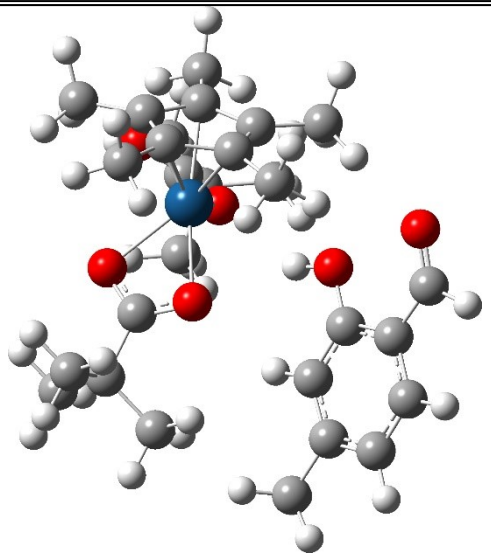
Frequencies

78.0089	109.1196	180.4274
208.1321	212.4068	302.4214
312.0853	388.5012	433.1349
457.5986	459.2802	552.2239
608.0983	632.4084	722.6339
753.8426	801.5857	809.5901
840.9984	950.2622	976.7368
1025.2979	1025.4938	1049.5891
1137.0226	1186.9915	1202.7707
1236.0378	1315.4716	1341.7424
1386.2596	1404.5550	1421.3819
1461.1408	1463.7987	1492.5942
1557.2434	1645.2235	1682.8128
1852.1558	2827.7520	3035.9226
3111.1864	3138.2979	3140.6324
3165.4874	3189.0755	3872.6950

C	-3.37195	0.23357	0.00005
H	-3.66870	0.81476	0.88134
H	-3.66865	0.81557	-0.88072
H	-3.94976	-0.69537	-0.00037

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.141607 Electronic Energy = -459.814783859
Internal Energy (E)= -459.664015859 Enthalpy (H)= -459.663071859
Gibbs Free Energy (G)=-459.707304859 Gibbs Free Energy of Solvation=-459.727870422

St.Pt.	General Structure	Ball & Stick model
I-5		

I-5

Cartesian co-ordinate

Atoms	X	Y	Z
C	2.97345	-0.23554	-1.10513
C	3.42503	-0.40798	0.24511
C	2.87558	-1.66009	0.75199
C	2.07389	-2.23607	-0.29616
C	2.10642	-1.34605	-1.44172
C	-2.54475	-0.75050	-1.34123
C	-1.61769	0.36218	3.00396
C	-0.48467	-0.01544	2.07816
O	0.65450	0.53152	2.19130
O	-0.66194	-0.81707	1.10769
C	3.11481	-2.21745	2.11143
H	3.02311	-1.43627	2.87409
H	2.38504	-2.99671	2.35162

Frequencies

34.4716	47.8959	50.3713
53.5523	65.0770	71.6910
72.2529	82.6975	89.5112
92.1569	96.9801	109.5326
120.5929	130.7291	131.7141
136.9930	141.9230	145.8340
156.6505	164.6272	181.6457
183.5859	187.7114	193.5541
196.0151	199.6523	206.5163
209.7342	216.2940	219.9944
225.3684	232.8149	238.4150
244.6519	250.9894	252.2354
257.7453	272.5943	279.8996
288.7364	293.5710	307.8774
315.4581	319.6490	322.0147
324.2404	328.1618	334.1201
338.0749	345.3090	373.8500

H	4.11712	-2.65728	2.19006	388.5172	391.0032	398.0697
C	1.25540	-3.47322	-0.21888	399.0469	418.2927	439.0184
H	0.29446	-3.33340	-0.72900	451.3779	458.0236	469.0425
H	1.77504	-4.30828	-0.70557	472.5459	476.3862	486.6073
H	1.05238	-3.75174	0.81983	535.0502	538.4470	544.5682
C	1.44764	-1.57383	-2.75622	549.5203	558.2021	567.4412
H	0.52753	-2.15971	-2.65708	582.4698	591.0779	602.2640
H	1.16582	-0.62004	-3.21746	610.5702	624.2264	628.3705
H	2.13092	-2.09272	-3.44156	628.9334	742.9187	754.6197
C	3.32605	0.89298	-2.00697	788.2228	800.2459	800.7546
H	2.51884	1.09434	-2.72023	803.6758	812.8338	816.0809
H	3.50908	1.81234	-1.44449	820.4405	834.4971	886.4541
H	4.22335	0.64119	-2.58708	907.8204	925.6236	936.7967
C	4.25529	0.56643	1.00330	944.6507	947.0882	949.2650
H	4.25947	0.33493	2.07275	950.8815	952.0414	956.6495
H	5.29347	0.56002	0.64792	958.0036	969.9527	977.9463
H	3.84256	1.57456	0.88007	979.7223	1027.7153	1031.0674
C	0.69615	2.46083	-0.55771	1035.6581	1039.0739	1040.0516
O	0.11292	1.28909	-0.52198	1042.5047	1043.5464	1048.4875
O	1.75909	2.71867	-0.00826	1049.4771	1050.2942	1050.6378
C	-0.07280	3.52868	-1.34995	1053.4944	1090.1665	1093.7999
O	-1.30088	-0.62601	-1.79680	1107.5602	1143.1088	1184.8825
C	-0.63251	2.94961	-2.64905	1187.5535	1216.4529	1232.8950
H	-1.39156	2.17954	-2.47228	1234.7488	1236.1462	1243.5298
H	-1.10039	3.74728	-3.24070	1257.6580	1261.9282	1263.6217
H	0.16151	2.50346	-3.26347	1270.7598	1346.8495	1362.9999
C	0.87341	4.68042	-1.67095	1376.3486	1377.6633	1378.8409
H	0.33957	5.46628	-2.22089	1382.9671	1383.8372	1386.4168
H	1.29366	5.10951	-0.75656	1388.5619	1394.3789	1397.1430
H	1.71297	4.33716	-2.28884	1404.1930	1407.7450	1409.1879
C	-1.21833	4.03754	-0.47191	1417.7353	1419.6150	1426.8462
H	-0.83840	4.43717	0.47688	1432.3348	1438.7157	1439.1236
H	-1.76186	4.83991	-0.98801	1444.2060	1445.1683	1449.8239
H	-1.93239	3.23710	-0.24108	1451.8496	1452.7955	1453.6636
C	-2.75771	-0.64576	2.90647	1456.0938	1457.7273	1458.9367
H	-2.44243	-1.63624	3.25595	1460.6777	1461.4982	1469.3140
H	-3.59611	-0.31613	3.53452	1471.1024	1473.9432	1474.3903
H	-3.11165	-0.75408	1.87450	1476.3166	1476.8706	1483.4743
C	-2.08351	1.74281	2.52202	1486.8214	1491.9870	1495.2364
H	-2.90793	2.10170	3.15200	1499.1016	1502.0280	1508.2961
H	-1.26103	2.46657	2.56728	1514.8546	1525.9678	1527.2691
H	-2.43495	1.68873	1.48297	1555.1272	1558.5005	1600.7677
C	-1.10593	0.46267	4.43914	1644.3809	1683.1166	1774.0333
H	-0.28728	1.18471	4.51878	1823.3232	2834.0792	3024.6020
H	-1.92051	0.78447	5.10034	3025.3971	3027.0795	3030.3390
H	-0.74249	-0.50713	4.80128	3033.1237	3033.6591	3034.7498
Ir	1.28600	-0.31631	0.24999	3036.2517	3036.9316	3037.4580
C	-3.22658	0.34249	-0.79156	3038.8607	3041.3989	3103.4349
C	-4.53543	0.23674	-0.34046	3107.0618	3112.5046	3114.1191
C	-5.19840	-0.99546	-0.45104	3115.1432	3116.7026	3116.7579
C	-3.20413	-1.99554	-1.43220	3116.9977	3117.2364	3119.9670
C	-4.53251	-2.07939	-0.98638	3123.2110	3124.1125	3125.5315
H	-5.03657	-3.04320	-1.06593	3131.2950	3135.1695	3136.6724
H	-0.89894	0.20636	-1.45880	3137.4999	3141.9016	3144.5842
H	-2.69486	1.29156	-0.71616	3146.4622	3146.5593	3147.3447
C	-2.58489	-3.22498	-1.91974	3158.2960	3158.4145	3171.2864
H	-3.30731	-4.08050	-1.93026	3180.0905	3185.7456	3513.2608
O	-1.43608	-3.40664	-2.27587			
H	-6.22688	-1.08812	-0.10734			
C	-5.21874	1.40806	0.29447			
H	-5.22314	1.30109	1.38813			

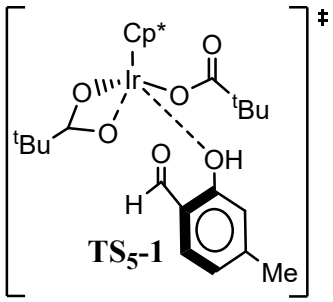
H	-4.71495	2.35172	0.05807	
H	-6.26410	1.48463	-0.02507	

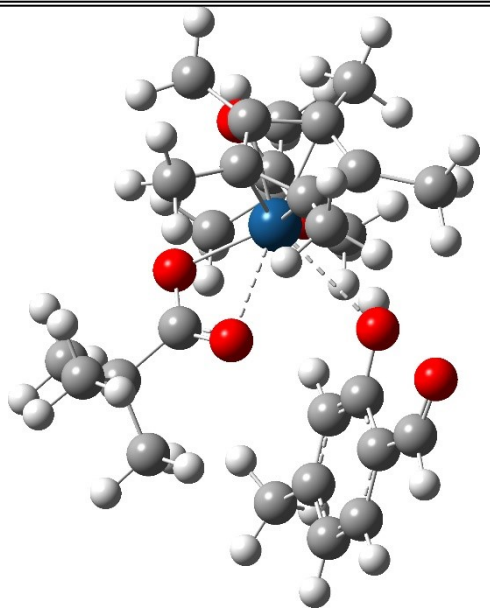
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.641441 Electronic Energy = -1646.80452365
Internal Energy (E)= -1646.12291665 Enthalpy (H)= -1646.12197265
Gibbs Free Energy (G)=-1646.23115065 Gibbs Free Energy of Solvation=-1646.28482665

St.Pt.	General Structure	Ball & Stick model

TS_5-1





Cartesian co-ordinate

Atoms	X	Y	Z
C	2.97709	-0.80627	-0.87304
C	3.11470	-0.66321	0.56364
C	2.31072	-1.70550	1.19374
C	1.67326	-2.45600	0.15790
C	2.06975	-1.89750	-1.12728
C	-2.24327	-0.89209	-1.39129
C	-1.76337	0.61034	2.94017
C	-0.80801	0.17633	1.83344
O	0.26142	0.84317	1.65056
O	-1.04620	-0.86703	1.18456
C	2.15151	-1.89001	2.66154
H	2.02747	-0.92239	3.16092
H	1.26915	-2.49576	2.88878
H	3.02841	-2.38716	3.09483
C	0.71389	-3.57317	0.33987
H	-0.09006	-3.52754	-0.40181
H	1.22861	-4.53634	0.22740
H	0.25267	-3.53931	1.33069
C	1.68270	-2.44378	-2.45657
H	0.67250	-2.86485	-2.43675
H	1.70376	-1.66525	-3.22731
H	2.38256	-3.23217	-2.76316
C	3.64971	0.03998	-1.89248
H	3.05884	0.08375	-2.81331
H	3.76079	1.06217	-1.51994
H	4.63721	-0.36973	-2.14072
C	3.96163	0.33454	1.26303
H	3.67547	0.42330	2.31558
H	5.01764	0.03713	1.21833
H	3.84001	1.31713	0.79615
C	1.25379	2.49228	-0.79862
O	0.59281	1.39108	-1.02256
O	2.38586	2.56412	-0.33638
C	0.42937	3.74962	-1.10968

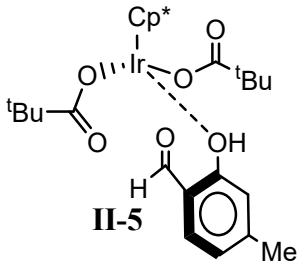
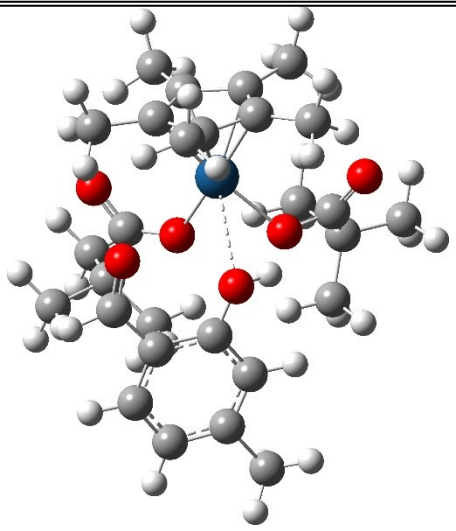
Frequencies

-80.9690	-14.0710	32.2481
38.6195	49.2165	57.7824
63.7244	70.4294	78.9112
84.8148	91.0780	96.0949
104.8893	106.3413	111.8745
119.8041	123.1831	128.9854
144.5797	154.2655	161.0617
166.8409	183.3179	185.3789
188.0043	190.7686	194.3122
197.0360	204.3298	209.0036
213.9380	222.2696	229.7927
234.5305	243.8838	256.7408
266.2263	271.0487	277.5104
293.1219	294.1990	308.4584
311.7757	320.0159	321.4177
323.5769	329.0406	338.0596
347.6983	365.9768	368.6557
380.4708	391.5941	393.0943
394.1134	410.5609	429.1350
437.7443	446.6298	455.2301
460.0454	469.4420	471.5682
533.5895	538.6861	544.7171
547.0519	554.9921	567.5556
583.4600	592.2075	603.2422
608.3597	612.1170	619.9127
627.0164	630.2603	740.0123
753.4374	785.3684	790.4420
807.9521	809.9347	810.6917
810.8527	815.8530	825.5430
903.2472	911.8827	925.4977
946.2842	946.8719	949.1650
950.9543	953.2167	955.7881
959.0705	972.7126	975.2171
976.7985	1020.3015	1024.5110
1032.3919	1035.6338	1036.6401
1038.2772	1039.7371	1041.1105
1044.1025	1044.5199	1047.1767
1047.9769	1096.3912	1099.4277

O	-0.95688	-1.20968	-1.65885	1111.6665	1142.7601	1186.0307
C	-0.26477	3.63662	-2.46602	1190.1214	1203.4771	1212.6022
H	-0.94943	2.78261	-2.50668	1235.8378	1237.0103	1241.2940
H	-0.84379	4.54848	-2.66547	1246.5464	1259.2187	1263.5509
H	0.46493	3.52187	-3.27782	1267.8881	1321.7877	1335.2108
C	1.32317	4.98235	-1.09142	1361.6369	1371.2602	1375.1466
H	0.72355	5.88515	-1.26782	1376.8314	1377.5909	1378.2174
H	1.83568	5.08188	-0.12977	1389.3164	1394.4616	1396.0219
H	2.09258	4.92355	-1.87041	1401.1196	1402.6020	1406.5233
C	-0.61626	3.84926	0.00755	1407.8722	1412.9782	1415.2688
H	-0.13099	3.98335	0.98309	1425.4275	1435.8992	1440.0343
H	-1.28600	4.70229	-0.16862	1443.1182	1444.5050	1446.4186
H	-1.21426	2.93005	0.06744	1447.3433	1453.5037	1455.9666
C	-3.19726	0.27276	2.54352	1456.4074	1460.6673	1462.8957
H	-3.30256	-0.78564	2.28363	1463.3525	1466.4714	1471.2112
H	-3.88232	0.50996	3.36787	1473.3876	1474.9155	1476.2194
H	-3.50686	0.85275	1.66429	1478.7456	1481.5457	1483.0422
C	-1.63329	2.09969	3.23643	1483.8223	1487.2898	1489.1414
H	-2.29637	2.37403	4.06733	1494.7818	1500.1330	1503.7309
H	-0.60580	2.36634	3.50513	1512.0065	1512.6527	1524.0255
H	-1.91563	2.70244	2.36400	1535.8867	1554.1953	1642.3656
C	-1.36117	-0.20002	4.17863	1668.5061	1682.1340	1771.7043
H	-0.32404	0.01695	4.46659	1827.7438	2838.0804	3019.4283
H	-2.01042	0.05787	5.02524	3022.8928	3027.5634	3030.5825
H	-1.45291	-1.27642	3.98884	3032.7868	3034.0275	3034.8771
Ir	1.08492	-0.37103	0.03344	3037.2167	3040.0598	3040.4532
C	-2.63033	0.44072	-1.26616	3042.8293	3043.8361	3105.0765
C	-3.94929	0.78704	-0.99269	3106.2901	3110.5435	3110.6568
C	-4.89821	-0.23083	-0.82551	3116.1382	3116.7584	3116.9221
C	-3.19101	-1.91916	-1.23790	3118.9534	3121.9340	3122.9073
C	-4.51242	-1.55259	-0.94496	3124.1029	3124.8384	3125.3158
H	-5.24934	-2.34751	-0.82741	3133.5351	3136.6157	3138.4306
H	-0.49732	-0.39328	-1.92184	3142.6539	3142.8554	3143.4721
H	-1.86028	1.21026	-1.35215	3143.6198	3152.7785	3160.3539
C	-2.90349	-3.34188	-1.41277	3160.7407	3166.3470	3167.4824
H	-3.81222	-3.97791	-1.26343	3170.2962	3185.1597	3728.2524
O	-1.84289	-3.85997	-1.70216			
H	-5.93286	0.02626	-0.60704			
C	-4.32730	2.22790	-0.83431			
H	-4.19758	2.55287	0.20813			
H	-3.69812	2.87862	-1.45203			
H	-5.37543	2.40168	-1.09966			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.639466 Electronic Energy = -1646.77865241
Internal Energy (E)= -1646.09980941 Enthalpy (H)= -1646.09886641
Gibbs Free Energy (G)=-1646.20677641 Gibbs Free Energy of Solvation=-1646.26706609

St.Pt.	General Structure	Ball & Stick model
II-5		

II-5

Cartesian co-ordinate

Atoms	X	Y	Z
C	3.02416	-0.12373	-1.26258
C	3.27011	0.09913	0.13266
C	2.84840	-1.09323	0.86757
C	2.33169	-2.04027	-0.07649
C	2.41632	-1.42173	-1.38650
Ir	1.16330	-0.19962	-0.11399
O	-0.56000	-0.35414	0.95090
O	0.17232	1.62405	-0.49937
O	-0.72886	-2.86742	-1.63729
C	-1.92773	-2.74339	-1.48575
H	-2.55769	-3.63574	-1.24208
C	-2.71343	-1.51298	-1.55576
C	-2.17291	-0.23508	-1.80600

Frequencies

25.7223	27.6998	43.3988
44.5469	58.4467	66.6848
68.4827	74.3853	78.8288
84.2209	88.8138	95.1447
100.9575	116.0874	120.8426
124.9560	133.3688	142.6187
149.5735	160.0029	164.9413
172.9008	178.2813	183.6323
186.4075	189.3159	198.4384
201.5190	207.3989	214.1769
220.3437	233.5641	235.7368
240.0978	243.6158	245.5386
258.7648	276.4809	280.8657
282.0983	292.3025	299.8368
304.1071	308.7961	312.9826
323.4926	325.8188	326.9843
327.0138	335.7810	347.9362
379.4425	385.3419	386.8147

C	-4.08569	-1.61094	-1.28162
C	-3.00046	0.88636	-1.72914
C	-4.90326	-0.49882	-1.22778
H	-4.49917	-2.60163	-1.08852
C	-4.35687	0.77385	-1.44133
H	-2.55915	1.86980	-1.89388
O	-0.87616	-0.10460	-2.13142
H	-0.57790	0.79873	-1.88771
C	-0.79575	-1.22633	1.89538
C	-2.16249	-1.06424	2.57853
C	0.72977	2.79835	-0.30900
C	-0.08832	3.68844	0.63210
O	1.80913	3.15207	-0.76125
O	-0.02854	-2.10718	2.26105
C	1.98845	-2.02522	-2.67570
H	1.47525	-2.97594	-2.52595
H	1.29294	-1.36612	-3.20717
H	2.86927	-2.18225	-3.31193
C	3.31684	0.81651	-2.37757
H	3.08693	1.84459	-2.08042
H	4.37219	0.74986	-2.67269
H	2.70818	0.57643	-3.25574
C	3.90368	1.30587	0.72083
H	3.62477	1.43039	1.77245
H	4.99685	1.21162	0.67418
H	3.60550	2.20878	0.17743
C	2.98117	-1.28537	2.33341
H	2.19298	-1.94287	2.70746
H	3.96334	-1.71497	2.57109
H	2.89430	-0.32910	2.86079
C	1.86506	-3.42308	0.20411
H	2.69736	-4.13000	0.08719
H	1.46057	-3.49715	1.21598
H	1.06374	-3.70682	-0.48456
C	-2.96243	0.11697	2.04298
H	-3.14980	0.02186	0.96758
H	-3.93101	0.16985	2.55920
H	-2.43747	1.06681	2.20664
C	-1.89736	-0.87502	4.07396
H	-2.84786	-0.80093	4.61850
H	-1.32465	-1.71612	4.47757
H	-1.33117	0.04764	4.26000
C	-2.94362	-2.36225	2.36251
H	-2.36531	-3.22600	2.70716
H	-3.89088	-2.32863	2.91690
H	-3.18405	-2.50412	1.29968
C	0.42843	5.11948	0.59868
H	0.32296	5.55633	-0.40159
H	-0.13593	5.74054	1.30645
H	1.48954	5.16207	0.86455
C	-1.57280	3.64385	0.27615
H	-1.94720	2.61380	0.30511
H	-2.14783	4.24840	0.99025
H	-1.75350	4.05536	-0.72750
C	0.11073	3.08640	2.03059
H	1.17611	3.07491	2.30171
H	-0.42238	3.68664	2.77985
H	-0.26748	2.05647	2.06690
H	-5.96305	-0.60030	-1.00295
C	-5.21909	1.99645	-1.38103
H	-4.63610	2.88622	-1.11965

397.7309	404.6079	418.0790
437.8120	444.9023	453.5044
463.0496	471.0815	476.0604
534.2855	539.3267	544.6888
553.0342	568.6144	570.6153
575.4890	579.8339	601.9764
602.5742	605.0728	631.1111
641.7203	734.6587	746.3126
772.6213	796.6633	801.3321
807.1851	810.3922	812.6762
813.4147	816.6150	821.7817
870.1006	908.3608	916.7668
937.9531	944.8018	950.8644
953.3196	958.2689	959.2674
960.4295	975.7496	976.1454
978.3439	1028.5433	1028.9119
1030.8266	1035.3572	1036.1262
1039.1391	1042.5295	1043.2693
1044.9823	1047.3683	1048.0387
1051.2762	1095.9076	1101.4868
1113.6152	1143.9398	1187.3998
1191.3255	1206.5604	1225.6304
1229.4806	1236.4899	1238.8781
1242.5172	1247.2919	1267.9181
1271.6786	1326.3413	1348.0343
1358.2453	1360.5106	1368.8329
1372.6620	1374.3850	1378.8859
1381.2192	1390.3347	1393.8046
1394.9468	1401.6634	1403.2310
1408.4766	1413.8159	1414.7875
1418.4808	1422.8746	1430.3671
1437.3482	1439.8805	1441.5830
1447.9362	1452.5549	1453.4679
1454.7296	1455.2918	1457.7417
1461.9428	1462.8695	1464.1191
1464.8691	1468.3321	1473.0383
1475.1762	1478.1807	1478.7010
1479.3435	1485.4732	1490.3136
1493.0996	1495.5917	1496.3699
1503.4744	1505.2819	1511.4038
1534.0292	1552.8233	1638.1669
1682.3815	1772.3864	1777.2440
1830.4913	2851.1912	3013.8115
3018.1083	3026.3277	3027.6517
3032.9313	3034.0697	3035.0128
3037.0608	3038.2131	3040.6457
3044.2151	3045.8113	3096.6472
3101.1675	3104.1011	3106.9869
3112.5864	3114.9900	3117.6072
3118.5990	3119.7228	3120.3660
3123.3279	3129.2816	3137.9651
3138.6656	3139.0799	3140.0413
3143.4314	3153.1374	3159.7116
3161.1890	3161.5086	3168.1526
3171.7610	3178.3982	3183.2707
3189.8071	3199.3028	3564.9018

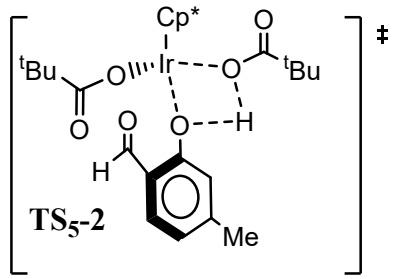
H	-5.69491	2.18838	-2.35132	
H	-6.02084	1.88193	-0.64389	

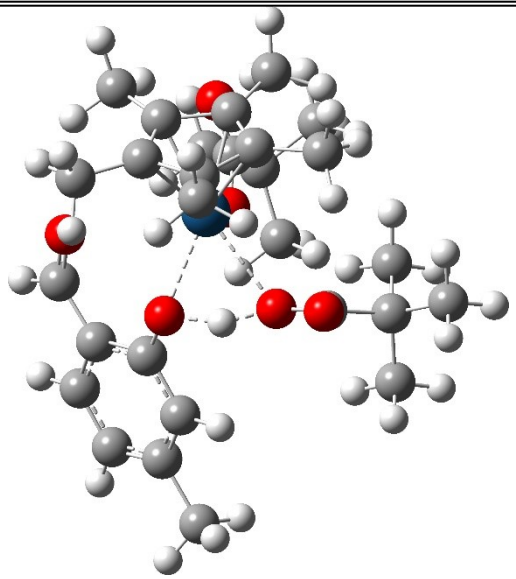
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.639640 Electronic Energy = -1646.78703081
Internal Energy (E)= -1646.10636681 Enthalpy (H)= -1646.10542281
Gibbs Free Energy (G)=-1646.21802981 Gibbs Free Energy of Solvation=-1646.27711615

St.Pt.	General Structure	Ball & Stick model

TS_5-2





Cartesian co-ordinate

Atoms	X	Y	Z
C	2.85860	-0.23120	-1.31877
C	3.06680	0.18308	0.04325
C	2.74173	-0.92041	0.92444
C	2.32791	-2.03217	0.08971
C	2.41745	-1.59482	-1.29448
Ir	0.99682	-0.39709	-0.18663
O	-0.69013	-0.49935	0.92424
O	-0.09578	1.79336	-0.39802
O	-0.48879	-2.81249	-1.34765
C	-1.69928	-2.67306	-1.33605
H	-2.35631	-3.56083	-1.16114
C	-2.45428	-1.44480	-1.52115
C	-1.88073	-0.16458	-1.71515
C	-3.85375	-1.55598	-1.45599
C	-2.74273	0.93928	-1.81233
C	-4.68457	-0.46112	-1.56362
H	-4.27897	-2.54876	-1.30234
C	-4.12357	0.81230	-1.74254
H	-2.30128	1.92637	-1.94687
O	-0.56418	0.04140	-1.82815
H	-0.32794	1.13034	-1.35352
C	-0.88466	-1.19109	2.01307
C	-2.27246	-0.98266	2.63525
C	0.58320	2.92491	-0.40597
C	0.25043	3.79722	0.80358
O	1.36016	3.25816	-1.28645
O	-0.08295	-1.96551	2.52126
C	2.11934	-2.39657	-2.50911
H	1.69130	-3.36828	-2.26136
H	1.40114	-1.87495	-3.15045
H	3.04637	-2.54459	-3.07806
C	3.02880	0.62411	-2.52512
H	2.60874	1.62359	-2.35548
H	4.09019	0.72994	-2.78464
H	2.51176	0.18755	-3.38544

Frequencies

-142.1958	37.8189	46.3991
50.4546	57.9453	70.4527
75.6746	82.3548	84.1101
91.5760	98.4781	104.0450
108.1659	114.4799	119.2467
123.4557	126.8623	134.3734
153.7486	164.1493	168.1513
176.9821	180.9795	186.8395
195.1866	200.1423	208.3257
210.6976	220.6929	226.8375
233.6371	237.2728	244.1761
248.9016	256.5826	265.6483
276.0043	289.5983	291.7678
297.9070	303.2198	309.2769
316.4148	319.5439	320.1341
323.3593	339.9204	342.3365
347.4554	352.6933	357.6478
375.6950	387.2572	388.8460
399.4533	401.9633	438.3464
442.0614	452.7704	454.5986
467.9826	478.0471	510.0434
532.3934	540.1803	549.6792
550.1749	575.7735	577.6793
584.0934	595.3604	599.3779
603.1190	626.0748	646.3540
656.7380	743.4858	755.8644
780.1463	789.3235	802.2513
809.8370	810.7850	812.4378
815.1603	819.4216	823.3002
907.6872	922.0857	926.8435
946.1463	948.6408	951.2884
952.5766	957.7025	957.8899
960.9860	966.5165	979.6217
980.7212	1014.3236	1028.5574
1028.9918	1040.4202	1041.5806
1042.9662	1043.9554	1044.6254
1045.5554	1046.6818	1047.3916
1050.8744	1100.4383	1100.7185
1112.8611	1149.9769	1188.1317

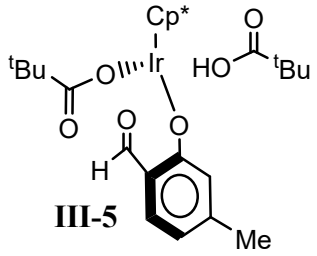
C	3.57948	1.51638	0.44459	1192.2176	1215.5806	1231.9727
H	3.32336	1.76036	1.48061	1235.7320	1238.3241	1243.9625
H	4.67509	1.51698	0.36636	1246.3725	1267.0586	1269.2395
H	3.19667	2.30631	-0.21155	1270.0452	1332.0846	1355.8436
C	2.89562	-0.94268	2.40267	1364.8009	1371.7875	1375.0944
H	2.07755	-1.50724	2.85961	1377.3769	1380.7745	1385.1261
H	3.85395	-1.40072	2.68083	1391.0699	1392.3632	1393.6499
H	2.87461	0.07093	2.81750	1395.8964	1399.2522	1409.4917
C	1.96259	-3.39221	0.55928	1412.5920	1415.1439	1417.3899
H	2.85496	-4.03161	0.59288	1428.7326	1433.3208	1441.1398
H	1.51240	-3.33771	1.55431	1443.6941	1445.7520	1448.0317
H	1.22330	-3.84202	-0.11031	1451.7246	1454.8819	1459.7346
C	-3.03438	0.17361	1.99698	1460.9827	1462.5463	1463.6892
H	-3.19640	0.01139	0.92555	1464.2685	1465.5882	1470.3782
H	-4.01261	0.28378	2.48491	1473.5043	1476.3923	1478.7496
H	-2.49081	1.12099	2.10849	1479.3562	1481.0061	1484.3974
C	-2.08628	-0.72535	4.13032	1485.1546	1490.7404	1498.0391
H	-3.06418	-0.63075	4.62036	1501.5232	1502.4040	1504.4198
H	-1.53325	-1.54357	4.60197	1507.0229	1508.8395	1514.8574
H	-1.53239	0.20692	4.30407	1525.0692	1549.5234	1618.2782
C	-3.04726	-2.28862	2.43549	1648.4232	1682.1419	1769.1250
H	-2.50251	-3.13347	2.87124	1809.4134	1810.7184	2847.0987
H	-4.03211	-2.21985	2.91620	3021.6463	3023.8805	3025.7225
H	-3.20953	-2.49105	1.36749	3027.8349	3033.3743	3033.7457
C	1.19681	4.98656	0.87522	3034.4405	3034.9000	3036.4433
H	1.16081	5.57764	-0.04577	3036.6006	3042.2961	3047.4446
H	0.92531	5.63269	1.71972	3100.6802	3102.0159	3106.7016
H	2.23502	4.66137	1.01694	3106.9314	3110.4797	3114.2962
C	-1.19143	4.28305	0.60200	3116.0485	3117.6878	3118.8998
H	-1.88680	3.43642	0.54935	3119.8868	3126.0673	3128.2299
H	-1.48987	4.92769	1.43867	3131.6231	3133.4027	3137.7197
H	-1.28361	4.86714	-0.32323	3138.4589	3143.7407	3144.9268
C	0.32882	2.96882	2.08801	3145.6578	3149.0812	3150.0413
H	1.36102	2.65395	2.29656	3153.9331	3173.4405	3179.7328
H	-0.00630	3.57274	2.94143	3184.8168	3189.8321	3193.2037
H	-0.29437	2.06887	2.02136			
H	-5.76521	-0.57386	-1.50206			
C	-5.00266	2.01822	-1.86874			
H	-4.45565	2.93956	-1.64285			
H	-5.39907	2.11034	-2.88808			
H	-5.86354	1.95518	-1.19398			

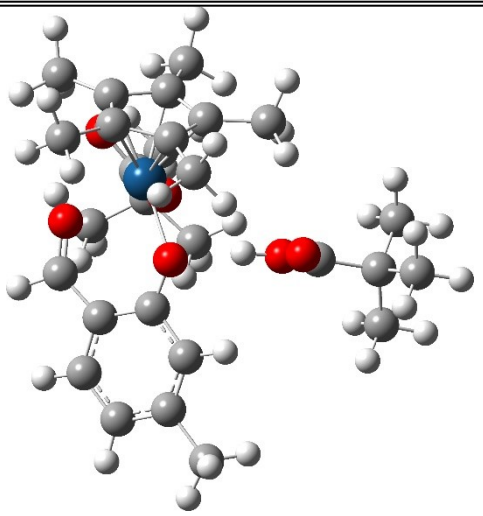
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.637230 Electronic Energy = -1646.77488159
Internal Energy (E)= -1646.09822759 Enthalpy (H)= -1646.09728359
Gibbs Free Energy (G)=-1646.20470659 Gibbs Free Energy of Solvation=-1646.25958208

St.Pt.	General Structure	Ball & Stick model

III-5





Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.72844	-1.98476	-1.49500
C	-1.39481	-2.27500	-0.11023
C	-2.41961	-1.67568	0.72246
C	-3.32477	-0.95822	-0.12489
C	-2.90599	-1.16740	-1.51059
Ir	-1.35281	-0.16075	-0.39182
O	-0.23174	0.69327	1.13804
O	2.16756	-0.92916	0.37138
O	-1.93680	1.89537	-0.75988
C	-1.13460	2.81748	-0.99841
H	-1.57325	3.83171	-1.04454
C	0.26357	2.75355	-1.24784
C	0.97989	1.53237	-1.44504
C	0.94875	3.98702	-1.36998
C	2.35185	1.63238	-1.78038
C	2.28824	4.04574	-1.64690
H	0.37911	4.90483	-1.22164
C	3.00521	2.84484	-1.86223
H	2.88502	0.70055	-1.96440
O	0.46103	0.34170	-1.37016
H	1.46045	-0.54759	-0.20647
C	-0.78834	1.18739	2.20421
C	0.26259	1.64550	3.22662
C	2.80329	-1.88992	-0.29207
C	3.97958	-2.44908	0.49594
O	2.45912	-2.28974	-1.38829
O	-1.99388	1.25646	2.42358
C	-3.59176	-0.60139	-2.70377
H	-3.87394	0.44296	-2.53097
H	-2.94180	-0.62611	-3.58364
H	-4.50383	-1.16413	-2.93981
C	-0.88474	-2.37753	-2.65535
H	0.17968	-2.24416	-2.42097
H	-1.05163	-3.43036	-2.91540
H	-1.11052	-1.76684	-3.53468
C	-0.28967	-3.14156	0.38433
H	0.21725	-2.67090	1.23716

Frequencies

36.1169	43.2191	46.1128
51.4388	68.2163	73.2173
75.4796	79.5306	85.4995
86.3715	100.1903	106.5387
112.4674	119.5285	125.3751
132.6152	138.3241	148.2696
155.4550	164.5536	178.7159
184.3556	187.6180	191.4455
197.1870	206.1574	211.7682
217.2044	231.0381	239.2485
244.8496	251.7548	255.0935
261.7534	270.6521	278.1778
284.6030	293.4642	298.8263
315.9582	321.2592	326.2547
328.6031	336.5394	339.2637
342.5064	355.6666	355.8256
361.9874	372.3038	374.1662
385.6157	387.6503	389.8750
397.8884	416.6114	422.1858
442.5837	446.5347	458.2994
466.7173	470.9541	534.3594
538.1034	544.1720	548.0730
564.8019	574.4927	583.5599
586.6265	593.9969	599.4965
606.3975	611.5773	642.5914
648.0700	752.6846	757.9219
761.3644	781.0993	787.3128
792.6142	808.8861	813.7232
816.9609	834.4674	888.3787
893.8844	917.2967	921.1454
938.9907	943.6142	945.0480
957.0092	958.2675	960.8586
965.0145	966.6115	983.0680
986.1668	1000.2553	1038.2291
1038.6464	1043.2466	1043.9675
1045.2550	1046.8532	1048.8626
1051.9381	1052.2779	1053.9609
1060.2274	1097.4626	1102.7673
1111.4612	1153.8989	1187.6387
1189.9293	1215.3427	1220.6275
1240.2508	1240.8425	1245.5170

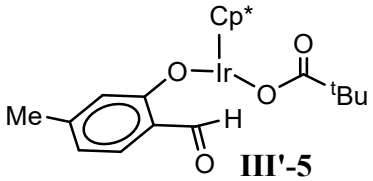
H	-0.67466	-4.11675	0.71095	1250.4884	1255.5852	1271.5326
H	0.46330	-3.31006	-0.39269	1275.1724	1289.5121	1351.8407
C	-2.49164	-1.79252	2.20164	1370.5306	1379.0691	1381.1288
H	-2.96866	-0.91634	2.64606	1384.3015	1384.7389	1386.8022
H	-3.05660	-2.69416	2.47355	1392.3246	1397.7149	1399.0339
H	-1.49010	-1.88157	2.63870	1403.8825	1406.7423	1409.0952
C	-4.46039	-0.11992	0.34717	1412.2190	1418.4966	1426.2012
H	-5.31330	-0.73759	0.65528	1433.0153	1435.9551	1438.4471
H	-4.13205	0.49093	1.19687	1444.6529	1446.8262	1448.5391
H	-4.80044	0.56222	-0.43825	1455.5184	1457.0797	1457.9711
C	1.31120	2.52151	2.53988	1458.8999	1461.2298	1464.0511
H	0.84857	3.40307	2.07530	1465.7718	1469.9644	1471.3742
H	2.04672	2.87641	3.27458	1473.4150	1479.2838	1480.9525
H	1.83960	1.96816	1.75514	1482.1366	1483.5995	1484.2563
C	0.93027	0.37831	3.77134	1490.1117	1493.2992	1495.2751
H	1.69603	0.64065	4.51383	1501.1387	1503.3224	1504.2434
H	0.19205	-0.26845	4.26618	1515.6933	1524.5395	1525.5354
H	1.40565	-0.18761	2.95994	1529.6672	1534.7422	1577.1854
C	-0.40536	2.41307	4.35848	1689.2179	1710.7750	1766.7024
H	-1.17360	1.80558	4.84786	1832.0643	2986.1641	3017.2963
H	0.34231	2.70676	5.10721	3020.8459	3028.8293	3031.3973
H	-0.89455	3.32042	3.98527	3032.2521	3033.7414	3035.4709
C	4.79069	-3.37650	-0.39874	3036.2912	3037.9260	3038.8800
H	5.20820	-2.83583	-1.25574	3039.9610	3040.9794	3097.1697
H	5.61941	-3.81507	0.17085	3098.8613	3106.1252	3109.9386
H	4.16818	-4.18592	-0.79370	3112.0567	3113.4833	3114.6718
C	4.85253	-1.30197	1.00761	3118.4515	3118.4811	3119.0483
H	4.29807	-0.64996	1.69040	3123.3394	3127.5245	3128.6477
H	5.72189	-1.70800	1.54036	3132.0724	3140.1365	3141.1569
H	5.22384	-0.68669	0.17760	3142.5616	3142.8880	3143.1791
C	3.41016	-3.23612	1.68155	3143.2433	3144.7651	3147.0978
H	2.77452	-4.06258	1.33680	3150.1757	3163.6855	3184.0207
H	4.23075	-3.66688	2.26927	3184.8553	3186.8733	3455.4976
H	2.81677	-2.59242	2.34100			
H	2.80430	5.00118	-1.71678			
C	4.46624	2.90980	-2.17874			
H	4.90108	1.91359	-2.30392			
H	4.64265	3.47851	-3.10023			
H	5.01417	3.42473	-1.37997			

Statistical Thermodynamic Analysis

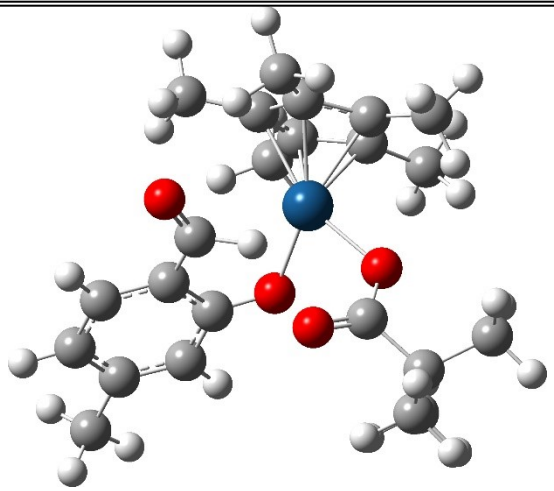
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.642645 Electronic Energy = -1646.80915655
Internal Energy (E)= -1646.12685455 Enthalpy (H)= -1646.12591155
Gibbs Free Energy (G)=-1646.23426655 Gibbs Free Energy of Solvation=-1646.28525476

St.Pt.	General Structure	Ball & Stick model

III'-5



III'-5



Cartesian co-ordinate

Atoms	X	Y	Z
C	1.44319	-2.34923	-0.76629
C	2.36568	-1.70815	0.11563
C	1.72691	-1.59897	1.42070
C	0.42983	-2.26096	1.33480
C	0.24750	-2.70829	-0.00984
C	-2.43589	-0.00385	-0.91529
Ir	0.54308	-0.52782	0.04184
C	-3.76094	-0.11315	-1.38313
C	-4.81131	0.34601	-0.62836
C	-2.17127	0.54826	0.36841
C	-4.56545	0.94219	0.63194
C	-3.27392	1.03609	1.11012
H	-3.06885	1.47691	2.08446
H	-5.83464	0.26809	-0.99191
H	-0.33902	0.17635	-1.53477
O	1.54675	1.27299	0.08632
C	1.12038	2.29792	-0.60531
C	1.73918	3.62318	-0.14706
O	0.27622	2.25460	-1.48887
H	-3.91576	-0.55589	-2.36530
C	-1.34187	-0.39163	-1.76627
O	-1.36527	-1.07601	-2.77181
O	-0.98024	0.59945	0.89665
C	1.58884	4.66898	-1.24458
H	0.54010	4.77916	-1.53585
H	1.96611	5.63911	-0.89512
H	2.15250	4.38531	-2.14170
C	0.93247	4.04383	1.08703
H	1.01120	3.29027	1.87970
H	1.30292	5.00243	1.47456
H	-0.12875	4.16045	0.83373
C	3.21020	3.46088	0.22700
H	3.80231	3.11258	-0.62955
H	3.62316	4.42646	0.54849
H	3.33866	2.74285	1.04396
C	3.69901	-1.13480	-0.21150
H	3.73010	-0.06922	0.04956
H	4.49167	-1.65174	0.34331

Frequencies

26.6105	30.7484	41.5268
54.9329	60.2795	72.5054
85.2707	99.5780	116.0286
118.6737	126.1874	138.3463
147.5191	158.7241	164.1982
175.3027	176.5042	181.9385
187.9135	192.7888	203.3822
210.6699	213.3768	217.5816
227.3221	238.9509	244.0991
252.4467	269.2982	283.4389
288.6972	300.6978	308.5964
313.8384	318.9079	327.6657
340.2310	355.5232	375.3783
390.5618	419.6083	426.3956
437.8629	439.8730	447.3763
467.5632	525.2599	535.9674
540.2636	543.1189	566.4282
577.3194	584.0625	592.9056
595.8119	603.7999	613.2970
644.3504	669.4427	741.2840
745.7905	791.6692	801.9438
803.1415	809.3499	818.4008
828.7873	869.4670	917.4480
951.8479	952.0746	953.3281
953.5780	958.4091	961.9688
970.3724	1023.5839	1038.4884
1039.8485	1041.9415	1043.9567
1044.6485	1045.5596	1048.9056
1049.4989	1062.3842	1088.6721
1092.7379	1104.7099	1127.4638
1179.9325	1183.9344	1190.5982
1216.3811	1236.5450	1246.3493
1266.7373	1270.6982	1323.3608
1357.1184	1376.0583	1377.9943
1380.0678	1389.3609	1393.1708
1395.5454	1399.2517	1401.7998
1402.7904	1415.1492	1435.0601
1437.3385	1438.4795	1440.8201
1443.7483	1447.6355	1452.6239
1454.8074	1457.1167	1458.5784
1460.1100	1460.4205	1463.8837
1467.0088	1468.8225	1469.1047

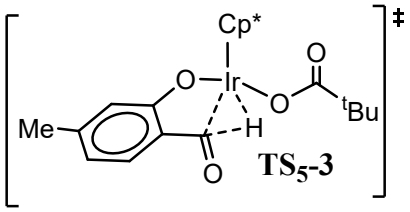
H	3.91975	-1.22031	-1.27914	1478.3105	1479.6066	1482.5118
C	1.61274	-2.61047	-2.22014	1485.2655	1494.6449	1505.2482
H	2.47853	-2.07820	-2.62386	1511.4212	1521.6675	1525.1070
H	1.75242	-3.68360	-2.40285	1543.2458	1598.2316	1680.2173
H	0.72513	-2.28282	-2.77656	1785.1752	1802.6694	2272.9922
C	-0.91140	-3.47115	-0.54778	3023.5330	3026.4000	3033.3347
H	-1.08474	-3.23483	-1.60204	3034.2405	3036.8752	3037.5175
H	-0.73454	-4.55098	-0.46063	3039.6161	3040.6015	3043.3233
H	-1.83177	-3.23371	-0.00434	3103.3562	3106.0981	3114.0368
C	-0.56150	-2.37531	2.43663	3115.6513	3115.9345	3120.6630
H	-1.58544	-2.32953	2.05084	3121.6699	3123.5257	3126.5838
H	-0.43890	-3.32505	2.97201	3130.8505	3136.6693	3140.0171
H	-0.44983	-1.55890	3.15661	3146.1143	3147.9985	3149.6709
C	2.35215	-0.99327	2.62618	3149.7484	3150.8425	3153.6504
H	1.59655	-0.68486	3.35504	3172.2234	3182.8559	3190.2562
H	3.03330	-1.70125	3.11631			
H	2.92493	-0.10104	2.35003			
C	-5.72028	1.45966	1.43307			
H	-6.46749	0.67436	1.60262			
H	-5.40060	1.84383	2.40653			
H	-6.23177	2.27121	0.90034			
C	4.79069	-3.37650	-0.39874			
H	5.20820	-2.83583	-1.25574			
H	5.61941	-3.81507	0.17085			
H	4.16818	-4.18592	-0.79370			
C	4.85253	-1.30197	1.00761			
H	4.29807	-0.64996	1.69040			
H	5.72189	-1.70800	1.54036			
H	5.22384	-0.68669	0.17760			
C	3.41016	-3.23612	1.68155			
H	2.77452	-4.06258	1.33680			
H	4.23075	-3.66688	2.26927			
H	2.81677	-2.59242	2.34100			
H	2.80430	5.00118	-1.71678			
C	4.46624	2.90980	-2.17874			
H	4.90108	1.91359	-2.30392			
H	4.64265	3.47851	-3.10023			
H	5.01417	3.42473	-1.37997			

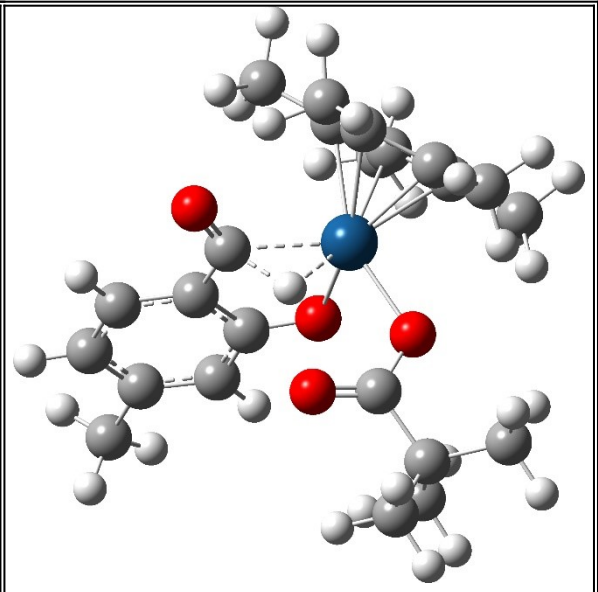
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.489776 Electronic Energy = -1299.93701883
Internal Energy (E)= -1299.41570883 Enthalpy (H)= -1299.41476583
Gibbs Free Energy (G)=-1299.50804083 Gibbs Free Energy of Solvation=-1299.55627304

St.Pt.	General Structure	Ball & Stick model

TS_5-3





Cartesian co-ordinate

Atoms	X	Y	Z
C	2.14894	-1.83176	-0.72822
C	2.77940	-0.78929	0.01802
C	2.26626	-0.82956	1.38296
C	1.33313	-1.90833	1.46540
C	1.21507	-2.50385	0.15895
C	-2.22574	-0.83077	-0.77558
Ir	0.61915	-0.37539	-0.03240
C	-3.43621	-1.27094	-1.33972
C	-4.62396	-1.01801	-0.69578
C	-2.20884	-0.14308	0.45724
C	-4.63009	-0.31162	0.53067
C	-3.44207	0.11737	1.09286
H	-3.43105	0.65921	2.03698
H	-5.56894	-1.34994	-1.12277
H	-0.14958	0.17812	-1.42178
O	0.96552	1.66824	0.08765
C	0.23539	2.47248	-0.63525
C	0.33854	3.93299	-0.18477
O	-0.51904	2.12834	-1.53724
H	-3.40169	-1.80053	-2.28945
C	-0.95373	-1.05060	-1.42796
O	-0.73222	-1.71761	-2.41492
O	-1.07999	0.22108	1.00238
C	-0.16331	4.85414	-1.28919
H	-1.18275	4.58953	-1.58502
H	-0.15318	5.89553	-0.94172
H	0.46921	4.78491	-2.18237
C	-0.57512	4.03926	1.04215
H	-0.25595	3.34157	1.82539
H	-0.55329	5.06091	1.44388
H	-1.61095	3.79521	0.77409
C	1.76956	4.30176	0.19766
H	2.45619	4.16306	-0.64778
H	1.81479	5.35740	0.49646
H	2.13120	3.69346	1.03331

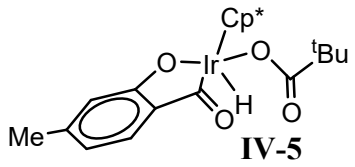
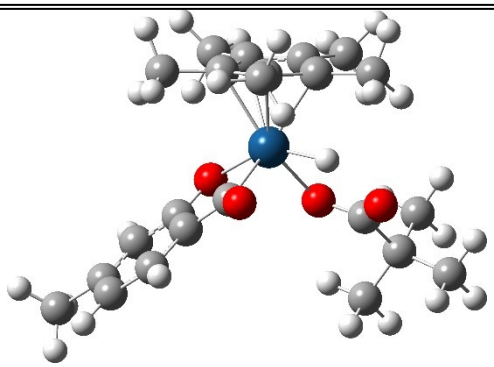
Frequencies

-171.5043	11.1779	31.8915
41.8265	57.6060	59.8187
80.1214	84.4650	115.1226
123.5449	134.6227	138.3710
150.5102	157.0774	164.6703
165.6334	167.2154	170.0969
182.7548	186.1587	193.0048
198.5877	214.8359	218.2196
224.0935	239.8515	256.1552
267.0643	269.7835	281.4630
281.9176	288.6035	298.1171
307.2600	323.1760	326.5725
348.6799	355.6522	368.7643
379.5685	393.1144	410.7664
430.5544	440.3749	442.2140
451.5443	498.2912	538.2118
540.3598	545.5786	558.8709
572.1938	588.9085	591.1016
597.7660	604.7050	609.7766
643.3125	669.9974	725.5758
747.4374	776.6908	791.5539
800.8050	809.7984	812.1703
822.3869	847.5489	860.4887
900.7781	922.9587	945.2749
949.4263	952.8152	953.2018
955.9935	959.2414	968.1347
1020.6007	1036.4750	1038.6307
1041.1571	1042.0981	1042.9286
1043.8747	1044.4946	1045.9411
1085.8382	1090.2060	1105.1659
1131.9418	1182.0746	1185.4240
1189.9640	1221.4309	1235.8004
1247.4509	1264.8954	1265.9059
1329.2537	1356.6958	1372.3765
1376.3226	1376.5018	1388.0072
1392.0057	1393.4949	1394.7284
1397.5422	1413.7700	1416.9013
1435.0332	1438.1363	1442.2066
1442.4767	1446.6927	1452.0687

C	3.78481	0.19567	-0.46300	1452.9615	1455.6692	1459.0059
H	3.46726	1.21612	-0.21596	1460.8331	1461.2870	1462.1332
H	4.75979	0.01567	0.00756	1464.2508	1468.0153	1468.5193
H	3.91180	0.14036	-1.54781	1469.9845	1478.8417	1483.1988
C	2.40117	-2.20747	-2.14471	1484.2424	1503.5299	1506.8435
H	3.06521	-1.48971	-2.63452	1510.4902	1518.4329	1519.8136
H	2.87120	-3.19769	-2.19812	1542.8495	1610.4518	1674.2673
H	1.46178	-2.24021	-2.70610	1746.8256	1788.1901	1875.1281
C	0.40973	-3.70744	-0.18858	3022.6802	3026.1929	3034.5477
H	0.11928	-3.69253	-1.24343	3034.7773	3034.9831	3039.4958
H	0.98394	-4.62381	-0.00002	3040.7277	3043.4871	3044.8718
H	-0.50958	-3.75651	0.40527	3104.8973	3108.4090	3112.7973
C	0.51681	-2.27673	2.65204	3113.2288	3115.3498	3120.8988
H	-0.48437	-2.60629	2.35445	3120.9558	3128.1681	3128.3673
H	0.99036	-3.09413	3.21010	3129.1343	3134.7678	3139.9144
H	0.39126	-1.42551	3.32735	3141.6935	3149.3346	3150.2210
C	2.68783	0.09460	2.47114	3151.4594	3153.1757	3158.4057
H	2.03803	0.00487	3.34645	3173.0911	3185.3915	3198.1490
H	3.71670	-0.11640	2.79032			
H	2.64329	1.13660	2.13386			
C	-5.93859	-0.03531	1.20600			
H	-6.48806	-0.96550	1.39726			
H	-5.80242	0.48242	2.16043			
H	-6.58221	0.58696	0.57169			
C	4.79069	-3.37650	-0.39874			
H	5.20820	-2.83583	-1.25574			
H	5.61941	-3.81507	0.17085			
H	4.16818	-4.18592	-0.79370			
C	4.85253	-1.30197	1.00761			
H	4.29807	-0.64996	1.69040			
H	5.72189	-1.70800	1.54036			
H	5.22384	-0.68669	0.17760			
C	3.41016	-3.23612	1.68155			
H	2.77452	-4.06258	1.33680			
H	4.23075	-3.66688	2.26927			
H	2.81677	-2.59242	2.34100			
H	2.80430	5.00118	-1.71678			
C	4.46624	2.90980	-2.17874			
H	4.90108	1.91359	-2.30392			
H	4.64265	3.47851	-3.10023			
H	5.01417	3.42473	-1.37997			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.486220 Electronic Energy = -1299.93193367
Internal Energy (E)= -1299.41461367 Enthalpy (H)= -1299.41366967
Gibbs Free Energy (G)=-1299.50644667 Gibbs Free Energy of Solvation=-1299.54780594

St.Pt.	General Structure	Ball & Stick model
IV-5	 **IV-5**	

Cartesian co-ordinate

Atoms	X	Y	Z
C	0.72182	-2.48248	-0.82492
C	1.93303	-1.90414	-0.27683
C	1.82344	-1.88696	1.17485
C	0.53306	-2.30131	1.51272
C	-0.19757	-2.60249	0.27312
C	-2.38428	0.46440	-0.88377
Ir	0.24685	-0.49450	-0.08708
C	-3.52883	0.84214	-1.59975
C	-4.63033	1.32063	-0.92241
C	-2.34669	0.55934	0.51743
C	-4.60906	1.42381	0.48514
C	-3.48066	1.04320	1.19505
H	-3.44950	1.12035	2.28046
H	-5.52456	1.62543	-1.46394
H	1.04772	0.00520	-1.37454
O	1.01271	1.38149	0.38468
C	1.88648	1.92929	-0.40899
C	2.45493	3.24299	0.14001
O	2.26885	1.45753	-1.47883
H	-3.51672	0.75070	-2.68371
C	-1.18503	-0.07632	-1.52326
O	-1.06691	-0.32057	-2.70167
O	-1.26108	0.18740	1.15878
C	-1.57992	-3.15843	0.23794
H	-2.01885	-3.07639	-0.76150
H	-1.58889	-4.21655	0.53068
H	-2.23361	-2.61129	0.92695

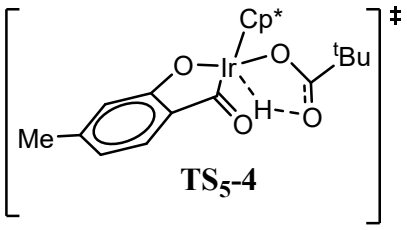
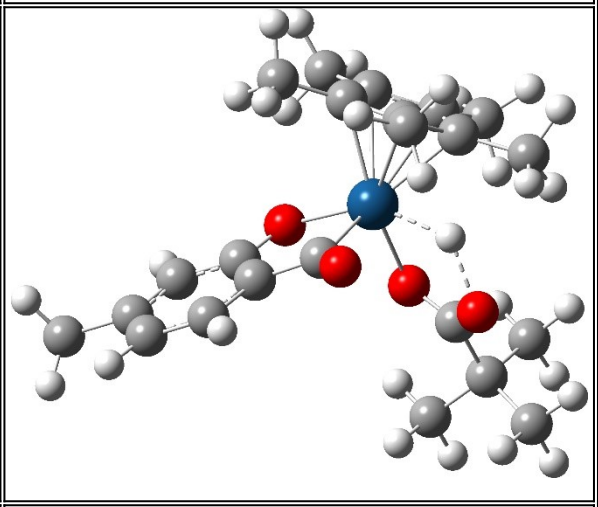
Frequencies

22.9964	31.6447	42.1115
52.0471	57.4981	81.1128
90.8762	111.3659	128.7715
133.0452	143.4725	153.7907
159.6384	163.8905	174.3739
179.8596	190.8101	199.9302
203.4891	207.7984	209.8923
219.5481	224.2265	233.8087
241.1311	257.1114	265.0346
269.0795	281.5696	285.3954
294.1156	298.0479	303.1460
305.8656	318.4330	323.1254
330.3514	362.5787	367.8558
370.8033	390.9406	420.3894
440.6943	444.0177	449.1253
455.1652	533.5826	533.9472
549.9085	560.2159	570.3347
592.5663	596.8096	600.2209
614.5464	619.6824	635.0255
645.1154	679.5154	736.3621
754.6458	774.8297	794.1056
807.0559	808.5372	813.2869
823.3750	865.7232	882.9264
906.9947	947.0641	950.0987
951.3245	951.9491	955.3880
960.9107	968.5337	970.9662
1019.9434	1022.9893	1037.6074
1038.0706	1039.4812	1045.0956
1047.1395	1049.9181	1055.6162
1085.8569	1090.3135	1107.5532
1128.2563	1175.3822	1182.8001
1188.3694	1215.3219	1242.4176

C	0.52568	-2.91087	-2.23691	1247.8151	1265.4043	1266.0934
H	1.20578	-3.73778	-2.47565	1325.6493	1360.1629	1365.9272
H	-0.49848	-3.25140	-2.41149	1374.7312	1376.9015	1388.1152
H	0.70607	-2.08685	-2.93506	1389.5240	1396.4498	1400.2202
C	3.19586	-1.63970	-1.02121	1401.3330	1404.0461	1412.1765
H	3.89895	-2.47204	-0.88415	1427.6292	1435.5295	1437.0392
H	3.00935	-1.51469	-2.09165	1448.9074	1450.4718	1454.2868
H	3.67502	-0.71976	-0.67015	1455.9376	1456.6850	1457.2082
C	2.88286	-1.35166	2.07196	1458.8446	1459.6261	1461.1131
H	3.84136	-1.85544	1.89683	1462.0074	1465.0980	1468.0330
H	3.03877	-0.27876	1.89144	1473.7525	1474.5494	1479.0935
H	2.62190	-1.47330	3.12691	1481.9641	1493.9349	1503.8100
C	-0.10982	-2.30249	2.84982	1507.4388	1513.9465	1516.9121
H	0.61095	-2.12186	3.65191	1585.9503	1625.2358	1667.8644
H	-0.87135	-1.51024	2.88823	1730.4528	1813.1137	2067.6947
H	-0.61226	-3.25789	3.04358	3015.9942	3030.4959	3031.6237
C	3.26999	2.90008	1.39011	3033.5654	3033.8615	3034.0116
H	3.73345	3.80760	1.79829	3036.5079	3040.1049	3044.9170
H	2.63415	2.45670	2.16468	3100.3564	3101.7529	3106.8924
H	4.07639	2.19218	1.14987	3108.0722	3111.7323	3114.3317
C	3.35521	3.89362	-0.90210	3123.7457	3128.5006	3129.5013
H	2.79780	4.12695	-1.81590	3131.1875	3138.1840	3138.9896
H	3.77118	4.82775	-0.50245	3139.6440	3145.2031	3148.3039
H	4.18285	3.23347	-1.18213	3149.5827	3154.4887	3157.8350
C	1.31126	4.18636	0.51089	3170.6863	3185.0037	3198.2494
H	1.71757	5.12287	0.91520			
H	0.70550	4.43630	-0.36899			
H	0.65249	3.73627	1.25958			
C	-5.81410	1.95598	1.20006			
H	-5.69099	1.91867	2.28692			
H	-6.00898	2.99853	0.91892			
H	-6.71341	1.38478	0.93879			
C	4.79069	-3.37650	-0.39874			
H	5.20820	-2.83583	-1.25574			
H	5.61941	-3.81507	0.17085			
H	4.16818	-4.18592	-0.79370			
C	4.85253	-1.30197	1.00761			
H	4.29807	-0.64996	1.69040			
H	5.72189	-1.70800	1.54036			
H	5.22384	-0.68669	0.17760			
C	3.41016	-3.23612	1.68155			
H	2.77452	-4.06258	1.33680			
H	4.23075	-3.66688	2.26927			
H	2.81677	-2.59242	2.34100			
H	2.80430	5.00118	-1.71678			
C	4.46624	2.90980	-2.17874			
H	4.90108	1.91359	-2.30392			
H	4.64265	3.47851	-3.10023			
H	5.01417	3.42473	-1.37997			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.488233 Electronic Energy = -1299.93912285
Internal Energy (E)= -1299.41974185 Enthalpy (H)= -1299.41879885
Gibbs Free Energy (G)=-1299.51083085 Gibbs Free Energy of Solvation=-1299.55372052

St.Pt.	General Structure	Ball & Stick model
TS_5-4	 **TS_5-4**	

Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.86114	-2.36535	0.97586
C	-2.02238	-1.78508	0.34201
C	-1.87823	-1.92085	-1.10427
C	-0.60572	-2.43465	-1.36314
C	0.07861	-2.64363	-0.07855
C	2.35478	0.48226	0.85936
Ir	-0.25668	-0.50133	0.02955
C	3.47365	0.90185	1.59165
C	4.61787	1.29184	0.92791
C	2.38501	0.44630	-0.54517
C	4.66474	1.26340	-0.48252
C	3.56069	0.84369	-1.20849
H	3.58263	0.81947	-2.29664
H	5.49375	1.62653	1.48191
H	-1.10190	0.25580	1.24426
O	-0.96008	1.39440	-0.57358
C	-1.69781	2.00424	0.28590
C	-2.32719	3.30590	-0.20177
O	-1.94507	1.55748	1.42184
H	3.40782	0.91249	2.67763
C	1.10842	0.03595	1.48305
O	0.92725	-0.07204	2.67612
O	1.32118	0.03838	-1.20048
C	1.42665	-3.26492	0.06007
H	1.83626	-3.10654	1.06296
H	1.38714	-4.34623	-0.12658
H	2.13267	-2.82430	-0.65302
C	-0.71594	-2.64326	2.43124
H	-1.46045	-3.38345	2.74945
H	0.27695	-3.03827	2.66374
H	-0.83785	-1.73122	3.02617
C	-3.28349	-1.39049	1.03052
H	-3.99456	-2.22746	1.03623
H	-3.09337	-1.09056	2.06514

Frequencies

-453.6414	20.6636	30.8249
40.7973	51.3734	74.4187
88.4874	100.8075	118.3407
131.0323	134.0540	146.3005
155.3012	155.8970	172.1018
186.4496	193.1429	197.5943
199.0893	205.5629	211.6310
215.4174	223.0741	230.5747
238.8871	244.7978	258.4828
264.9951	270.9601	274.0724
278.0002	288.1896	292.9949
297.4035	309.0891	328.3497
331.3735	352.6480	364.9269
374.4007	390.0442	414.3980
434.9222	443.6239	448.3805
455.7734	478.1230	533.1047
537.6745	551.7731	566.0378
589.4786	595.6993	598.4248
602.5081	620.2227	623.4931
637.5578	649.3569	681.5756
754.0187	755.3557	784.5013
804.1794	809.4429	812.4426
832.8198	847.4413	862.8667
893.5364	942.0805	947.5787
948.9727	953.2653	954.7474
957.7021	958.2968	969.6836
1019.8608	1033.5462	1035.6202
1042.8310	1043.1512	1046.4408
1046.7317	1055.0302	1058.4608
1083.6988	1091.0721	1106.8233
1127.6635	1175.8627	1182.0674
1187.4625	1215.7124	1240.0256
1253.8812	1265.9767	1267.4515
1326.8634	1368.0009	1374.2828
1377.5906	1378.2063	1388.2835
1396.9111	1399.1780	1400.2919
1401.6871	1404.1388	1422.3293
1427.4445	1438.5597	1440.8104
1449.0320	1449.5438	1455.7975

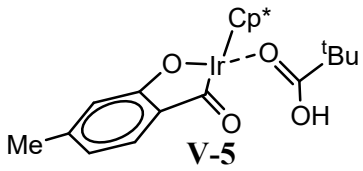
H	-3.76422	-0.54227	0.53037	1457.4889	1458.7938	1459.8158
C	-2.88668	-1.41868	-2.07670	1460.2416	1461.6124	1463.1889
H	-3.85028	-1.92807	-1.94950	1465.9845	1468.2251	1469.1061
H	-3.06204	-0.34397	-1.92880	1473.2387	1473.9400	1480.6892
H	-2.56138	-1.56073	-3.11100	1483.7815	1499.2403	1504.0262
C	0.07743	-2.58414	-2.67352	1507.9679	1512.9692	1516.1306
H	-0.60570	-2.42497	-3.51236	1557.6591	1589.5277	1624.5735
H	0.88826	-1.84415	-2.74746	1668.2205	1753.8881	1812.0059
H	0.52319	-3.58101	-2.77565	3020.1106	3020.6705	3030.8929
C	-3.39908	2.90764	-1.22327	3032.6346	3032.9043	3034.8006
H	-3.92305	3.80172	-1.58437	3036.4767	3040.2061	3041.8900
H	-2.95022	2.39784	-2.08355	3098.1804	3099.7454	3105.9620
H	-4.14644	2.24106	-0.77012	3106.1711	3113.9140	3117.0270
C	-2.96909	4.05364	0.95960	3117.7658	3126.2219	3126.3229
H	-2.22540	4.31853	1.71929	3133.3257	3134.9664	3135.9168
H	-3.43181	4.97854	0.59249	3144.2845	3145.1242	3148.0095
H	-3.73822	3.44669	1.44797	3149.6479	3150.5818	3152.0936
C	-1.26947	4.17855	-0.87520	3169.4406	3186.6804	3196.6229
H	-1.73418	5.10085	-1.24706			
H	-0.48153	4.46094	-0.16657			
H	-0.79887	3.65890	-1.71499			
C	5.91690	1.69675	-1.18335			
H	5.82683	1.60411	-2.27020			
H	6.15515	2.74250	-0.95201			
H	6.77813	1.09820	-0.86136			
C	4.79069	-3.37650	-0.39874			
H	5.20820	-2.83583	-1.25574			
H	5.61941	-3.81507	0.17085			
H	4.16818	-4.18592	-0.79370			
C	4.85253	-1.30197	1.00761			
H	4.29807	-0.64996	1.69040			
H	5.72189	-1.70800	1.54036			
H	5.22384	-0.68669	0.17760			
C	3.41016	-3.23612	1.68155			
H	2.77452	-4.06258	1.33680			
H	4.23075	-3.66688	2.26927			
H	2.81677	-2.59242	2.34100			
H	2.80430	5.00118	-1.71678			
C	4.46624	2.90980	-2.17874			
H	4.90108	1.91359	-2.30392			
H	4.64265	3.47851	-3.10023			
H	5.01417	3.42473	-1.37997			

Statistical Thermodynamic Analysis

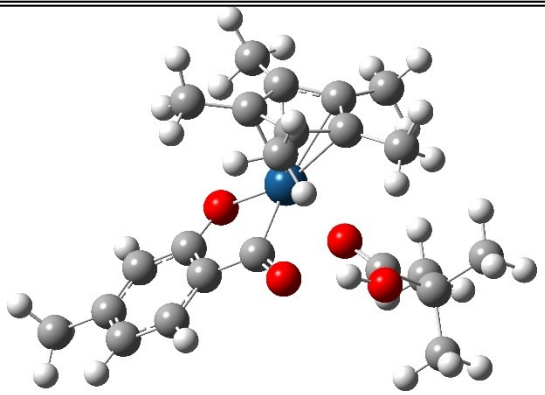
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.486031 Electronic Energy = -1299.93809793
Internal Energy (E)= -1299.42132393 Enthalpy (H)= -1299.42038093
Gibbs Free Energy (G)=-1299.51142793 Gibbs Free Energy of Solvation=-1299.55310108

St.Pt.	General Structure	Ball & Stick model

V-5



V-5



Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.51576	-2.22823	1.27057
C	-1.75984	-1.77659	0.71999
C	-1.77885	-2.13331	-0.70649
C	-0.53944	-2.67835	-1.04557
C	0.30859	-2.65837	0.15648
C	2.27005	0.85014	0.74141
Ir	-0.10007	-0.59450	-0.07421
C	3.26060	1.51364	1.48145
C	4.45607	1.84614	0.88363
C	2.46590	0.54479	-0.62744
C	4.67504	1.54034	-0.47991
C	3.69318	0.90752	-1.22318
H	3.84929	0.68130	-2.27695
H	5.24032	2.35094	1.44621
H	-1.02445	1.39321	1.77679
O	-1.11710	1.28815	-0.65365
C	-1.82972	1.96310	0.09984
C	-2.88081	2.90415	-0.45960
O	-1.80245	1.91427	1.40354
H	3.05642	1.74932	2.52459
C	0.94799	0.51272	1.23123
O	0.47508	0.91761	2.30786
O	1.50759	-0.03493	-1.30163
C	1.68578	-3.22337	0.22429
H	2.22744	-2.83419	1.09320
H	1.67357	-4.31964	0.28847
H	2.25898	-2.93818	-0.66493
C	-0.13578	-2.21153	2.70952
H	-0.59319	-3.05443	3.24264
H	0.95001	-2.28110	2.83062
H	-0.44879	-1.27779	3.18903
C	-2.93908	-1.28656	1.49006
H	-3.65198	-2.09829	1.69109
H	-2.63378	-0.86305	2.45304
H	-3.48086	-0.50137	0.94740
C	-2.91857	-1.81399	-1.60941
H	-3.82181	-2.36731	-1.31998
H	-3.16467	-0.74375	-1.56588
H	-2.69237	-2.05608	-2.65204
C	-0.03006	-3.05971	-2.39037
H	-0.78219	-2.90619	-3.17001

Frequencies

24.6788	33.1241	52.9583
67.8620	81.1034	82.5639
101.6501	110.1548	124.6280
126.3130	140.0289	145.3193
159.9377	163.8643	173.8486
175.4448	188.1638	197.7448
203.1055	212.6923	219.7138
224.7642	230.7086	233.8043
248.6487	259.8838	263.9112
270.5729	271.5223	284.2599
301.1226	306.5835	311.5249
317.0489	322.7041	336.0246
361.2515	373.3006	386.9155
392.7601	398.9491	411.1347
417.6291	443.6220	465.5141
468.6563	532.1709	538.4501
550.4847	555.2827	570.3732
583.1024	593.3097	604.5727
606.9294	612.8889	625.2454
660.7097	696.6275	752.2725
759.9626	780.9741	789.2452
804.9771	806.5855	810.5690
862.5651	893.7930	908.9381
937.4117	949.0036	952.6424
955.1814	960.5443	963.3496
965.1437	966.5504	1020.6011
1037.0233	1040.2387	1043.4510
1044.8842	1047.9094	1048.9740
1050.5296	1055.0069	1087.2077
1090.6286	1106.9323	1125.2917
1178.4464	1182.7620	1185.9458
1217.6260	1237.9531	1248.9735
1264.4639	1276.9938	1328.2743
1342.8772	1369.1978	1375.1007
1383.2541	1389.8616	1391.3983
1395.3540	1399.6035	1400.3650
1405.6424	1413.8284	1429.1337
1433.7849	1442.2725	1450.4568
1451.8163	1453.0037	1455.8941
1458.4549	1459.7208	1462.1322
1462.2445	1463.1058	1464.4173
1466.2892	1468.1382	1468.7854
1476.1257	1479.1881	1485.0973
1497.2420	1505.8476	1508.0774
1511.9034	1521.3494	1525.6628

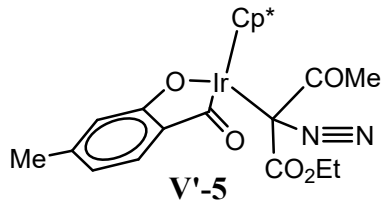
H	0.84745	-2.45194	-2.64683	1592.4322	1609.0576	1650.9981
H	0.27409	-4.11420	-2.41487	1673.9024	1740.8648	3020.5895
C	-4.24832	2.30558	-0.10125	3024.8653	3028.7904	3031.8967
H	-5.04278	2.94578	-0.50364	3032.0638	3033.2256	3038.8608
H	-4.37372	1.30512	-0.53952	3039.6194	3044.3037	3060.7691
H	-4.38131	2.22930	0.98332	3090.2094	3099.7422	3104.6571
C	-2.73614	4.28337	0.18561	3105.6399	3115.4867	3115.6414
H	-1.75538	4.72273	-0.03211	3123.5329	3124.2052	3132.7962
H	-3.50251	4.95577	-0.21866	3133.0745	3135.6889	3136.7786
H	-2.85645	4.23339	1.27185	3137.3913	3139.9869	3140.8642
C	-2.74112	3.00913	-1.97299	3141.4120	3142.3939	3151.6392
H	-3.51497	3.67998	-2.36501	3167.2439	3182.3905	3191.1681
H	-1.76182	3.40895	-2.25724			
H	-2.85133	2.03205	-2.45545			
C	5.98296	1.91582	-1.10912			
H	6.01575	1.64707	-2.16966			
H	6.16523	2.99463	-1.02604			
H	6.82039	1.41535	-0.60652			
C	4.79069	-3.37650	-0.39874			
H	5.20820	-2.83583	-1.25574			
H	5.61941	-3.81507	0.17085			
H	4.16818	-4.18592	-0.79370			
C	4.85253	-1.30197	1.00761			
H	4.29807	-0.64996	1.69040			
H	5.72189	-1.70800	1.54036			
H	5.22384	-0.68669	0.17760			
C	3.41016	-3.23612	1.68155			
H	2.77452	-4.06258	1.33680			
H	4.23075	-3.66688	2.26927			
H	2.81677	-2.59242	2.34100			
H	2.80430	5.00118	-1.71678			
C	4.46624	2.90980	-2.17874			
H	4.90108	1.91359	-2.30392			
H	4.64265	3.47851	-3.10023			
H	5.01417	3.42473	-1.37997			

Statistical Thermodynamic Analysis

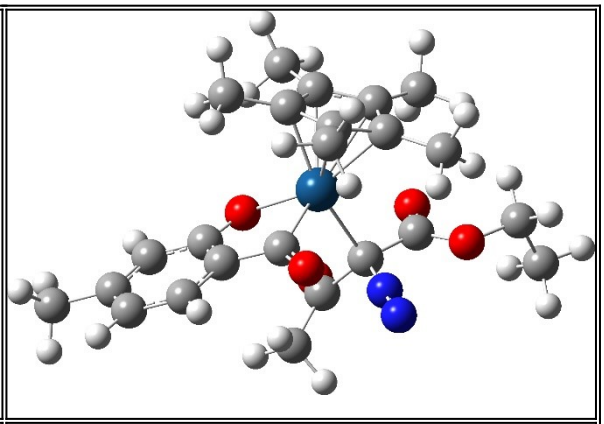
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.492217 Electronic Energy = -1299.97237081
Internal Energy (E)= -1299.44934981 Enthalpy (H)= -1299.44840581
Gibbs Free Energy (G)=-1299.53913681 Gibbs Free Energy of Solvation=-1299.57723098

St.Pt.	General Structure	Ball & Stick model

V'-5



V'-5



Cartesian co-ordinate

Atoms	X	Y	Z
C	0.10599	2.60465	0.69010
C	1.44946	2.09625	0.72616
C	1.90396	1.94616	-0.65890
C	0.81699	2.17431	-1.50871
C	-0.33863	2.52541	-0.67729
C	-2.58379	-0.31005	0.80878
Ir	0.07580	0.51632	0.00114
C	-2.52405	-0.55568	-0.58068
C	-3.69726	-0.98101	-1.23791
C	-3.77765	-0.49218	1.52135
C	-4.87972	-1.13911	-0.53239
C	-4.91879	-0.89295	0.85820
H	-3.77256	-0.30733	2.59426
H	-5.85728	-1.02621	1.39480
H	-3.65235	-1.18063	-2.30744
C	1.06110	-1.47283	0.15689
C	2.45283	-1.40720	-0.41921
C	0.17285	-2.57815	-0.46560
O	0.36395	-2.91244	-1.60358
N	1.09583	-1.54545	1.54280
N	1.06026	-1.57182	2.66631
C	3.29949	1.63584	-1.06893
H	3.33945	0.94991	-1.92126
H	3.82092	2.56077	-1.34831
H	3.86492	1.18599	-0.24543
C	2.28751	2.00302	1.95601
H	3.09637	1.27333	1.83582
H	2.74453	2.96657	2.22085
H	1.67575	1.67234	2.80434
C	-0.66200	3.09721	1.86520
H	-0.53909	2.42839	2.72370
H	-0.31920	4.10095	2.14729
H	-1.73436	3.15164	1.64980
C	-1.66949	2.91419	-1.22128
H	-2.44241	2.88444	-0.44660
H	-1.64721	3.92569	-1.64788
H	-1.97497	2.21666	-2.00948
C	0.76629	2.02891	-2.98897
H	0.63469	3.00113	-3.48308
H	1.67969	1.56886	-3.37827
H	-0.07469	1.38918	-3.28324

Frequencies

-55.1838	16.5379	25.8976
42.7901	53.7673	57.7252
73.3541	87.3000	97.2025
101.4918	105.7298	110.7063
117.7488	120.0990	127.3650
142.3918	145.8140	154.1401
159.2749	160.0009	163.8731
177.9843	185.3362	187.6965
196.9454	200.3207	202.5690
217.3289	242.4819	247.6884
251.3640	259.9729	264.1892
274.3452	282.8610	285.4167
305.6106	314.3840	322.2610
338.7263	343.0487	354.1144
363.5978	369.5687	377.2310
401.3936	439.1117	444.3549
456.6200	462.9943	495.5172
499.7049	532.2385	535.5782
538.3990	550.8087	568.7210
577.7529	583.1051	597.6809
601.7037	605.4413	610.0559
619.7976	664.1512	682.9260
752.4234	759.3002	764.5540
777.9646	800.8443	807.0269
814.9132	819.4120	862.8723
878.8463	886.8990	949.2367
951.4179	958.4189	965.2130
965.5818	984.6595	1016.7697
1018.9633	1026.9610	1029.3136
1042.2195	1042.6521	1048.4991
1049.8187	1061.2578	1091.2359
1091.5572	1100.5982	1110.0502
1119.7906	1122.7632	1178.4869
1180.6949	1183.7300	1186.3570
1197.3405	1210.1849	1262.9338
1264.4206	1327.0730	1328.0355
1371.3189	1372.3683	1376.3405
1385.1464	1387.5775	1393.6684
1400.4220	1401.3380	1403.1593
1414.0983	1425.2253	1427.9299
1431.9971	1444.0884	1448.0421
1449.6646	1454.3198	1459.1803
1459.9753	1462.8278	1463.3103
1464.9920	1466.2745	1469.6543
1476.3395	1481.6044	1487.7103

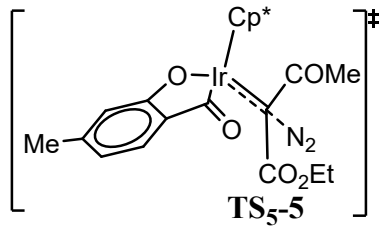
C	-1.30672	0.06457	1.41681	1489.7837	1493.2535	1504.9491
O	-1.38313	-0.42366	-1.21058	1506.1227	1512.8581	1514.5539
O	-1.10580	0.13549	2.62291	1579.1723	1611.8956	1666.2489
O	2.68614	-1.33191	-1.59578	1741.5348	1854.1194	1897.8824
C	4.75828	-1.50293	0.10592	2265.6043	3025.2346	3027.3680
H	5.33280	-1.11377	0.95215	3032.2265	3034.8120	3035.4763
H	4.88225	-0.83123	-0.75003	3039.4062	3044.3069	3052.5359
O	3.38753	-1.45037	0.54896	3077.5206	3101.7663	3102.3874
C	5.14884	-2.91632	-0.24727	3104.5354	3112.6487	3118.2034
H	4.56745	-3.26978	-1.10443	3122.5106	3124.6318	3134.5318
H	6.20969	-2.95863	-0.51454	3135.6230	3137.8474	3139.2146
H	4.98086	-3.59080	0.59844	3139.9958	3141.9057	3144.4605
C	-0.84230	-3.22946	0.42859	3145.5565	3158.2726	3169.4012
H	-1.52119	-3.80996	-0.19944	3182.2060	3183.2780	3192.3740
H	-0.33306	-3.91199	1.12185			
H	-1.42005	-2.51178	1.02011			
C	-6.13171	-1.57430	-1.23314			
H	-6.52811	-2.50003	-0.79736			
H	-6.92054	-0.81762	-1.13654			
H	-5.96000	-1.74892	-2.29989			
H	5.61941	-3.81507	0.17085			
H	4.16818	-4.18592	-0.79370			
C	4.85253	-1.30197	1.00761			
H	4.29807	-0.64996	1.69040			
H	5.72189	-1.70800	1.54036			
H	5.22384	-0.68669	0.17760			
C	3.41016	-3.23612	1.68155			
H	2.77452	-4.06258	1.33680			
H	4.23075	-3.66688	2.26927			
H	2.81677	-2.59242	2.34100			
H	2.80430	5.00118	-1.71678			
C	4.46624	2.90980	-2.17874			
H	4.90108	1.91359	-2.30392			
H	4.64265	3.47851	-3.10023			
H	5.01417	3.42473	-1.37997			

Statistical Thermodynamic Analysis

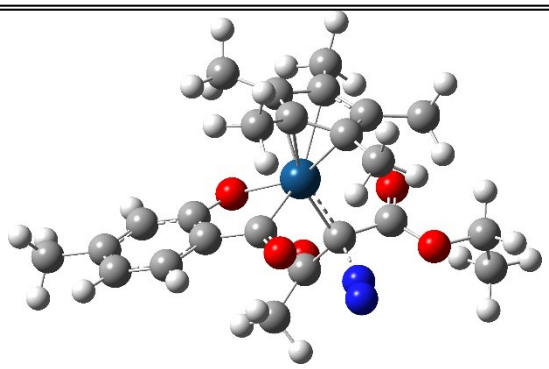
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.486535 Electronic Energy = -1521.39903556
Internal Energy (E)= -1520.87796056 Enthalpy (H)= -1520.87701656
Gibbs Free Energy (G)=-1520.97725256 Gibbs Free Energy of Solvation=-1521.02019183

St.Pt.	General Structure	Ball & Stick model

TS_5-5



TS_5-5



Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.35592	2.65528	0.46582
C	0.96199	2.28868	0.92221
C	1.77429	2.04258	-0.25554
C	0.95790	2.16652	-1.41217
C	-0.37688	2.49953	-0.95593
C	-2.53743	-0.43288	0.80444
Ir	0.08087	0.49468	-0.04110
C	-2.48415	-0.67598	-0.58546
C	-3.65346	-1.12610	-1.23331
C	-3.72164	-0.63957	1.52774
C	-4.82589	-1.30905	-0.51780
C	-4.85907	-1.06260	0.87342
H	-3.71251	-0.45587	2.60074
H	-5.79043	-1.21448	1.41728
H	-3.61314	-1.32525	-2.30299
C	1.12444	-1.27233	0.06859
C	2.55788	-1.22291	-0.39938
C	0.40360	-2.50145	-0.51602
O	0.65492	-2.83528	-1.64763
N	1.25178	-1.59477	1.68140
N	1.05643	-1.41816	2.76872
C	3.24790	1.83569	-0.23562
H	3.60279	1.37354	-1.16113
H	3.75501	2.80251	-0.11978
H	3.55955	1.20369	0.60485
C	1.42909	2.32508	2.33746
H	2.40466	1.83692	2.44306
H	1.53038	3.35433	2.70652
H	0.72449	1.79218	2.98874
C	-1.47946	3.10620	1.33485
H	-1.37772	2.70605	2.34858
H	-1.49770	4.20161	1.40295
H	-2.45058	2.77614	0.94992
C	-1.55246	2.68047	-1.85119
H	-2.48375	2.75389	-1.28098
H	-1.44918	3.59126	-2.45460
H	-1.65045	1.82729	-2.53261
C	1.36707	2.00342	-2.83509
H	1.71793	2.95145	-3.26635
H	2.16422	1.26153	-2.94118
H	0.52421	1.65538	-3.44192
C	-1.26299	-0.03639	1.39915

Frequencies

-399.4252	27.6311	31.7733
38.1497	42.5626	61.5166
77.4072	86.1548	94.3776
99.4596	109.8690	117.1312
126.3129	138.9246	143.5690
149.5409	154.2503	158.6342
170.7837	178.3688	181.2054
185.1629	201.1648	208.8435
217.7116	221.7661	227.7859
240.6958	248.2080	252.7326
260.4435	269.2379	278.6510
285.6565	289.0252	297.9145
310.3686	320.5910	326.7993
328.2518	340.7373	352.3729
355.6479	364.7168	380.8239
403.3070	415.3351	417.0294
431.2185	445.3394	446.9142
463.3366	505.7224	533.3723
540.3854	552.8217	566.0848
568.5601	582.6274	591.9156
599.0973	603.0182	604.7907
609.9265	659.2442	680.3388
709.2735	751.9906	755.8273
758.7497	798.2419	808.1049
817.2531	820.8482	862.2235
877.4565	886.5397	902.0935
948.2396	949.7083	963.7713
964.7761	980.8230	1006.3089
1016.4167	1035.6933	1039.2385
1040.0495	1041.6610	1044.3382
1048.6639	1051.1855	1088.3202
1096.3913	1098.0979	1117.0436
1120.3504	1122.5599	1181.0294
1183.0749	1185.7392	1190.3533
1203.3427	1210.7850	1264.2674
1277.7341	1326.8791	1333.7740
1377.6532	1382.1924	1386.1727
1390.2893	1393.9269	1397.1561
1399.6825	1402.7189	1416.0637
1423.6667	1439.2257	1441.6669
1450.8937	1452.8304	1456.2267
1458.8991	1459.3182	1461.8811
1462.8914	1463.4579	1464.1178
1465.8353	1472.1540	1479.8848
1481.4953	1484.3379	1487.7849
1497.1382	1502.9565	1505.8729

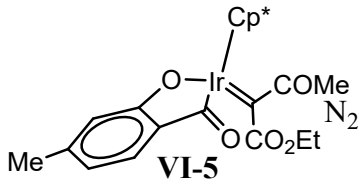
O	-1.35448	-0.51443	-1.22731	1509.9733	1513.0052	1521.5941
O	-1.05234	0.03988	2.60300	1548.8192	1610.7603	1665.1269
O	2.84990	-0.98194	-1.54279	1732.0787	1837.0991	1878.5274
C	4.83308	-1.49718	0.17257	2265.2469	3027.6047	3028.5516
H	5.39079	-1.24056	1.07828	3032.9187	3035.1250	3037.7533
H	4.99939	-0.72197	-0.58307	3038.9526	3045.8888	3051.0516
O	3.45011	-1.46333	0.57746	3070.4533	3103.5769	3105.4717
C	5.19709	-2.86277	-0.35353	3108.6871	3111.1159	3117.9618
H	4.62296	-3.08936	-1.25724	3118.7922	3128.3801	3130.1982
H	6.26158	-2.89785	-0.60728	3136.2384	3138.7956	3143.3730
H	4.99738	-3.63547	0.39577	3144.0913	3145.7519	3149.4833
C	-0.56546	-3.25648	0.35076	3156.9284	3159.6003	3170.7946
H	-1.21670	-3.83894	-0.30491	3178.3487	3184.9560	3193.5006
H	-0.00839	-3.95260	0.99155			
H	-1.17406	-2.61515	0.99526			
C	-6.07410	-1.77121	-1.20757			
H	-6.45104	-2.70048	-0.76238			
H	-6.87546	-1.02780	-1.11111			
H	-5.90601	-1.95041	-2.27408			
H	5.61941	-3.81507	0.17085			
H	4.16818	-4.18592	-0.79370			
C	4.85253	-1.30197	1.00761			
H	4.29807	-0.64996	1.69040			
H	5.72189	-1.70800	1.54036			
H	5.22384	-0.68669	0.17760			
C	3.41016	-3.23612	1.68155			
H	2.77452	-4.06258	1.33680			
H	4.23075	-3.66688	2.26927			
H	2.81677	-2.59242	2.34100			
H	2.80430	5.00118	-1.71678			
C	4.46624	2.90980	-2.17874			
H	4.90108	1.91359	-2.30392			
H	4.64265	3.47851	-3.10023			
H	5.01417	3.42473	-1.37997			

Statistical Thermodynamic Analysis

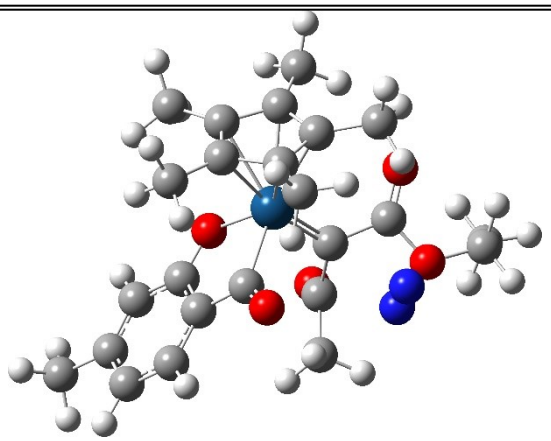
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.486816 Electronic Energy = -1521.39198819
Internal Energy (E)= -1520.87092719 Enthalpy (H)= -1520.86998319
Gibbs Free Energy (G)=-1520.96864219 Gibbs Free Energy of Solvation=-1521.00824618

St.Pt.	General Structure	Ball & Stick model

VI-5



VI-5



Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.76420	2.48520	0.57324
C	0.53295	2.19565	1.13629
C	1.48799	2.15225	0.05004
C	0.77599	2.40133	-1.17307
C	-0.60760	2.58624	-0.84073
C	-2.48870	-0.75950	0.76453
Ir	0.02415	0.42426	-0.12845
C	-2.56247	-0.69456	-0.63815
C	-3.77302	-1.03864	-1.26980
C	-3.58866	-1.17935	1.52590
C	-4.86303	-1.44343	-0.51461
C	-4.76664	-1.51322	0.89310
H	-3.48492	-1.22599	2.60811
H	-5.63470	-1.83035	1.46905
H	-3.82964	-0.99199	-2.35583
C	1.16958	-1.06852	-0.38395
C	2.61558	-0.86538	-0.72030
C	0.85466	-2.52838	-0.57042
O	1.57382	-3.15508	-1.33391
N	1.88191	-1.56407	2.73429
N	2.45719	-0.68278	3.07127
C	2.96868	2.10673	0.21206
H	3.45856	1.75433	-0.70023
H	3.34898	3.11062	0.44204
H	3.26743	1.44543	1.03501
C	0.85318	2.17049	2.59028
H	1.89337	1.88133	2.76753
H	0.70112	3.16698	3.02549
H	0.21785	1.45846	3.12726
C	-2.01305	2.70171	1.35885
H	-1.98395	2.14580	2.30190
H	-2.14300	3.76481	1.60019
H	-2.90272	2.37068	0.81163
C	-1.70067	2.77754	-1.83248
H	-2.68410	2.62504	-1.37718
H	-1.67342	3.78877	-2.25701
H	-1.60859	2.05785	-2.65331
C	1.37032	2.49070	-2.53456
H	1.85132	3.46662	-2.68688

Frequencies

21.0129	25.8839	38.2618
42.1515	54.0859	64.5381
73.8957	79.4173	87.0265
89.6490	105.8758	116.8720
121.5339	129.6169	136.0038
137.3059	141.7531	142.2183
147.4749	155.0354	163.0427
165.4633	169.6490	178.0319
192.8873	202.8960	210.6280
217.2904	218.4419	232.2728
245.1003	248.7760	261.8581
264.9881	283.9128	287.8479
294.9027	308.2349	312.8962
315.2886	326.1768	338.4368
353.9514	358.2029	364.6696
369.8104	379.2591	400.1890
424.2271	445.0398	453.0980
457.2953	490.2167	530.5416
540.5753	553.0690	563.4453
574.5322	589.9325	592.6214
601.4836	602.5351	605.2868
641.8227	671.7768	679.5196
738.7655	750.6555	752.5934
754.4619	806.7974	812.9972
818.6579	819.7722	863.5015
867.5898	890.3840	957.1210
959.3447	960.2637	967.5484
973.1920	1012.4081	1018.3724
1021.1454	1032.7389	1038.0354
1042.1422	1042.4177	1045.2792
1046.7344	1050.8291	1091.3890
1095.8635	1113.6893	1118.0777
1126.5930	1128.4993	1179.9280
1183.5203	1187.1771	1189.3479
1214.3496	1246.3029	1264.8945
1290.2768	1315.3738	1324.0767
1380.7035	1384.5608	1387.0442
1390.5296	1395.0411	1396.3098
1397.9496	1401.2387	1404.3870
1420.1655	1434.4572	1439.7643
1444.0992	1448.1838	1451.5235
1455.6274	1458.9906	1461.3054
1462.5973	1465.3299	1468.4446
1469.3705	1470.8951	1473.2569

H	2.12097	1.70941	-2.68571	1478.9613	1485.9067	1493.7732
H	0.60443	2.37369	-3.30767	1501.8916	1504.3426	1506.0927
C	-1.19998	-0.38632	1.34303	1512.3274	1513.6483	1522.5010
O	-1.50064	-0.33949	-1.32443	1534.2978	1620.7331	1665.8470
O	-0.92790	-0.43138	2.52292	1778.6696	1798.1240	1821.7748
O	3.01795	-0.30473	-1.71674	2461.7378	3034.7448	3035.4817
C	4.81756	-1.42226	-0.07661	3036.1987	3038.3240	3041.0197
H	5.30390	-1.49728	0.90100	3042.5828	3054.8138	3056.6142
H	5.11066	-0.47700	-0.54773	3066.2759	3108.7182	3112.1853
O	3.41084	-1.38372	0.22292	3114.9232	3118.3872	3123.3532
C	5.12706	-2.60553	-0.96043	3124.0691	3125.1673	3137.8355
H	4.62868	-2.49992	-1.92887	3140.5889	3144.9430	3145.9721
H	6.20630	-2.68418	-1.12878	3146.0539	3158.5960	3161.7905
H	4.77588	-3.53254	-0.49614	3163.4620	3166.3812	3168.5245
C	-0.28331	-3.18090	0.14719	3169.3471	3187.2120	3195.0086
H	-1.23609	-2.87769	-0.30133			
H	-0.17659	-4.26377	0.05192			
H	-0.31225	-2.89292	1.20395			
C	-6.15332	-1.81732	-1.17866			
H	-6.42588	-2.85515	-0.95047			
H	-6.97776	-1.18840	-0.82048			
H	-6.09546	-1.71435	-2.26649			
H	5.61941	-3.81507	0.17085			
H	4.16818	-4.18592	-0.79370			
C	4.85253	-1.30197	1.00761			
H	4.29807	-0.64996	1.69040			
H	5.72189	-1.70800	1.54036			
H	5.22384	-0.68669	0.17760			
C	3.41016	-3.23612	1.68155			
H	2.77452	-4.06258	1.33680			
H	4.23075	-3.66688	2.26927			
H	2.81677	-2.59242	2.34100			
H	2.80430	5.00118	-1.71678			
C	4.46624	2.90980	-2.17874			
H	4.90108	1.91359	-2.30392			
H	4.64265	3.47851	-3.10023			
H	5.01417	3.42473	-1.37997			

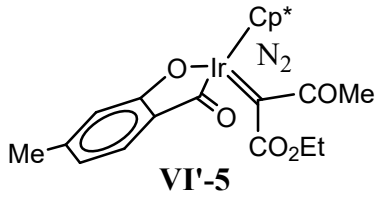
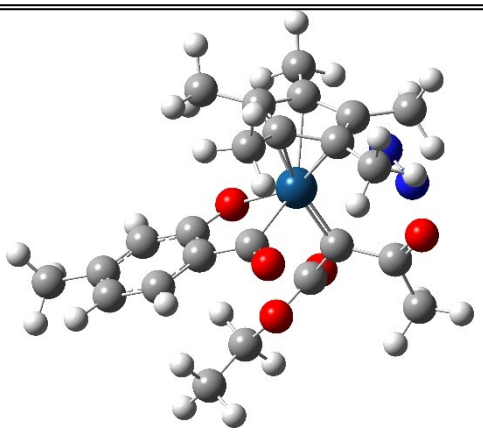
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm

Zero-point correction= 0.486584 Electronic Energy = -1521.44291333

Internal Energy (E)= -1520.92034233 Enthalpy (H)= -1520.91939833

Gibbs Free Energy (G)=-1521.02332833 Gibbs Free Energy of Solvation=-1521.05766464

St.Pt.	General Structure	Ball & Stick model
VI'-5	 **VI'-5**	

Cartesian co-ordinate

Atoms	X	Y	Z
C	1.31031	-2.50515	-0.54444
C	2.33060	-1.53819	-0.90866
C	2.81365	-0.94226	0.30515
C	2.00912	-1.45372	1.39405
C	1.10653	-2.43796	0.85519
C	-2.12268	-0.80929	-0.72942
Ir	0.67205	-0.31078	-0.00246
C	-2.12774	-0.41808	0.62467
C	-3.34830	-0.46563	1.33061
C	-3.30425	-1.21296	-1.37035
C	-4.51009	-0.88218	0.70165
C	-4.48538	-1.25774	-0.66141
H	-3.25658	-1.48950	-2.42164
H	-5.40736	-1.58624	-1.13867
H	-3.35331	-0.16573	2.37754
C	0.61793	1.53532	-0.44976
C	1.65215	2.28276	-1.22861
C	-0.49810	2.36969	0.08472
C	-2.77953	2.89754	-0.02441
H	-2.92293	2.50070	0.99004
H	-2.56339	3.96899	0.06801
C	-3.95633	2.61629	-0.91887
H	-4.85838	3.08724	-0.51448
H	-3.78480	3.01063	-1.92593
H	-4.13303	1.53761	-0.99767
O	-1.63797	2.23800	-0.59872
O	-0.35537	3.10483	1.03837
C	3.99997	-0.05531	0.43318
H	4.08810	0.35494	1.44388
H	4.91486	-0.62520	0.22490
H	3.95070	0.77403	-0.27881
C	2.89170	-1.37625	-2.27752
H	3.52966	-0.49257	-2.33477
H	3.47562	-2.26111	-2.56563
H	2.08532	-1.24521	-3.00839
C	0.65632	-3.43764	-1.50022

Frequencies

23.7094	30.5663	34.0542
42.7894	55.1920	65.1935
68.5019	75.2929	76.8280
94.3638	99.8307	103.7179
105.5377	110.6675	113.5325
120.8048	129.3387	134.1688
142.3686	155.0652	158.8561
167.5950	173.4084	184.8788
187.4820	199.4641	207.0766
211.0731	213.0780	223.3395
232.6495	233.9713	238.9479
260.2052	265.7945	272.5539
275.5784	281.9013	287.9952
292.6622	305.1512	316.2683
326.1591	337.3829	357.5120
366.8546	377.3974	393.3983
405.7405	411.7245	440.5346
452.9183	477.4601	532.6405
539.0505	551.7264	557.6585
579.6703	584.2231	588.3870
597.8520	600.4696	604.0821
627.9984	662.8089	676.0621
735.6888	748.4205	753.2031
799.1626	800.4556	807.3053
809.6015	819.8897	849.7978
871.1438	890.5611	934.3486
951.0619	957.2736	963.1616
965.9022	1016.2651	1022.5289
1024.1808	1031.7974	1032.8549
1037.8968	1041.2652	1042.8851
1055.7519	1060.1888	1085.2321
1090.4662	1107.0050	1109.9636
1125.2213	1140.9131	1172.2311
1179.5495	1184.6622	1186.2967
1213.7279	1233.2304	1262.2448
1274.8970	1316.2939	1325.6854
1369.3423	1374.5230	1378.5646
1383.8074	1387.8007	1394.0924
1399.2577	1400.3630	1409.0805
1421.3878	1431.4281	1438.8681

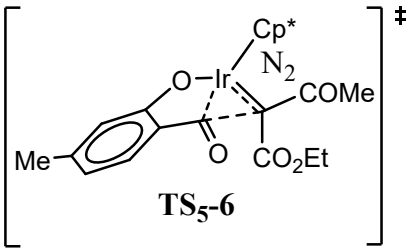
H	0.49440	-2.95995	-2.47092	1443.4874	1444.9710	1450.6315
H	1.29420	-4.31790	-1.65409	1451.0718	1455.6076	1456.9717
H	-0.31558	-3.78428	-1.13261	1457.6659	1458.6872	1462.3713
C	0.09454	-3.17930	1.65810	1462.6534	1467.9440	1471.6460
H	-0.59115	-3.74472	1.01985	1474.6681	1476.9696	1481.7800
H	0.57713	-3.88484	2.34628	1493.9413	1502.0940	1502.3792
H	-0.50621	-2.48473	2.25766	1509.8161	1512.2483	1513.4820
C	2.13709	-1.13747	2.84349	1552.2843	1616.8380	1666.1436
H	2.70215	-1.91847	3.37030	1772.6612	1822.8114	1828.4217
H	2.64577	-0.18344	3.00767	2466.7888	3033.2636	3033.8370
H	1.14977	-1.06356	3.31311	3036.4662	3036.8207	3039.0348
C	-0.84487	-0.71669	-1.41699	3040.0623	3044.4429	3044.9269
O	-1.02369	-0.00936	1.19761	3047.9965	3098.7363	3106.4335
O	-0.62314	-0.89680	-2.58738	3109.6126	3116.9167	3119.2895
N	2.64284	2.98681	1.80727	3120.1335	3121.5280	3131.1570
N	2.48359	2.43050	2.74862	3141.1934	3141.6651	3142.0371
C	1.43888	3.75775	-1.44958	3143.7855	3152.6342	3165.2522
H	1.42003	4.29256	-0.49387	3169.3032	3174.3723	3175.5355
H	2.23813	4.14618	-2.08351	3177.9662	3178.8958	3194.8944
H	0.46835	3.93314	-1.93177			
O	2.62147	1.71594	-1.71165			
C	-5.80731	-0.93009	1.45031			
H	-6.26920	-1.92220	1.37639			
H	-5.67363	-0.69446	2.51056			
H	-6.52757	-0.21477	1.03332			
H	5.61941	-3.81507	0.17085			
H	4.16818	-4.18592	-0.79370			
C	4.85253	-1.30197	1.00761			
H	4.29807	-0.64996	1.69040			
H	5.72189	-1.70800	1.54036			
H	5.22384	-0.68669	0.17760			
C	3.41016	-3.23612	1.68155			
H	2.77452	-4.06258	1.33680			
H	4.23075	-3.66688	2.26927			
H	2.81677	-2.59242	2.34100			
H	2.80430	5.00118	-1.71678			
C	4.46624	2.90980	-2.17874			
H	4.90108	1.91359	-2.30392			
H	4.64265	3.47851	-3.10023			
H	5.01417	3.42473	-1.37997			

Statistical Thermodynamic Analysis

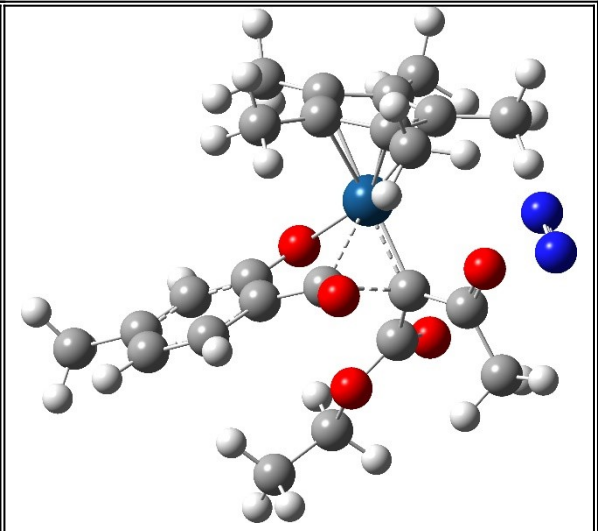
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.484692 Electronic Energy = -1521.44764523
Internal Energy (E)= -1520.92622623 Enthalpy (H)= -1520.92528223
Gibbs Free Energy (G)=-1521.03108323 Gibbs Free Energy of Solvation=-1521.06525554

St.Pt.	General Structure	Ball & Stick model

TS_5-6



TS_5-6



Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.39676	-2.39035	0.55440
C	-2.28040	-1.36786	1.11230
C	-2.94198	-0.72122	0.02763
C	-2.42859	-1.30727	-1.20610
C	-1.52900	-2.37754	-0.85727
C	1.99307	-0.55194	0.88525
Ir	-0.78669	-0.34109	-0.15418
C	2.03852	-0.66055	-0.52771
C	3.24742	-1.09014	-1.11629
C	3.10491	-0.90016	1.66934
C	4.34262	-1.42659	-0.33764
C	4.26578	-1.33699	1.07060
H	3.02418	-0.80535	2.75032
H	5.13147	-1.61105	1.67125
H	3.29098	-1.15702	-2.20230
C	-0.19111	1.42837	0.40632
C	-0.93317	2.24450	1.40885
C	0.78878	2.18643	-0.43995
C	3.03200	2.73107	-0.86805
H	2.91733	2.25003	-1.84907
H	2.83554	3.80198	-1.00280
C	4.38040	2.45827	-0.25698
H	5.17332	2.86998	-0.88979
H	4.45995	2.91365	0.73566
H	4.54128	1.37839	-0.15403
O	2.04617	2.18104	0.01847
O	0.44133	2.81093	-1.41848
C	-4.00897	0.30834	0.14916
H	-4.20811	0.79525	-0.81038
H	-4.94664	-0.15054	0.48909
H	-3.71917	1.07640	0.87553
C	-2.53010	-1.16687	2.56558
H	-3.23834	-0.35342	2.73495
H	-2.93697	-2.08964	3.00039
H	-1.60998	-0.90476	3.09968
C	-0.53165	-3.28917	1.36769
H	-0.25732	-2.81563	2.31565

Frequencies

-253.1598	28.5803	34.7098
40.6851	51.7692	59.5493
61.8677	77.2662	83.3825
85.0664	92.6710	96.8808
100.2211	113.6564	120.1490
127.9704	135.3375	140.3340
146.5829	154.0166	166.8223
173.1167	177.9833	190.7277
200.6125	202.2789	205.4325
206.8543	218.9806	224.7763
230.7723	232.4510	263.8238
272.1725	279.0103	284.8877
295.5573	301.3043	308.7020
317.2000	319.1232	331.0236
332.6960	354.6856	365.1906
382.4251	394.5588	398.2048
414.1588	420.2004	441.2047
446.5385	473.5297	523.9531
537.8029	543.4489	545.5436
551.8791	577.5295	581.0538
590.6835	600.7160	607.4747
610.6207	658.6068	679.5478
723.5941	744.1182	756.3182
805.4373	810.8836	811.9835
816.3328	819.6462	828.4285
866.2533	891.4942	928.2920
960.8616	961.8459	968.3192
971.0625	1018.5477	1019.7239
1029.1777	1034.8589	1038.0133
1040.6559	1041.0274	1046.5513
1048.0436	1050.8892	1091.5707
1096.5119	1108.7083	1113.5196
1129.5430	1140.4666	1180.3376
1183.2188	1183.6144	1189.7632
1212.6653	1238.8421	1261.4255
1299.3775	1314.3828	1326.5350
1373.0375	1376.2722	1380.1520
1382.6703	1395.4131	1396.2598
1401.7286	1405.0051	1405.5029
1426.9996	1434.5349	1440.9437
1442.7936	1447.6268	1452.2109

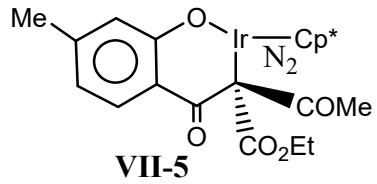
H	-1.05495	-4.22588	1.60102	1453.2118	1456.2604	1458.3585
H	0.39563	-3.54182	0.84257	1461.0959	1461.2639	1462.9551
C	-0.74345	-3.18602	-1.82943	1465.7718	1469.8943	1475.1556
H	0.13196	-3.64037	-1.35374	1476.1247	1482.5347	1497.3715
H	-1.35112	-3.99129	-2.26089	1498.8859	1508.4492	1514.8367
H	-0.37730	-2.55924	-2.65008	1516.9982	1527.0993	1535.3396
C	-2.85441	-0.94699	-2.58568	1554.4656	1604.0946	1669.2671
H	-3.74692	-1.51537	-2.88134	1781.4352	1825.9768	1843.4145
H	-3.09112	0.11925	-2.66602	2463.4864	3031.4074	3035.6164
H	-2.06353	-1.16065	-3.31174	3036.1873	3037.7786	3039.3135
C	0.79312	-0.02343	1.50643	3039.8581	3042.1306	3044.0011
O	1.00743	-0.34956	-1.26705	3046.5537	3095.4556	3105.1149
O	0.52380	0.04607	2.67515	3117.3689	3120.5450	3121.4003
N	-2.55815	3.23213	-1.27379	3121.8610	3123.1730	3129.0549
N	-2.76682	2.66042	-2.19601	3139.2399	3140.1812	3142.8817
C	-0.51824	3.68132	1.59212	3143.1644	3145.7872	3153.9954
H	-0.58048	4.23215	0.64671	3164.1564	3166.8960	3170.8947
H	-1.15901	4.15190	2.34030	3175.4191	3183.3256	3193.4903
H	0.52787	3.72342	1.92195			
O	-1.83132	1.75835	2.07700			
C	5.62561	-1.86506	-0.97500			
H	5.98579	-2.80510	-0.53990			
H	5.51633	-2.00613	-2.05465			
H	6.41402	-1.11866	-0.81176			
H	5.61941	-3.81507	0.17085			
H	4.16818	-4.18592	-0.79370			
C	4.85253	-1.30197	1.00761			
H	4.29807	-0.64996	1.69040			
H	5.72189	-1.70800	1.54036			
H	5.22384	-0.68669	0.17760			
C	3.41016	-3.23612	1.68155			
H	2.77452	-4.06258	1.33680			
H	4.23075	-3.66688	2.26927			
H	2.81677	-2.59242	2.34100			
H	2.80430	5.00118	-1.71678			
C	4.46624	2.90980	-2.17874			
H	4.90108	1.91359	-2.30392			
H	4.64265	3.47851	-3.10023			
H	5.01417	3.42473	-1.37997			

Statistical Thermodynamic Analysis

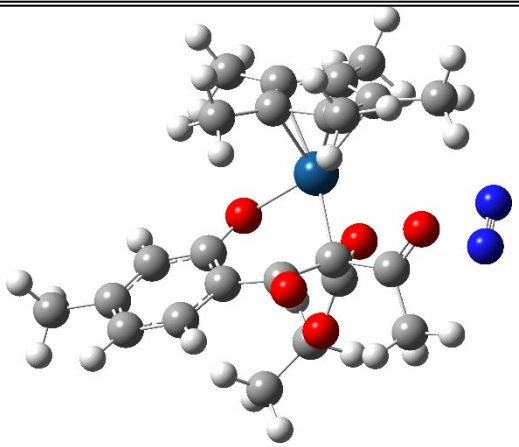
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.485524 Electronic Energy = -1521.43039227
Internal Energy (E)= -1520.90933327 Enthalpy (H)= -1520.90838927
Gibbs Free Energy (G)=-1521.01070427 Gibbs Free Energy of Solvation=-1521.04896899

St.Pt.	General Structure	Ball & Stick model

VII-5



VII-5



Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.10051	-2.27035	0.77243
C	-2.07040	-1.32518	1.29019
C	-2.90302	-0.91397	0.19725
C	-2.49695	-1.68030	-0.97869
C	-1.42637	-2.53744	-0.62505
C	2.31433	0.09701	1.03285
Ir	-0.79815	-0.43780	-0.21490
C	2.25080	-0.58167	-0.21010
C	3.43339	-1.17860	-0.69772
C	3.51688	0.10140	1.75360
C	4.62361	-1.14128	0.01298
C	4.66073	-0.49269	1.25972
H	3.51705	0.61148	2.71500
H	5.59095	-0.46265	1.82502
H	3.37411	-1.69297	-1.65698
C	0.06981	1.28024	0.70326
C	-0.87298	2.23734	1.44024
C	0.39061	1.75775	-0.66464
C	2.04579	2.42500	-2.21692
H	1.70993	1.51573	-2.72790
H	1.61911	3.29292	-2.73304
C	3.54438	2.49114	-2.08783
H	4.00802	2.50694	-3.07929
H	3.85447	3.39056	-1.54659
H	3.91234	1.61263	-1.54332
O	1.51924	2.39470	-0.86902
O	-0.41019	1.45163	-1.56631
C	-4.08793	-0.01698	0.28201
H	-4.38245	0.34936	-0.70679
H	-4.94809	-0.55222	0.70636
H	-3.87158	0.85026	0.91259
C	-2.15739	-0.90540	2.71574
H	-2.88698	-0.10505	2.85055
H	-2.44463	-1.76358	3.33754
H	-1.19447	-0.52650	3.08060
C	-0.05631	-2.97007	1.56868
H	0.32763	-2.32402	2.36576
H	-0.46393	-3.87861	2.03259
H	0.79158	-3.26332	0.94033

Frequencies

28.5298	48.5699	54.0207
64.0718	65.8146	78.9188
82.9487	85.3313	99.6278
100.4563	103.9483	117.1439
119.7648	126.8261	131.6504
137.9863	143.8175	152.5534
155.9766	168.4347	179.2814
180.4276	181.5574	183.7797
202.3213	207.3922	212.9108
219.0616	226.6682	237.4760
246.9108	253.7932	261.3473
268.8582	276.6596	284.6621
296.8773	302.0141	306.5116
311.0775	316.8507	326.6996
356.4300	357.6302	359.0409
391.4502	404.4530	421.1466
427.3823	456.6521	474.0268
491.1444	522.1726	537.7000
539.2412	549.0030	555.2830
564.2355	588.9360	594.6545
597.9185	607.5962	610.7040
651.0006	670.5321	726.3409
744.9122	753.8367	788.6898
802.0462	806.3148	814.8559
824.0998	847.5772	856.2184
866.2846	897.9578	950.9320
958.6740	970.6668	972.4282
995.3763	1014.5507	1018.2581
1036.9143	1039.0447	1041.1464
1042.9164	1044.5450	1050.7442
1056.6569	1081.8523	1091.7802
1095.2452	1112.8097	1128.7326
1134.4547	1161.4837	1179.3618
1182.2131	1186.5222	1189.0279
1209.7783	1250.8754	1288.1575
1295.0856	1327.8633	1356.3129
1362.6151	1375.2381	1378.7915
1383.6368	1392.7462	1395.6364
1398.5370	1399.7575	1407.1249
1429.1645	1435.6634	1438.4491
1444.1985	1446.7804	1449.8034
1453.4848	1454.2779	1455.2911
1458.5097	1459.0328	1460.0750

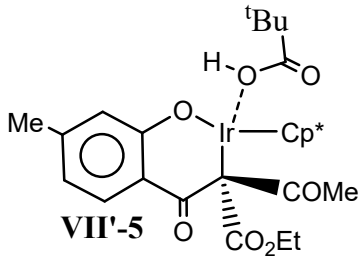
C	-0.62048	-3.42395	-1.50736	1467.5563	1471.5912	1473.0867
H	0.43000	-3.10056	-1.50604	1476.4594	1482.8269	1487.5599
H	-0.65956	-4.46506	-1.16335	1493.4982	1495.4597	1500.8259
H	-0.97546	-3.39621	-2.54170	1501.7656	1518.7107	1521.2597
C	-3.09741	-1.50766	-2.32980	1555.1126	1606.8454	1668.1891
H	-4.07288	-2.00710	-2.39160	1678.4350	1731.8418	1845.0893
H	-3.25391	-0.44565	-2.55302	2470.4430	3026.9101	3032.6074
H	-2.45286	-1.91762	-3.11271	3033.4065	3037.8081	3038.0272
C	1.17216	0.83024	1.60583	3039.7100	3043.2467	3053.3252
O	1.15962	-0.69824	-0.93914	3067.1870	3102.5441	3105.6261
O	1.07753	1.04981	2.81404	3114.2588	3115.4209	3118.3361
N	-2.57532	3.33238	-0.94418	3124.8516	3130.9073	3132.9431
N	-3.28462	2.67534	-1.47876	3136.0337	3140.3514	3142.0267
C	-0.30021	3.59974	1.71701	3147.2929	3148.1305	3154.6774
H	-0.16815	4.13689	0.76801	3156.8037	3169.4767	3171.1153
H	-0.98235	4.16611	2.35499	3174.9735	3179.6887	3197.7945
H	0.68217	3.51179	2.19109			
O	-2.00530	1.94788	1.75860			
C	5.85561	-1.80716	-0.52183			
H	6.12078	-2.68697	0.07841			
H	5.72131	-2.13810	-1.55679			
H	6.71855	-1.13114	-0.48848			
H	5.61941	-3.81507	0.17085			
H	4.16818	-4.18592	-0.79370			
C	4.85253	-1.30197	1.00761			
H	4.29807	-0.64996	1.69040			
H	5.72189	-1.70800	1.54036			
H	5.22384	-0.68669	0.17760			
C	3.41016	-3.23612	1.68155			
H	2.77452	-4.06258	1.33680			
H	4.23075	-3.66688	2.26927			
H	2.81677	-2.59242	2.34100			
H	2.80430	5.00118	-1.71678			
C	4.46624	2.90980	-2.17874			
H	4.90108	1.91359	-2.30392			
H	4.64265	3.47851	-3.10023			
H	5.01417	3.42473	-1.37997			

Statistical Thermodynamic Analysis

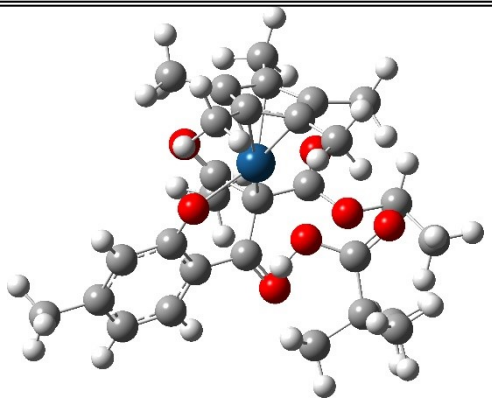
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.487601 Electronic Energy = -1521.46765674
Internal Energy (E)= -1520.94468274 Enthalpy (H)= -1520.94373874
Gibbs Free Energy (G)=-1521.04447474 Gibbs Free Energy of Solvation=-1521.08319338

St.Pt.	General Structure	Ball & Stick model

VII'-5



VII'-5



Cartesian co-ordinate

Atoms	X	Y	Z
C	2.58138	-0.94036	-1.97070
C	2.11509	0.40321	-2.07991
C	2.50621	1.13948	-0.87976
C	3.16323	0.22830	-0.00144
C	3.16034	-1.07715	-0.65503
O	-1.47439	0.85528	-1.43173
C	-1.81707	2.15385	-1.35772
O	-0.97206	2.99693	-1.55804
C	-3.28059	2.50229	-1.08186
C	-1.32244	-2.24632	-0.18963
H	-2.20506	0.27550	-1.16458
C	1.37300	1.01066	-3.21377
H	0.69538	1.79364	-2.85485
H	2.07587	1.46180	-3.92743
H	0.77384	0.26510	-3.74596
C	2.32400	2.60446	-0.71733
H	2.93355	3.13768	-1.45917
H	1.27596	2.89202	-0.86659
H	2.64226	2.93600	0.27500
C	3.72806	-2.31842	-0.06957
H	3.48308	-3.19242	-0.68048
H	4.82114	-2.24087	0.00165
H	3.32318	-2.47717	0.93615
C	2.35896	-2.05714	-2.92921
H	1.75365	-1.73281	-3.78065
H	3.30867	-2.44358	-3.31896
H	1.82332	-2.88099	-2.44219
C	3.79435	0.50639	1.31571
H	4.88357	0.59148	1.20668
H	3.41447	1.42813	1.76568
H	3.57430	-0.30028	2.02329
Ir	1.13947	-0.48045	-0.33992
C	-3.78772	3.25324	-2.31715
H	-3.79695	2.60798	-3.20507
H	-4.81354	3.59997	-2.14131
H	-3.15635	4.12181	-2.52990
C	-4.16019	1.28361	-0.81479
H	-3.84721	0.75531	0.09613
H	-5.19448	1.61205	-0.65879
H	-4.18030	0.58661	-1.66533

Frequencies

14.7934	28.6661	32.7441
56.9114	61.3538	68.0985
77.5898	78.3598	79.4173
87.9339	88.6956	89.3541
99.3701	105.4989	112.1894
125.3565	127.7769	136.4404
139.8682	145.4004	148.4700
150.6560	156.2870	162.5539
168.0341	180.8143	190.8474
200.7305	205.5449	205.9752
218.6983	226.1198	231.2091
232.0568	238.7035	245.3296
250.6092	261.2302	275.5428
276.0696	283.1891	290.1774
291.9795	295.2212	305.0069
308.1747	312.5300	324.8224
343.4170	360.6063	368.9413
369.9658	386.7402	392.2298
403.3385	418.6155	423.8407
428.2273	448.9411	455.0842
459.2037	485.9905	518.1256
528.1103	533.1865	538.7240
542.2633	552.4033	571.5419
573.0335	574.5500	584.5903
594.6717	597.1934	604.9189
623.2100	658.8236	688.1061
722.8497	750.2143	765.0839
768.5567	775.5138	785.6036
797.2275	811.4699	813.5794
813.8814	867.1209	875.6926
885.2680	907.0282	916.6056
947.8070	953.4510	962.0546
967.1965	968.8209	970.8692
977.5737	991.5476	1009.9456
1023.0072	1030.1331	1032.4164
1036.7157	1037.0705	1039.1017
1043.5735	1045.0641	1047.2966
1053.8880	1089.5733	1095.0634
1102.3109	1113.0065	1122.3716
1143.3710	1156.0809	1170.6815
1183.1528	1186.9455	1189.8287
1190.2586	1193.0136	1244.4906
1247.4887	1255.0844	1270.2059
1275.8725	1276.6911	1297.7450
1322.7118	1364.1598	1369.0399

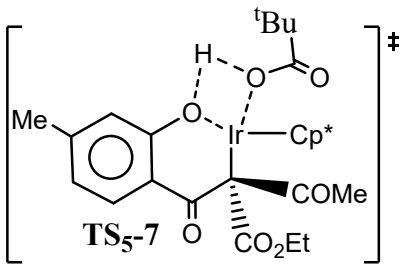
C	-3.30523	3.42642	0.13596	1375.1000	1375.6357	1377.0179
H	-2.87953	2.92055	1.01210	1379.0768	1383.4044	1390.1594
H	-2.72857	4.33517	-0.06646	1390.5553	1397.4026	1398.8075
H	-4.34081	3.71030	0.36107	1401.8672	1409.0010	1422.3496
O	-0.16749	-1.96333	-0.75588	1431.0985	1432.1223	1434.6296
C	-1.98656	-1.42685	0.75494	1443.3091	1446.3154	1448.6189
C	-3.27054	-1.80063	1.19553	1449.2597	1453.0931	1455.3274
C	-1.97679	-3.41845	-0.62754	1457.7379	1458.2401	1461.5249
C	-3.88727	-2.95183	0.75728	1463.6353	1466.4087	1466.7763
C	-3.23063	-3.78231	-0.17013	1467.8115	1471.8042	1474.7894
C	-1.41134	-0.19357	1.33831	1478.1428	1480.5396	1483.6937
O	-2.15718	0.68530	1.76243	1493.7184	1496.9937	1498.9829
H	-1.45539	-4.02912	-1.36317	1500.7077	1510.2491	1519.6034
H	-4.87324	-3.22877	1.12706	1521.7727	1532.8768	1554.9511
H	-3.75643	-1.14513	1.91661	1602.8035	1674.5615	1743.7209
C	0.08561	-0.12377	1.50278	1793.1231	1825.1566	1857.5503
C	0.53234	-1.22030	2.50398	3018.8463	3030.5429	3031.7600
C	0.55377	1.16539	2.10111	3035.1768	3036.7743	3037.2998
C	0.54566	3.50247	2.05528	3038.1186	3038.9453	3040.2804
H	1.64085	3.57682	1.98931	3042.0530	3045.4461	3055.1318
H	0.29972	3.48847	3.12359	3095.8785	3106.6357	3108.5862
C	-0.13767	4.62804	1.32576	3115.5933	3118.9437	3119.2024
H	0.27984	5.58882	1.64490	3123.7300	3124.0588	3124.5366
H	-0.01716	4.52752	0.24039	3129.0012	3132.5020	3134.9017
H	-1.21022	4.63431	1.54124	3140.0770	3141.8743	3143.0273
O	0.12654	2.26592	1.46248	3145.2260	3147.2613	3151.5768
O	1.29606	1.22088	3.06619	3151.9322	3157.3818	3158.9201
O	1.53002	-1.89384	2.34500	3160.3460	3176.2797	3176.9702
C	-0.33323	-1.39026	3.72343	3187.5506	3195.3033	3781.1051
H	0.20934	-1.95885	4.48155			
H	-0.64602	-0.41944	4.12073			
H	-1.24144	-1.94169	3.44682			
C	-3.88954	-5.03986	-0.64841			
H	-4.02335	-5.75130	0.17606			
H	-4.88769	-4.83512	-1.05455			
H	-3.30053	-5.53532	-1.42647			

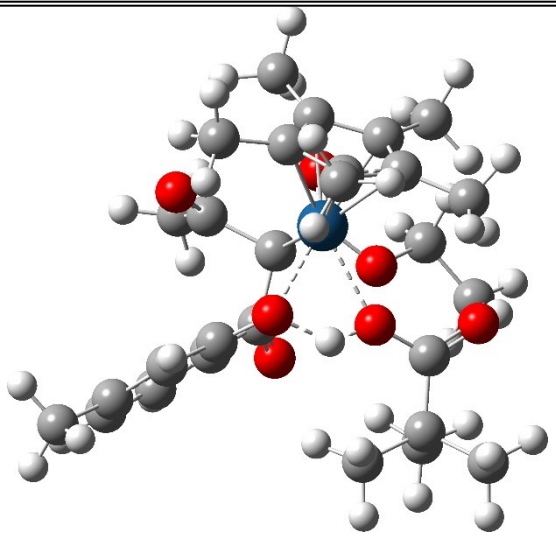
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.628829 Electronic Energy = -1758.83872554
Internal Energy (E)= -1758.16816154 Enthalpy (H)= -1758.16721854
Gibbs Free Energy (G)=-1758.28200254 Gibbs Free Energy of Solvation=-1758.33875626

St.Pt.	General Structure	Ball & Stick model

TS_5-7





Cartesian co-ordinate

Atoms	X	Y	Z
C	0.61491	-2.39855	-2.03105
C	1.87414	-1.82566	-1.72043
C	2.15043	-2.05600	-0.30472
C	1.07276	-2.85204	0.23153
C	0.07944	-2.98780	-0.80714
O	0.53943	1.20630	-1.13306
C	1.38163	2.23512	-1.24030
O	2.57840	2.05674	-1.17670
C	0.75216	3.61642	-1.40254
C	-2.51789	0.39847	-0.50816
H	-0.51783	1.05130	-1.36507
C	2.75504	-1.02574	-2.61246
H	3.00762	-0.06473	-2.14614
H	3.68908	-1.56757	-2.81019
H	2.27417	-0.81691	-3.57289
C	3.41128	-1.68752	0.39342
H	4.18806	-2.44631	0.22752
H	3.79052	-0.72712	0.02301
H	3.24638	-1.59514	1.47312
C	-1.22527	-3.69393	-0.70747
H	-1.95303	-3.25121	-1.39747
H	-1.11371	-4.75533	-0.96637
H	-1.63645	-3.60419	0.30156
C	-0.12283	-2.33685	-3.32242
H	0.40611	-1.72320	-4.05753
H	-0.25357	-3.33924	-3.74932
H	-1.11766	-1.89695	-3.17882
C	1.05539	-3.48476	1.57503
H	1.69876	-4.37465	1.55858
H	1.43490	-2.80167	2.34213
H	0.04668	-3.79081	1.85911
Ir	0.34808	-0.90725	-0.40280
C	1.42834	4.30473	-2.58835
H	1.18820	3.80292	-3.53458
H	1.08170	5.34300	-2.66052
H	2.51600	4.30638	-2.46647

Frequencies

-925.7234	28.8694	50.4500
53.5814	60.0424	65.1433
75.7700	84.2476	91.3872
95.6860	103.7571	114.5089
114.8663	119.3438	122.7087
135.4858	138.6767	144.7634
151.3937	157.0479	160.2763
162.4309	167.1926	176.1645
182.0748	188.4012	201.7188
206.3908	218.2032	219.7201
221.6773	230.0703	235.3295
239.6241	243.8610	248.2475
254.3487	263.1643	277.5080
287.9721	291.1700	300.9060
304.9892	306.5383	315.1485
338.6693	341.2844	342.7975
343.1223	357.6760	365.6888
369.1658	383.0388	384.4424
404.5761	410.6247	412.9439
422.0118	433.0412	436.3735
440.8122	460.6874	493.8056
524.0264	535.0335	538.3202
550.0865	551.2253	554.5512
572.8525	588.8062	595.8664
599.9311	603.6398	614.2824
634.6983	640.1085	678.3559
731.7968	746.4015	765.3060
774.3831	789.6637	809.7000
811.3801	815.1060	817.5016
833.0041	873.9442	880.0801
890.7981	908.3232	935.0039
945.2638	950.3502	953.3674
963.3435	963.6192	976.1060
985.4293	989.0210	1011.7946
1018.2956	1026.1321	1037.1021
1039.3695	1039.4818	1046.1454
1046.3045	1047.5738	1049.6655
1050.1929	1090.2150	1094.7972
1102.4963	1117.2166	1120.6996
1141.1774	1151.6061	1178.5886
1179.3968	1185.3854	1187.8116

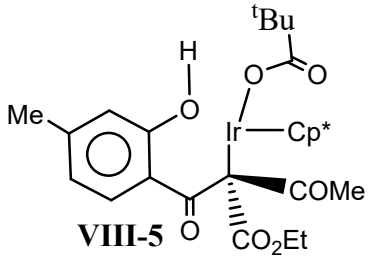
C	-0.75856	3.57400	-1.60448	1192.0474	1202.7812	1222.5239
H	-1.27505	3.17468	-0.72237	1236.2807	1251.5009	1268.1779
H	-1.13034	4.59356	-1.76225	1285.4457	1289.3854	1312.4326
H	-1.04533	2.98297	-2.48488	1319.0740	1344.3432	1368.7055
C	1.06921	4.37771	-0.10859	1371.5661	1376.3786	1380.7427
H	0.65212	3.86210	0.76700	1384.0126	1384.3157	1386.7739
H	2.15230	4.47548	0.02422	1395.5927	1400.0048	1403.7002
H	0.63068	5.38221	-0.16284	1406.4172	1414.3247	1421.2622
O	-1.44657	0.07621	-1.25410	1433.1342	1436.5834	1440.7000
C	-2.37108	1.05425	0.72554	1444.3265	1446.6092	1449.7027
C	-3.51018	1.52883	1.38286	1451.9348	1454.2201	1458.5361
C	-3.79750	0.16561	-1.01524	1460.2779	1462.4066	1463.3683
C	-4.77573	1.29729	0.86937	1465.0160	1465.5752	1467.9232
C	-4.93188	0.60179	-0.33582	1469.9739	1474.9644	1477.8921
C	-1.05116	1.23155	1.38250	1483.6391	1484.3831	1486.5429
O	-0.76784	2.29120	1.92000	1487.5935	1493.5552	1499.0227
H	-3.88263	-0.34605	-1.97371	1506.4478	1513.5823	1520.7364
H	-5.65693	1.64744	1.40461	1526.4740	1528.8359	1553.5857
H	-3.37570	2.06192	2.32270	1619.9678	1672.5226	1768.3371
C	-0.20225	-0.02535	1.51381	1779.7905	1827.2112	1830.0158
C	-1.08105	-0.98154	2.34488	2094.7379	3024.1046	3026.8665
C	1.10884	0.17845	2.20391	3028.0048	3033.8048	3033.9558
C	3.06779	1.45243	2.41345	3034.4559	3034.7492	3035.7265
H	3.70809	0.59683	2.16019	3042.6089	3047.6371	3056.1577
H	2.94992	1.45209	3.50400	3059.7933	3104.2048	3109.8884
C	3.63481	2.74771	1.89762	3110.7768	3110.8360	3111.3421
H	4.63155	2.91167	2.32102	3113.5705	3114.2298	3116.3459
H	3.71146	2.72634	0.80463	3116.7725	3128.8626	3135.5214
H	2.99730	3.59056	2.18568	3136.0822	3136.1845	3137.3665
O	1.77994	1.26445	1.81040	3140.8548	3144.3431	3145.5633
O	1.57293	-0.61250	3.01323	3146.2424	3147.8627	3154.1416
O	-1.62521	-1.96151	1.87854	3167.9762	3168.1472	3169.4278
C	-1.29851	-0.60475	3.78887	3175.1291	3184.8062	3192.0424
H	-2.24262	-1.03137	4.13631			
H	-0.47587	-1.02589	4.37660			
H	-1.28149	0.47970	3.94520			
C	-6.29740	0.37186	-0.91032			
H	-7.04493	0.22870	-0.12241			
H	-6.62186	1.23200	-1.51025			
H	-6.31691	-0.50676	-1.56367			

Statistical Thermodynamic Analysis

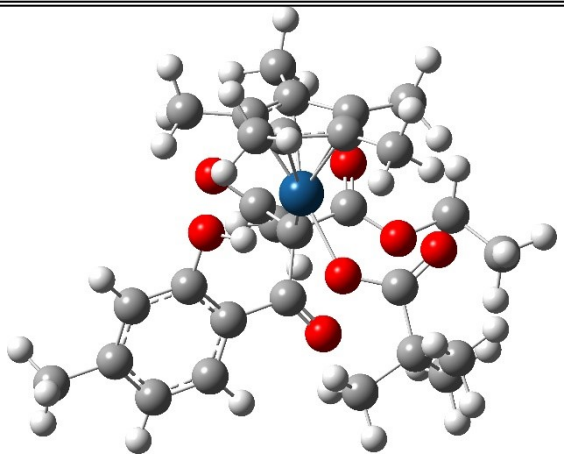
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.626036 Electronic Energy = -1758.82826313
Internal Energy (E)= -1758.16204213 Enthalpy (H)= -1758.16109913
Gibbs Free Energy (G)=-1758.26991013 Gibbs Free Energy of Solvation=-1758.31707414

St.Pt.	General Structure	Ball & Stick model

VIII-5



VIII-5



Cartesian co-ordinate

Atoms	X	Y	Z
C	0.56661	-2.56828	-1.78851
C	1.84040	-2.08060	-1.40762
C	1.93888	-2.17082	0.04729
C	0.74360	-2.84694	0.53385
C	-0.13002	-3.01510	-0.58408
O	0.64097	1.02720	-1.14126
C	1.75715	1.70364	-1.14851
O	2.84029	1.26857	-0.77913
C	1.61405	3.14397	-1.66222
C	-2.64653	0.61056	-0.73027
H	-0.98016	0.72935	-1.70333
C	2.88635	-1.51910	-2.30181
H	3.41737	-0.70026	-1.80963
H	3.60659	-2.30118	-2.57608
H	2.45223	-1.12050	-3.22504
C	3.14199	-1.80763	0.84124
H	3.91910	-2.57819	0.74935
H	3.54607	-0.85207	0.48285
H	2.88370	-1.70106	1.90051
C	-1.49040	-3.61606	-0.57394
H	-2.11077	-3.18391	-1.36732
H	-1.43340	-4.69942	-0.74482
H	-1.99703	-3.42604	0.37532
C	-0.02006	-2.59144	-3.15584
H	0.59452	-2.02747	-3.86366
H	-0.10762	-3.62035	-3.52813
H	-1.02285	-2.14888	-3.15652
C	0.51547	-3.32713	1.92220
H	1.05278	-4.27288	2.07258
H	0.87233	-2.60407	2.66418
H	-0.54769	-3.50050	2.11056
Ir	0.29306	-0.90036	-0.34674
C	2.62630	3.34224	-2.79003
H	2.38677	2.71221	-3.65752
H	2.62150	4.38829	-3.12305
H	3.63495	3.08645	-2.44981
C	0.20598	3.45813	-2.15701
H	-0.52852	3.36695	-1.34675
H	0.16898	4.49081	-2.52825

Frequencies

31.3061	39.1215	52.2474
67.0505	72.3162	76.7526
84.0498	87.5359	96.5939
99.2408	108.8966	119.8574
124.3065	136.5499	137.7274
138.8169	140.2781	147.4984
152.7858	157.4565	166.3557
168.7590	177.4897	185.6520
187.0613	191.8248	198.5018
209.6585	219.3955	225.7632
228.9221	233.8832	245.5891
252.0523	261.4774	267.4551
271.3829	282.8331	288.1737
299.1602	300.6669	309.7855
318.7189	322.1805	323.2403
331.8245	341.4365	357.4828
365.8861	369.7101	373.1758
381.8684	386.2329	390.0732
401.3023	410.7141	415.1874
432.4730	436.7330	446.7406
475.6102	478.1085	503.0092
532.3366	536.8663	543.8798
554.4759	556.9764	564.9765
577.8096	587.3694	590.4118
601.5230	606.0095	628.8466
631.8170	670.7007	718.0023
740.6303	757.7581	787.9745
793.7933	806.4469	809.2498
812.8970	816.0766	833.6424
834.9614	876.5751	884.6953
892.9338	910.5675	924.2249
947.7477	953.4176	956.6501
963.6084	968.8968	972.3617
985.9740	990.6274	1012.5720
1013.2497	1020.1902	1025.6921
1037.4637	1039.9030	1045.2931
1046.0293	1057.6368	1060.0984
1062.1150	1091.9512	1099.2459
1106.6949	1120.3004	1121.0474
1143.1902	1155.4484	1168.2691
1170.9879	1188.7001	1193.2028
1199.9016	1233.5290	1239.1280
1245.5747	1267.0100	1275.6509

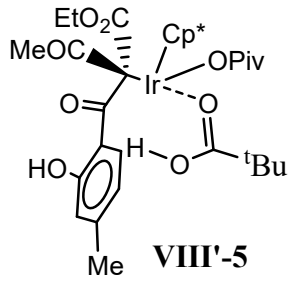
H	-0.09214	2.79880	-2.98293	1286.4059	1296.1889	1323.8318
C	1.95039	4.07466	-0.49402	1338.4108	1361.7227	1368.6871
H	1.28099	3.89157	0.35723	1372.6352	1374.1630	1378.0811
H	2.98435	3.92536	-0.16516	1383.2324	1384.4603	1387.0180
H	1.83533	5.12021	-0.80978	1398.3998	1399.0968	1403.3989
O	-1.62170	0.02208	-1.45144	1407.6432	1415.9978	1429.1391
C	-2.36406	1.40622	0.38034	1431.6393	1439.6958	1443.5038
C	-3.42952	2.06869	0.99334	1446.2008	1451.8415	1453.4019
C	-3.94471	0.42173	-1.17479	1454.9817	1455.9068	1459.1941
C	-4.73356	1.88394	0.55599	1459.8660	1460.7790	1466.2186
C	-5.01100	1.04634	-0.52682	1466.6175	1467.8524	1469.3061
C	-1.01109	1.52436	1.02186	1473.7282	1479.9463	1485.7264
O	-0.58468	2.62585	1.31447	1487.2021	1489.7128	1491.0340
H	-4.11052	-0.20452	-2.04996	1495.2017	1500.7830	1505.7084
H	-5.55328	2.39013	1.06338	1508.5170	1518.4300	1527.6269
H	-3.21171	2.71306	1.84312	1534.8359	1536.0813	1557.4150
C	-0.37790	0.20754	1.42393	1632.7446	1687.3873	1766.9506
C	-1.46984	-0.56740	2.17992	1771.9705	1792.6068	1829.1376
C	0.84033	0.30881	2.28639	3021.3805	3025.8382	3035.3272
C	2.89418	1.33634	2.73661	3036.7100	3037.1164	3038.4543
H	3.40759	0.36902	2.67020	3040.3348	3041.4482	3042.3736
H	2.62708	1.48602	3.79047	3044.6054	3051.7770	3060.4945
C	3.74148	2.45206	2.18958	3101.7524	3105.8025	3114.2329
H	4.68211	2.51345	2.74732	3118.3648	3118.3807	3122.9441
H	3.95995	2.27097	1.13130	3123.3169	3124.5568	3125.4004
H	3.22357	3.41281	2.27902	3126.0485	3128.7758	3137.9200
O	1.68953	1.27854	1.95973	3138.4066	3140.5572	3145.8688
O	1.06858	-0.47867	3.19581	3148.3578	3149.1864	3153.7794
O	-2.07742	-1.50378	1.70073	3154.0897	3161.0136	3167.5382
C	-1.82407	-0.05960	3.55630	3173.5734	3174.6182	3184.4652
H	-2.87195	-0.28906	3.76647	3186.3095	3191.2254	3453.6414
H	-1.19067	-0.57552	4.28510			
H	-1.63356	1.01447	3.66672			
C	-6.41341	0.86132	-1.02130			
H	-7.14351	0.99805	-0.21687			
H	-6.65386	1.59041	-1.80566			
H	-6.56038	-0.13579	-1.44993			

Statistical Thermodynamic Analysis

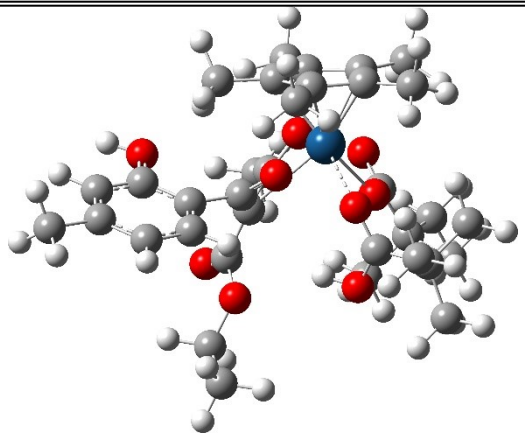
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.631786 Electronic Energy = -1758.84160623
Internal Energy (E)= -1758.16959123 Enthalpy (H)= -1758.16864723
Gibbs Free Energy (G)=-1758.27746323 Gibbs Free Energy of Solvation=-1758.32816514

St.Pt.	General Structure	Ball & Stick model

VIII'-5



VIII'-5



Cartesian co-ordinate

Atoms	X	Y	Z
H	0.92761	1.35305	0.23530
C	-2.01769	-2.69253	-1.19023
C	-1.64767	-2.94015	0.16551
C	-2.60818	-2.26807	1.03433
C	-3.58058	-1.61346	0.19828
C	-3.19323	-1.82860	-1.18653
C	-2.77057	1.95825	-0.16261
O	-1.88977	1.19402	0.41210
O	-3.62493	1.59349	-0.96498
C	-2.62101	3.44616	0.19882
O	0.03797	-0.43317	1.45030
C	0.47742	0.61822	1.91737
O	0.93698	1.60661	1.19299
C	0.54796	0.83158	3.41781
C	-4.76351	-0.84361	0.66080
H	-5.62196	-1.51538	0.79213
H	-4.56391	-0.35339	1.62016
H	-5.01788	-0.06240	-0.05927
C	-3.91783	-1.31962	-2.37970
H	-4.84680	-1.88241	-2.53964
H	-4.15401	-0.25915	-2.23957
H	-3.30192	-1.41267	-3.27905
C	-2.63083	-2.34924	2.51785
H	-1.61778	-2.29944	2.93112
H	-3.21006	-1.52788	2.95189
H	-3.08284	-3.29339	2.84921
C	-0.46019	-3.70254	0.63471
H	-0.17908	-3.39271	1.64689
H	-0.67389	-4.77876	0.65300
H	0.40051	-3.50829	-0.01252
C	-1.31122	-3.15015	-2.41448
H	-0.32544	-3.55589	-2.17861
H	-1.90095	-3.92025	-2.92792
H	-1.16097	-2.31158	-3.10222
C	-0.88629	0.73171	3.94527
H	-0.89680	0.91214	5.02715
H	-1.53550	1.46997	3.45885
H	-1.30317	-0.26160	3.75041
C	1.15007	2.18230	3.78632

Frequencies

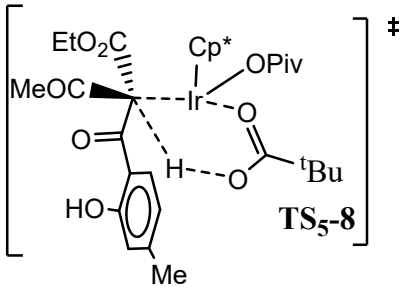
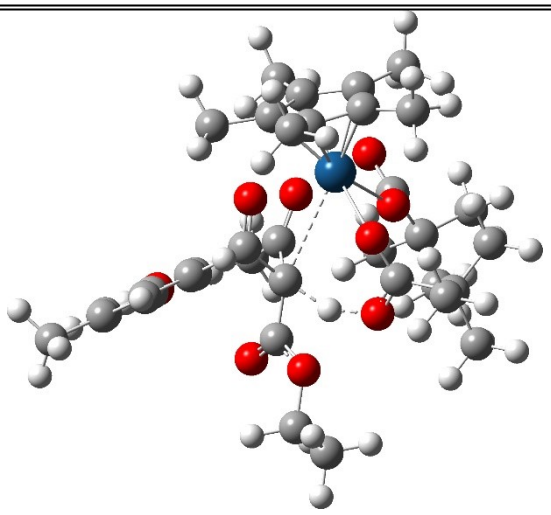
10.3433	24.2476	33.5285
41.8820	51.0847	55.8557
63.0694	70.4084	74.1185
78.2640	81.7468	86.9996
95.6843	102.8240	104.7709
108.3877	109.9198	113.9672
124.6394	128.1938	137.4903
139.6968	148.5638	153.4042
159.0837	159.8654	168.0237
174.1374	176.2612	186.2005
187.4797	193.9479	203.1503
207.8556	213.6470	219.5811
222.3244	223.4954	232.8964
237.3852	239.1036	240.8594
243.5952	254.7742	263.0503
266.9497	270.3256	277.4981
290.4386	294.7878	297.7373
304.1452	310.2639	314.1803
315.1161	318.0545	318.6000
322.3075	327.3508	329.6337
333.4648	335.8221	341.0393
354.7165	370.0296	382.4480
390.6641	393.8118	396.3586
403.1443	420.1233	421.5766
432.0062	439.3572	444.1435
452.8164	474.4843	476.3985
504.2421	526.5961	536.5836
539.0406	541.4033	546.0316
554.7917	572.5942	579.8028
588.9176	592.6273	593.4565
602.4231	612.5661	628.5772
631.0276	645.1736	726.4326
741.2299	749.8895	769.2647
778.6752	794.4395	799.4840
804.9433	809.2761	810.8125
816.5218	819.9020	832.0361
837.3347	846.6231	882.5300
896.4792	903.7451	915.6842
948.4084	949.6952	952.3292
960.1794	961.9324	965.1534
969.7167	972.1867	978.0185
1014.3634	1017.1346	1027.0602
1032.4206	1033.4342	1035.2555
1038.8502	1043.9330	1044.8517

H	1.19175	2.27470	4.87865	1045.7209	1046.7721	1047.5641
H	2.16641	2.29226	3.39343	1049.2203	1055.0395	1056.9227
H	0.54754	3.01103	3.39734	1093.1882	1096.1822	1108.0334
C	1.40156	-0.30097	3.99730	1112.1015	1137.2688	1145.3592
H	0.97659	-1.28042	3.74805	1172.8054	1178.1972	1181.5648
H	2.42753	-0.26313	3.60736	1185.7565	1189.5212	1209.6914
H	1.44702	-0.20831	5.08924	1237.0969	1238.2170	1240.8084
C	-3.94006	4.16930	-0.04611	1248.3972	1268.0089	1272.7213
H	-4.73013	3.78196	0.60926	1281.8464	1289.5892	1298.0520
H	-3.82525	5.24247	0.15585	1310.1904	1320.6877	1328.4199
H	-4.27358	4.03697	-1.07939	1367.3250	1367.9622	1371.1693
C	-1.54446	4.00970	-0.73470	1372.0110	1376.3615	1376.9195
H	-1.40123	5.08209	-0.54613	1381.4890	1383.5569	1384.2546
H	-0.58015	3.50688	-0.57604	1385.8341	1386.5575	1390.0890
H	-1.83468	3.88364	-1.78555	1397.9059	1400.9102	1407.9077
C	-2.18318	3.64026	1.64749	1418.4071	1420.6850	1426.5915
H	-2.12078	4.71198	1.87952	1427.9737	1434.8048	1435.8984
H	-2.90121	3.18865	2.34574	1441.5636	1442.9435	1447.4908
H	-1.19858	3.19317	1.82433	1450.9660	1452.6337	1453.3249
Ir	-1.64629	-0.80419	-0.19541	1453.6041	1455.1685	1458.4284
C	1.43501	0.67365	-1.62544	1461.8985	1462.5756	1465.4228
C	1.76876	-0.64191	-1.10048	1466.1082	1466.8703	1467.5700
O	0.95796	-1.57523	-1.06028	1469.9113	1471.9182	1473.1867
C	3.13885	-0.95227	-0.55967	1475.3274	1475.6463	1477.0135
C	4.32807	-0.81114	-1.28471	1478.1817	1479.9713	1483.1594
C	3.21457	-1.48980	0.72096	1485.9254	1488.0537	1494.0602
C	5.54807	-1.16056	-0.71627	1496.2882	1501.1215	1507.1095
C	4.43541	-1.81957	1.30262	1513.6886	1514.2154	1537.9548
H	2.28247	-1.63344	1.26804	1557.1794	1575.9547	1646.8448
C	5.62016	-1.65947	0.58729	1680.0424	1707.9808	1758.5876
H	6.46403	-1.04184	-1.30013	1764.2429	1834.1440	3022.9513
O	4.23639	-0.32598	-2.54976	3024.4038	3031.1081	3032.5537
H	5.11608	-0.25814	-2.93565	3034.3822	3036.7598	3038.6727
C	0.15657	0.87909	-2.22972	3039.6161	3040.9662	3041.4589
C	2.46912	1.71371	-1.79984	3041.9697	3043.6240	3046.8874
C	4.40801	2.62052	-0.80007	3047.8087	3055.0970	3088.7156
H	4.08948	3.66026	-0.94905	3099.8340	3106.6456	3110.7407
H	4.98772	2.33569	-1.69033	3114.2314	3117.8841	3119.7812
C	5.19194	2.43216	0.47373	3120.9125	3122.6860	3125.2720
H	6.10210	3.04089	0.46352	3126.0789	3129.4365	3133.3742
H	4.59073	2.72418	1.34128	3134.4102	3134.4260	3134.5413
H	5.47329	1.37843	0.59466	3135.3864	3138.1410	3142.4470
O	3.26199	1.78049	-0.70356	3144.2326	3144.6285	3147.7819
O	2.60938	2.47763	-2.73256	3149.4232	3151.0216	3151.6551
C	-0.06005	1.93749	-3.27505	3152.9484	3157.6869	3165.0007
H	-1.12728	1.97109	-3.51022	3169.4354	3175.9475	3181.1979
H	0.28829	2.91661	-2.93360	3185.8347	3404.1935	3894.4708
H	0.52955	1.71761	-4.17100			
O	-0.88099	0.21394	-1.94997			
H	4.46877	-2.21364	2.31763			
C	6.94637	-2.03121	1.17882			
H	6.87024	-2.18970	2.25941			
H	7.33636	-2.95692	0.73657			
H	7.69784	-1.25189	1.00400			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm

Zero-point correction= 0.778869	Electronic Energy = -2105.66414392
Internal Energy (E)= -2104.83499792	Enthalpy (H)= -2104.83405492
Gibbs Free Energy (G)=-2104.96575892	Gibbs Free Energy of Solvation=-2105.03417223

St.Pt.	General Structure	Ball & Stick model
TS_5-8		

Cartesian co-ordinate

Atoms	X	Y	Z
H	1.09602	1.20586	-0.09302
C	-1.94199	-2.61991	-1.28184
C	-1.52491	-2.95070	0.04016
C	-2.50204	-2.39557	0.97276
C	-3.53827	-1.75110	0.20143
C	-3.16481	-1.83049	-1.19486
C	-2.95075	1.88381	-0.07377
O	-2.08738	1.14248	0.55370
O	-3.79669	1.48754	-0.87101
C	-2.76580	3.38551	0.19629
O	-0.02023	-0.44665	1.36360
C	0.42559	0.65797	1.76608
O	0.85904	1.58501	1.00896
C	0.50837	0.88390	3.27241
C	-4.74973	-1.07766	0.73693
H	-5.61311	-1.75217	0.66845
H	-4.61919	-0.80097	1.78815
H	-4.95752	-0.16437	0.17038
C	-3.93153	-1.30817	-2.35547

Frequencies

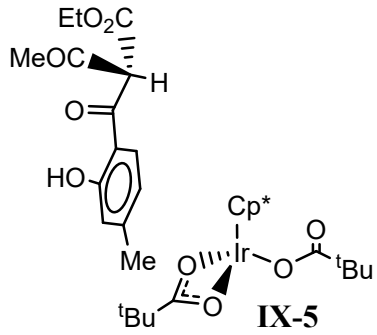
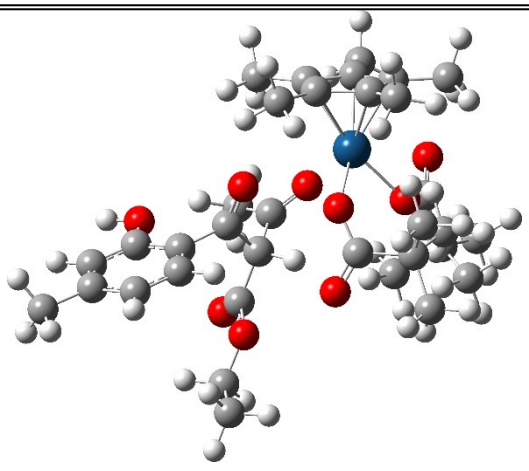
-503.7060	-33.7740	-31.7518
16.5558	28.9045	35.3647
43.4956	49.3365	55.0199
66.0899	69.0262	81.4783
85.1740	90.7286	92.3025
95.4783	98.0593	111.1518
112.8898	115.9745	122.9523
129.0899	132.9807	136.3511
144.5869	152.8951	159.9623
163.1486	172.2392	175.3577
184.0663	184.6280	191.5824
195.6957	203.7074	203.7890
216.7168	218.1708	220.7516
228.0563	233.5563	234.6075
241.3253	247.0815	260.5756
261.7995	267.2370	276.9612
281.1919	285.0050	292.1300
300.4091	305.8874	307.7007
309.8235	315.6338	327.4611
331.0529	335.0999	338.1087
343.3034	345.2107	348.4715
356.4457	364.7980	374.5050
392.2258	396.6510	404.5035
407.2071	411.8640	424.5144

H	-4.60025	-2.07827	-2.76283	427.7155	429.5113	440.8358
H	-4.51010	-0.42710	-2.06830	450.8009	452.4738	462.2753
H	-3.24422	-0.99472	-3.14847	472.0018	517.3812	522.9499
C	-2.44682	-2.55673	2.44955	535.2746	538.1955	549.2645
H	-1.43505	-2.34755	2.81588	550.8125	565.4213	568.9578
H	-3.13057	-1.86532	2.95205	579.2877	590.0784	592.0527
H	-2.71438	-3.57938	2.74497	602.5947	609.7966	618.2192
C	-0.29560	-3.68983	0.43474	632.9343	641.6841	696.9930
H	0.03715	-3.37695	1.43105	729.7280	745.8615	766.4064
H	-0.48405	-4.77073	0.46487	789.9277	794.3368	802.5224
H	0.52370	-3.48121	-0.25990	803.4424	805.4352	811.7904
C	-1.28023	-2.99165	-2.55891	815.4975	815.8920	825.1564
H	-0.28597	-3.40955	-2.39458	838.8101	859.0036	893.5807
H	-1.89725	-3.73083	-3.08671	902.9578	910.0061	922.2357
H	-1.16669	-2.11998	-3.21103	941.9954	948.8467	950.7158
C	-0.90180	0.75678	3.85201	954.3172	957.3708	961.9334
H	-0.86766	0.89407	4.94036	964.9131	965.9806	980.6336
H	-1.57435	1.51154	3.42818	983.5141	1011.2768	1014.0535
H	-1.32796	-0.22920	3.63720	1030.7870	1033.4214	1035.2449
C	1.09287	2.25186	3.60205	1036.1931	1038.7210	1042.6969
H	1.16548	2.36855	4.69094	1044.3232	1044.9120	1045.4178
H	2.09301	2.37128	3.17202	1046.0950	1051.0321	1053.4120
H	0.46594	3.06146	3.21252	1094.3850	1096.8816	1101.5062
C	1.40963	-0.21196	3.85238	1110.1184	1130.7032	1142.0475
H	1.01157	-1.21070	3.63652	1163.6628	1169.8374	1176.1322
H	2.42504	-0.14889	3.43835	1185.8580	1188.6924	1197.0855
H	1.47977	-0.09526	4.94121	1223.5707	1235.9833	1240.9066
C	-4.06377	4.13131	-0.08540	1248.3969	1252.6263	1260.1833
H	-4.85774	3.81600	0.60318	1269.0147	1269.8457	1270.7693
H	-3.91389	5.21176	0.04111	1299.8902	1313.3581	1327.2250
H	-4.41287	3.93915	-1.10416	1356.8229	1359.1074	1366.8247
C	-1.67810	3.84200	-0.78384	1372.5389	1373.5015	1374.4718
H	-1.48849	4.91751	-0.66774	1377.6815	1378.4424	1380.4470
H	-0.73751	3.30554	-0.59225	1383.7661	1388.5329	1391.6574
H	-1.98708	3.65718	-1.82112	1395.3688	1401.4562	1405.1724
C	-2.29675	3.65975	1.62119	1405.6255	1408.7848	1412.0756
H	-2.20016	4.74200	1.78195	1420.7493	1423.7092	1426.9082
H	-3.01010	3.27203	2.36079	1433.7240	1437.3877	1438.6812
H	-1.32163	3.19443	1.80225	1442.6718	1449.3206	1450.5320
Ir	-1.65100	-0.79122	-0.12827	1451.4621	1455.4952	1456.7136
C	1.42888	0.80498	-1.41082	1458.3907	1461.5186	1463.6159
C	1.81521	-0.60735	-1.16640	1463.8220	1465.9595	1469.5325
O	1.06699	-1.54693	-1.40733	1470.7172	1471.6658	1472.9476
C	3.14517	-0.93655	-0.54903	1474.0736	1475.6778	1478.1880
C	4.35265	-0.79570	-1.23821	1480.4131	1481.4233	1484.4704
C	3.16727	-1.49267	0.72340	1487.3417	1490.1260	1492.0244
C	5.55138	-1.16872	-0.64371	1495.2874	1502.5637	1509.4416
C	4.36869	-1.84840	1.33159	1517.2619	1527.6693	1533.8767
H	2.21832	-1.62798	1.24253	1544.8678	1556.1870	1648.9638
C	5.57530	-1.69170	0.65313	1663.7733	1682.5648	1714.8958
H	6.48645	-1.04842	-1.19568	1757.8489	1775.4111	1847.1983
O	4.28576	-0.27640	-2.49233	3014.2568	3023.0359	3024.9743
H	5.17002	-0.21691	-2.86916	3032.0731	3033.4052	3035.7238
C	0.17103	0.99734	-2.12936	3036.6200	3037.9095	3038.4386
C	2.52162	1.79539	-1.65549	3039.6732	3042.9922	3045.3622
C	4.51886	2.64361	-0.73479	3046.2545	3048.6629	3059.0675
H	4.21202	3.68864	-0.86799	3096.0141	3101.4886	3103.4346
H	5.05860	2.35118	-1.64662	3107.3957	3108.2000	3110.6633
C	5.34435	2.43570	0.50869	3111.9488	3116.4736	3119.5644
H	6.27227	3.01465	0.45765	3123.6557	3124.6392	3125.5187
H	4.78966	2.75110	1.39822	3126.4873	3130.2060	3131.4384

H	5.59678	1.37425	0.62418	3136.2325	3138.2033	3139.4413
O	3.35837	1.82468	-0.60087	3141.1884	3142.0628	3142.7114
O	2.65214	2.53850	-2.60387	3145.6842	3146.2544	3147.0413
C	0.04708	1.93127	-3.29295	3149.9149	3156.0696	3156.9433
H	-0.97958	1.89043	-3.66485	3157.0217	3162.8382	3173.1124
H	0.30102	2.95328	-2.99394	3178.5868	3183.1777	3895.4418
H	0.76748	1.67232	-4.07454			
O	-0.87983	0.41782	-1.79278			
H	4.36794	-2.25868	2.34049			
C	6.87860	-2.08961	1.27787			
H	6.76777	-2.26710	2.35238			
H	7.27183	-3.01115	0.82996			
H	7.64312	-1.31542	1.14073			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.772116 Electronic Energy = -2105.65232994
Internal Energy (E)= -2104.83158794 Enthalpy (H)= -2104.83064394
Gibbs Free Energy (G)=-2104.95830094 Gibbs Free Energy of Solvation=-2105.0242863

St.Pt.	General Structure	Ball & Stick model
IX-5	 **IX-5**	

Cartesian co-ordinate

Atoms	X	Y	Z
H	1.15591	1.05171	-0.30637
C	-2.04145	-2.20820	-1.68695

Frequencies

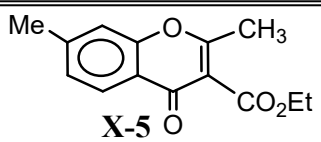
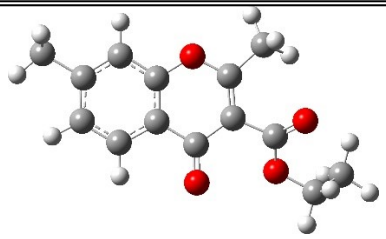
22.5662	28.8241	36.7964
41.5777	49.9133	60.6248
68.9620	75.5318	76.1612
79.7021	83.4495	89.7605
91.3383	98.1861	102.9619
109.1358	110.6605	118.6709

C	-1.58489	-2.82811	-0.48551	121.9288	125.3483	128.7284
C	-2.52818	-2.48011	0.56933	143.8248	145.8834	152.1546
C	-3.58316	-1.67077	-0.02025	154.6358	162.6213	167.4337
C	-3.26507	-1.47183	-1.40837	170.5736	181.7793	185.1105
C	-2.92223	1.98304	0.23733	189.8449	195.1525	198.6044
O	-2.08544	1.13133	0.75303	208.0317	215.4126	219.5524
O	-3.84044	1.71546	-0.53267	222.4858	226.4863	229.1329
C	-2.58741	3.43232	0.61607	234.3996	244.0311	252.3086
O	0.00293	-0.60981	1.15183	254.3844	258.5812	267.7326
C	0.38538	0.40660	1.87335	278.0996	285.1045	291.4483
O	0.75356	1.49228	1.42860	294.4638	298.6178	307.3966
C	0.37171	0.15671	3.38855	309.1675	313.8105	314.9803
C	-4.74891	-1.09908	0.70317	321.1088	325.6271	337.2526
H	-5.61518	-1.76873	0.62775	339.2310	339.9777	345.2782
H	-4.51713	-0.95565	1.76428	350.5869	352.8494	357.5422
H	-5.00227	-0.11902	0.28795	359.1496	382.6911	389.8139
C	-4.07649	-0.74217	-2.41764	389.8694	402.0104	410.3814
H	-4.80418	-1.41723	-2.88796	424.8463	426.9663	428.6674
H	-4.59615	0.10193	-1.95812	434.3853	444.3951	457.4717
H	-3.43670	-0.33287	-3.20657	463.1861	471.9566	481.6545
C	-2.47074	-2.99441	1.96297	503.9417	525.4501	536.0542
H	-1.45476	-2.92193	2.36759	537.8443	548.0218	548.6721
H	-3.13608	-2.43436	2.62696	558.7167	579.9483	582.2987
H	-2.77274	-4.04962	1.99284	588.1275	597.5489	602.0523
C	-0.34732	-3.63352	-0.29791	607.4038	611.9351	619.0566
H	0.04493	-3.49709	0.71673	643.5219	664.1105	687.1370
H	-0.54332	-4.70366	-0.44361	744.8220	756.6682	791.9343
H	0.43951	-3.31749	-0.99178	799.9358	805.9572	811.9342
C	-1.41302	-2.27887	-3.03177	812.2161	813.4967	814.8950
H	-0.41332	-2.71371	-2.99345	817.8606	818.2121	846.4992
H	-2.04367	-2.88654	-3.69397	862.3142	865.3558	903.7429
H	-1.32878	-1.28054	-3.47598	910.4828	916.3494	949.9727
C	-1.09602	0.12552	3.82746	952.2788	953.8139	959.5253
H	-1.16017	-0.06094	4.90823	960.4368	965.8513	967.5327
H	-1.59625	1.07773	3.61079	972.0013	979.8612	1001.5333
H	-1.64498	-0.66531	3.30287	1014.5330	1018.2423	1024.9862
C	1.10116	1.27898	4.11603	1036.5638	1037.7309	1040.6097
H	1.08156	1.10031	5.19956	1043.2688	1044.0971	1044.8404
H	2.14746	1.34287	3.79429	1045.7306	1047.1980	1049.1695
H	0.63599	2.24940	3.91399	1050.1515	1055.2608	1071.4475
C	1.03506	-1.18120	3.71332	1097.2655	1099.0078	1110.4319
H	0.53694	-2.01096	3.19823	1111.7382	1137.5759	1143.5489
H	2.09274	-1.17850	3.41510	1174.8873	1179.7669	1187.0357
H	0.99491	-1.36983	4.79441	1189.3128	1195.6257	1235.4911
C	-3.77888	4.33596	0.33041	1236.7397	1240.9429	1246.8710
H	-4.63855	4.06593	0.95630	1252.7329	1263.4708	1273.9143
H	-3.51847	5.38204	0.53982	1276.0797	1276.5384	1284.3291
H	-4.09392	4.25207	-0.71440	1296.8410	1311.0325	1328.1816
C	-1.40012	3.82130	-0.27605	1361.4695	1365.3305	1368.0167
H	-1.09630	4.85607	-0.06805	1371.4190	1376.1410	1377.0987
H	-0.54720	3.15854	-0.07902	1377.7999	1383.2812	1388.1063
H	-1.67054	3.75229	-1.33880	1390.6759	1391.4879	1394.5504
C	-2.16724	3.55009	2.07960	1398.5939	1402.4249	1410.0900
H	-1.96705	4.60254	2.32290	1412.0887	1414.2853	1417.8511
H	-2.96005	3.19696	2.75316	1430.7733	1433.1984	1434.0326
H	-1.25685	2.97180	2.27292	1435.7732	1440.0017	1443.7696
Ir	-1.69025	-0.68763	-0.14854	1446.2801	1451.7847	1454.2532
C	1.50305	0.92164	-1.36234	1455.7079	1456.3094	1458.7602
C	1.98639	-0.52337	-1.41035	1459.8910	1463.8901	1465.0496
O	1.32997	-1.35958	-2.00080	1465.8673	1466.3259	1469.3059
C	3.20158	-0.91593	-0.63798	1470.4887	1474.2265	1475.2416

C	4.47921	-0.65415	-1.13719	1477.0702	1478.8502	1483.0195
C	3.06760	-1.61766	0.55357	1486.4201	1488.8824	1489.7281
C	5.60416	-1.07828	-0.44307	1489.8002	1498.2814	1502.1018
C	4.19670	-2.03130	1.25614	1503.0216	1506.1426	1507.9091
H	2.06298	-1.80415	0.93674	1518.1421	1543.3642	1545.8576
C	5.47483	-1.76973	0.76562	1555.0668	1647.9016	1685.5708
H	6.59796	-0.87038	-0.84579	1734.6144	1761.0306	1769.6493
O	4.54494	0.02415	-2.31490	1810.4653	1866.3211	2841.9257
H	5.46419	0.13376	-2.58090	3016.8393	3017.7363	3021.0455
C	0.28146	1.02963	-2.24058	3028.2226	3029.8937	3032.9069
C	2.57361	1.97625	-1.53828	3036.5135	3036.5418	3036.9067
C	4.50097	2.83372	-0.49752	3038.3008	3039.0538	3044.6120
H	4.15999	3.87320	-0.57456	3045.6180	3046.7081	3051.7567
H	5.07766	2.61019	-1.40539	3094.0571	3097.9346	3102.5523
C	5.28165	2.56736	0.76254	3102.9369	3109.9338	3110.5167
H	6.18474	3.18531	0.79299	3113.9158	3115.4814	3116.2972
H	4.67511	2.79281	1.64508	3119.0952	3123.2168	3125.4762
H	5.57447	1.51136	0.81273	3126.5913	3129.7293	3131.7383
O	3.36065	1.96923	-0.46280	3135.2645	3138.2640	3139.2364
O	2.70040	2.73723	-2.46890	3139.3338	3142.5955	3142.8264
C	0.41583	1.40361	-3.67472	3142.8575	3143.9262	3146.4526
H	-0.55562	1.33404	-4.16954	3150.7722	3151.0845	3154.4411
H	0.84525	2.40510	-3.76947	3176.3338	3178.9353	3183.8794
H	1.13825	0.71972	-4.14090	3185.4546	3195.0766	3898.7636
O	-0.82157	0.73921	-1.78702			
H	4.08352	-2.56804	2.19681			
C	6.69843	-2.22914	1.49920			
H	6.45287	-2.57315	2.50867			
H	7.18771	-3.06026	0.97571			
H	7.43913	-1.42552	1.58687			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.779889 Electronic Energy = -2105.66129882
Internal Energy (E)= -2104.83166382 Enthalpy (H)= -2104.83072082
Gibbs Free Energy (G)=-2104.96041082 Gibbs Free Energy of Solvation=-2105.02892363

St.Pt.	General Structure	Ball & Stick model
X-5	 **X-5**	
Cartesian co-ordinate		**Frequencies**

Atoms	X	Y	Z
C	1.81018	0.61657	0.04012
C	1.34411	-0.67962	-0.13500
C	-0.09281	-0.94618	-0.31854
C	-0.37532	1.49548	-0.08612
O	0.95244	1.68173	0.05068
C	2.27921	-1.72133	-0.14013
C	3.16234	0.89962	0.21071
C	3.62144	-1.45718	0.03126
C	4.08185	-0.13937	0.20856
H	1.89867	-2.72978	-0.28296
H	3.47352	1.93339	0.34347
O	-0.50928	-2.07034	-0.55052
C	-0.93471	0.25953	-0.23323
C	-1.07971	2.80539	-0.04831
H	-1.27309	3.15610	-1.06774
H	-2.05235	2.72967	0.43911
H	-0.44999	3.53768	0.46287
C	-2.41142	0.17336	-0.36966
C	-4.31399	-1.13778	0.07548
H	-4.44124	-2.22231	0.13836
H	-4.64731	-0.79535	-0.91001
C	-5.05058	-0.42239	1.18165
H	-6.11917	-0.65821	1.14156
H	-4.66847	-0.72901	2.16079
H	-4.93538	0.66088	1.08019
O	-3.10092	1.02329	-0.89663
O	-2.89811	-0.93622	0.18827
H	4.34429	-2.27154	0.02956
C	5.54474	0.12639	0.38795
H	6.11292	-0.18183	-0.49796
H	5.74570	1.18739	0.56365
H	5.94692	-0.43966	1.23636

32.5165	47.4386	61.8071
75.6153	101.2547	103.3479
123.4647	143.4394	174.0340
203.3549	232.1416	234.6206
271.7986	287.9519	289.8329
346.0650	356.3923	367.9744
395.1312	448.5379	461.0795
476.0373	513.5026	559.4619
570.9010	596.7050	613.1381
686.1969	693.0604	744.8602
767.7938	782.8700	807.7422
830.9653	841.8079	869.1744
895.1868	920.1198	945.3127
987.9439	995.7879	1029.2539
1035.3953	1042.3164	1049.4795
1113.3726	1127.3668	1130.6956
1163.8833	1173.8476	1201.2541
1236.9494	1274.3036	1287.5419
1314.4628	1341.7739	1381.0672
1390.3665	1397.8458	1402.1414
1410.7750	1423.1478	1451.0579
1454.3290	1459.8922	1461.8304
1469.8747	1474.6428	1489.9877
1493.6114	1536.7401	1626.9446
1668.5143	1693.6486	1803.7775
1828.5280	3037.4559	3047.8991
3064.7774	3071.3005	3112.6347
3128.9127	3140.0409	3141.5403
3147.5946	3152.9088	3176.0152
3183.9217	3197.1045	3204.5630

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.254024 Electronic Energy = -842.321789870
Internal Energy (E)= -842.05089287 Enthalpy (H)= -842.04994887
Gibbs Free Energy (G)=-842.11302787 Gibbs Free Energy of Solvation=-842.133393962

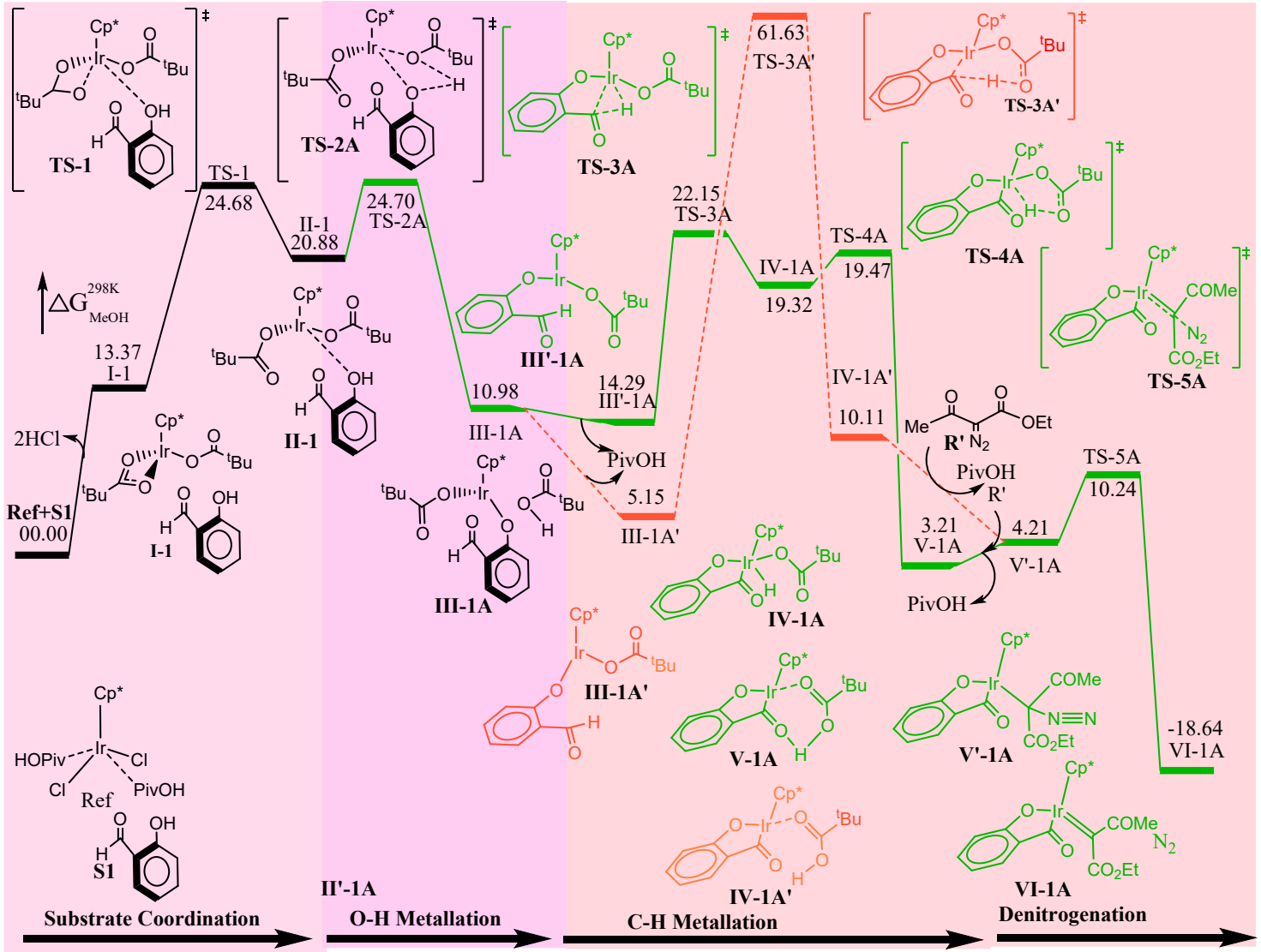


Fig-18: PES with Gibbs free energy (kcal/mol) and the structures of the stationary points for S1 M06 functional and 6-31G(d,p) basis set (green, orange and black colour represent path-A, path-A' and common path respectively)

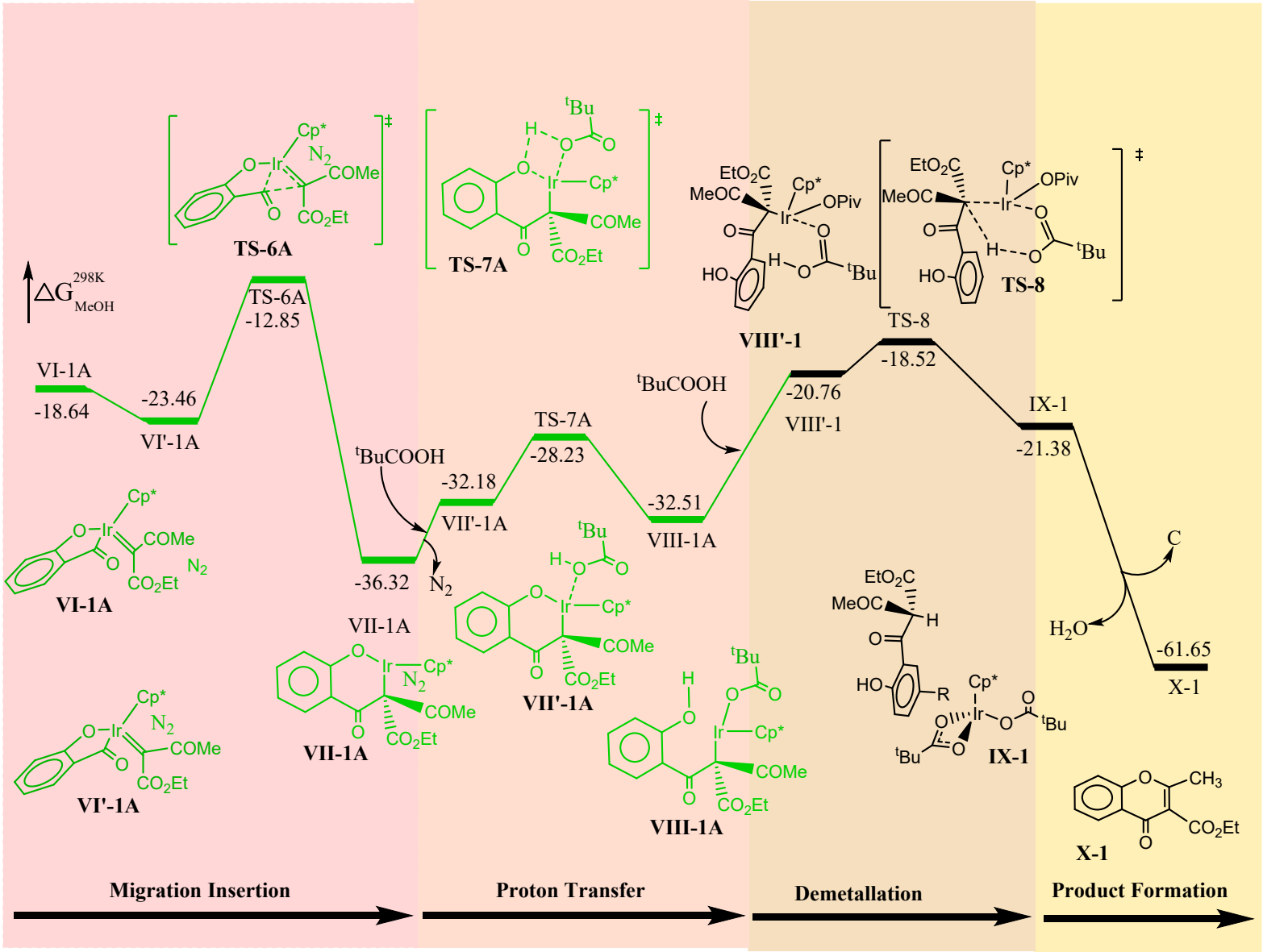


Fig-19: PES with Gibbs free energy (kcal/mol) and the structures of the stationary points for S1 using M06 functional and 6-31G(d,p) basis set (green and black colour represent path-A, and common path respectively)

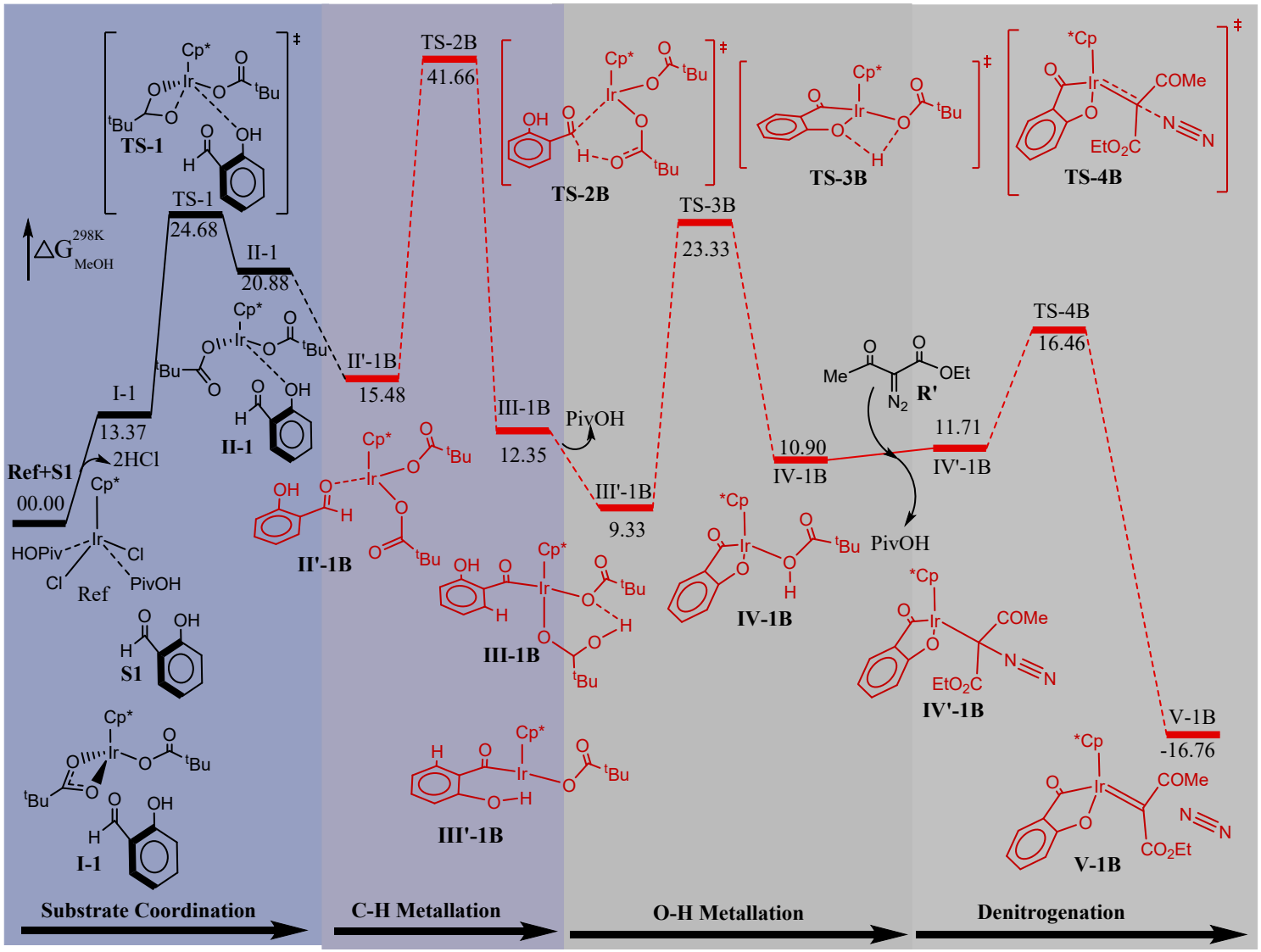


Fig-20: PES with Gibbs free energy (kcal/mol) and the structures of the stationary points for S1 using M06 functional and 6-31G(d,p) basis set (red and black colours represent path-B, and common path respectively)

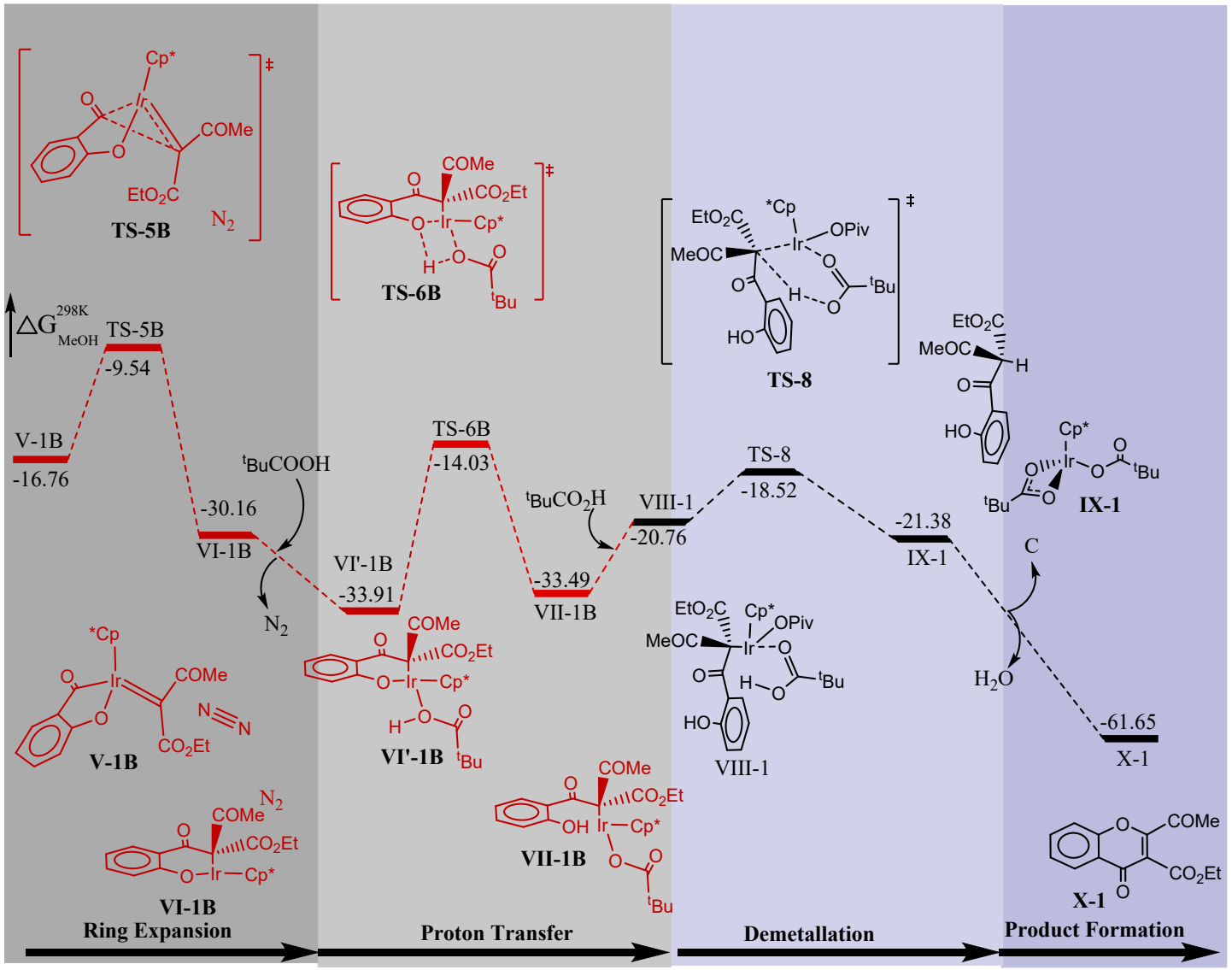


Fig-21: PES with Gibbs free energy (kcal/mol) and the structures of the stationary points for S1 using M06 functional and 6-31G(d,p) basis set (red and black colours represent path-B, and common path respectively)

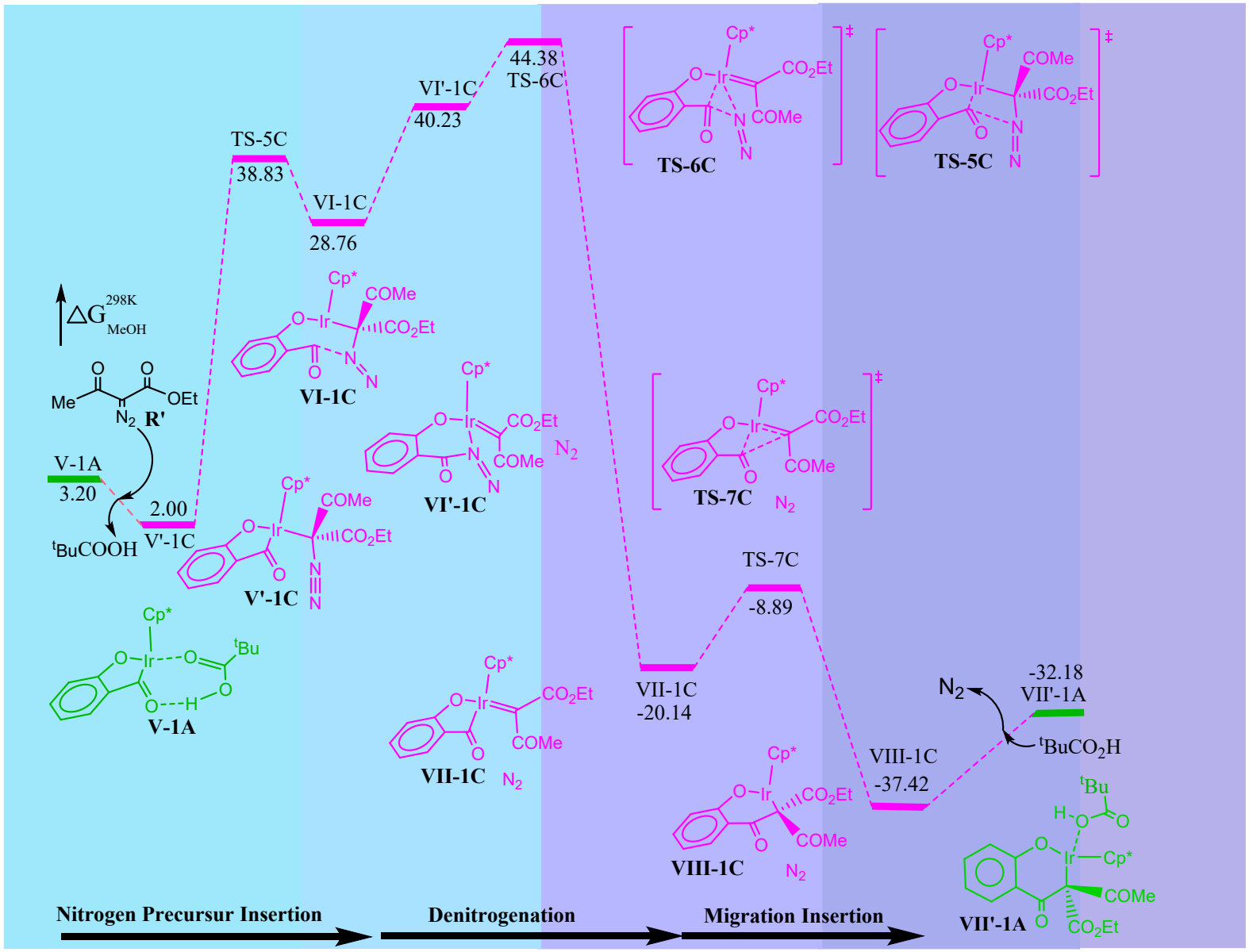


Fig-22: PES with Gibbs free energy (kcal/mol) and the structures of the stationary points for S1 using M06 functional and 6-31G(d,p) basis set (green and pink colours represent path-A, and path-C respectively)

As the structures and ball & stick models are already given before so, here only the coordinates are given.

St.Pt.	General Structure	Ball & Stick model
S1		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.01946	0.85724	0.00008
O	-0.98850	1.78803	0.00040
C	1.33244	1.20679	-0.00014
C	2.31566	0.22773	-0.00030
C	-0.38096	-0.50492	0.00026
C	1.97465	-1.12238	-0.00019
C	0.63319	-1.46736	0.00019
H	0.33776	-2.51660	0.00042
H	2.74506	-1.88767	-0.00029
H	3.36135	0.52627	-0.00052
C	-1.77286	-0.98506	0.00053
H	-1.82981	-2.10381	0.00242
O	-2.77830	-0.31496	-0.00110
H	1.60805	2.26137	-0.00031
H	-0.58400	2.66361	0.00124

Frequencies

94.4723	194.1531	195.2168
264.0076	394.7275	414.7653
420.3882	447.7625	553.2002
575.7265	668.0339	726.5674
760.5006	775.5017	849.3556
883.1663	950.6734	982.2974
1024.9241	1071.3042	1125.9927
1166.2432	1186.0961	1233.0601
1320.3752	1344.0107	1388.0075
1417.0381	1493.2463	1542.7352
1654.1962	1676.6399	1853.6786
2830.8546	3155.1590	3159.9234
3184.0258	3209.4341	3876.9588

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.114055 Electronic Energy = -420.525646372
Internal Energy (E)= -420.404091372 Enthalpy (H)= -420.403147372
Gibbs Free Energy (G)=-420.443605372 Gibbs Free Energy of Solvation=-420.463492583

St.Pt.	General Structure	Ball & Stick model
I-1		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.57125	-2.05432	1.31663
C	-2.82338	-1.38560	1.09888
C	-3.12470	-1.42685	-0.32509
C	-2.03443	-2.10526	-0.97562
C	-1.05840	-2.47648	0.03107
C	1.90832	-0.49111	-1.93986
C	-0.94514	3.41155	-1.51014

Frequencies

29.1295	36.1937	42.8825
49.5544	51.4046	62.5574
67.6684	76.6554	80.9445
97.3404	97.8765	102.8569
109.8153	123.3783	134.2404
143.1125	149.4423	151.5996
162.1310	166.6169	175.6805
181.8346	182.2141	192.8374
198.5297	202.4932	210.5203
218.0793	226.2262	229.6837
235.2949	239.4130	242.2945

C	-1.19469	2.01286	-0.98586	268.6714	277.8211	285.1888
O	-1.83354	1.80161	0.08574	293.3010	298.9695	302.8242
O	-0.75531	1.00517	-1.62742	309.5829	318.9939	321.4630
C	-4.33922	-0.86051	-0.97384	333.0314	339.2226	341.3353
H	-4.63512	0.08059	-0.49770	350.3164	364.5844	377.5995
H	-4.15381	-0.64457	-2.03090	390.7188	398.1820	405.5328
H	-5.18762	-1.55407	-0.91306	407.1093	408.6601	418.3524
C	-1.86459	-2.31212	-2.43804	426.9388	433.8787	441.5497
H	-0.83686	-2.07246	-2.73723	450.4543	461.0371	463.1900
H	-2.07689	-3.35496	-2.70636	468.5569	534.4324	538.1229
H	-2.54004	-1.66749	-3.00891	548.1682	555.5634	559.4538
C	0.21107	-3.22882	-0.16299	573.3790	577.1438	581.3857
H	0.49530	-3.28325	-1.21550	590.8768	605.9033	620.6115
H	1.03686	-2.72802	0.35930	643.7149	666.4001	729.1447
H	0.11873	-4.24668	0.23950	769.2851	777.4275	791.5769
C	-0.91514	-2.31765	2.62406	794.4145	808.5821	818.5486
H	0.17607	-2.29202	2.52696	820.4509	829.7898	852.5166
H	-1.19385	-1.57177	3.37066	882.2993	920.9226	935.7560
H	-1.19553	-3.31687	2.98404	946.8784	948.1223	949.0745
C	-3.61682	-0.70408	2.15630	952.0169	954.6766	962.7543
H	-4.35806	-0.02606	1.72248	965.1571	969.4921	991.0174
H	-4.14538	-1.43323	2.78336	997.1496	1030.4480	1034.6005
H	-2.94744	-0.10913	2.78855	1040.2134	1043.0370	1043.4463
C	0.44624	0.80170	2.04888	1045.1697	1045.3842	1048.0075
O	0.48462	0.44203	0.79535	1057.8528	1058.8094	1073.4058
O	-0.52012	0.68837	2.79633	1097.8052	1102.1818	1124.2632
C	1.78122	1.37420	2.54609	1128.1600	1161.3989	1184.9480
O	1.29952	-1.43818	-2.39572	1188.8061	1193.0516	1234.4551
C	2.82335	0.25473	2.47537	1241.9754	1242.9469	1246.6710
H	2.91782	-0.13525	1.45555	1257.6220	1263.4580	1270.6407
H	3.80677	0.62380	2.79852	1319.0878	1336.9291	1365.6614
H	2.54229	-0.57579	3.13820	1368.4608	1372.4287	1378.3787
C	1.64283	1.86021	3.98206	1379.6073	1385.8352	1389.3416
H	2.60318	2.25632	4.33913	1389.4531	1397.5966	1399.6377
H	0.88887	2.65119	4.06122	1408.7448	1412.2150	1413.5741
H	1.33157	1.04597	4.64496	1433.2329	1434.4080	1439.3934
C	2.18996	2.53420	1.64081	1441.5705	1444.4183	1445.1488
H	1.45454	3.34971	1.69280	1448.4223	1453.5319	1455.3891
H	3.16602	2.93785	1.94412	1456.8189	1459.8797	1461.3423
H	2.25260	2.19961	0.60077	1461.8213	1469.7792	1470.7283
C	0.52900	3.52238	-1.90152	1473.9427	1476.2154	1477.9949
H	0.78058	2.81379	-2.69857	1483.0246	1483.5430	1483.9156
H	0.74696	4.53813	-2.25540	1485.3624	1491.7231	1496.3855
H	1.17630	3.31600	-1.03732	1500.0890	1507.4053	1514.7033
C	-1.28750	4.44767	-0.44695	1518.6829	1529.4474	1541.5192
H	-1.11466	5.45639	-0.84343	1542.7375	1611.7534	1653.9073
H	-2.33437	4.36915	-0.13624	1676.4312	1766.2871	1823.1619
H	-0.66695	4.31479	0.44741	2927.9081	3019.7191	3022.3071
C	-1.82703	3.60668	-2.74743	3026.3517	3026.5090	3028.3502
H	-2.89084	3.53668	-2.48764	3031.7008	3033.5156	3038.1372
H	-1.64963	4.60017	-3.17907	3038.3962	3039.8981	3041.3555
H	-1.60579	2.85217	-3.51055	3096.5624	3097.3966	3098.8829
Ir	-1.29062	-0.35180	0.02504	3113.1789	3114.9511	3116.7538
H	1.44614	0.52072	-1.92149	3116.9341	3119.4237	3119.6435
C	3.26579	-0.52257	-1.37099	3126.9621	3129.0001	3129.9900
C	3.85712	0.71166	-1.08044	3134.2283	3138.8155	3139.4464
C	3.99147	-1.69812	-1.09534	3141.3552	3146.3398	3148.5837
C	5.12471	0.81165	-0.52974	3155.6260	3157.3437	3158.1337
H	3.28167	1.61126	-1.30206	3161.9379	3171.5281	3173.0650
C	5.26487	-1.60063	-0.53038	3189.2656	3208.4296	3878.9438
C	5.82407	-0.36016	-0.25209			

H	5.55827	1.78325	-0.30988
H	5.81920	-2.51315	-0.30893
H	6.81754	-0.31254	0.18815
O	3.43671	-2.89561	-1.37013
H	4.05237	-3.59029	-1.10959

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.613366 Electronic Energy = -1607.49765833
Internal Energy (E)= -1606.84537833 Enthalpy (H)= -1606.84443433
Gibbs Free Energy (G)=-1606.95229533 Gibbs Free Energy of Solvation=-1607.01340136

St.Pt.	General Structure	Ball & Stick model
TS-1		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.54294	-2.42706	0.68683
C	-2.61754	-1.48861	0.95603
C	-3.10933	-0.98900	-0.32336
C	-2.31333	-1.58593	-1.35413
C	-1.33667	-2.46850	-0.73771
C	1.55073	0.31504	-1.82878
C	-1.33401	3.68083	-0.54775
C	-1.27953	2.15882	-0.48201
O	-1.30730	1.59907	0.66153
O	-1.18525	1.48883	-1.53497
C	-4.19363	0.01586	-0.49940
H	-4.14957	0.77481	0.29002
H	-4.09230	0.53639	-1.45667
H	-5.18410	-0.45474	-0.46400
C	-2.39890	-1.32591	-2.81434
H	-1.39648	-1.20073	-3.23406
H	-2.88879	-2.16826	-3.32026
H	-2.96177	-0.41402	-3.02975
C	-0.37051	-3.33322	-1.46534
H	0.11803	-2.78485	-2.27608
H	0.41820	-3.68366	-0.79206
H	-0.87942	-4.21340	-1.88159
C	-0.81632	-3.25164	1.68705
H	0.24633	-3.32397	1.43031
H	-0.87382	-2.80722	2.68178
H	-1.23365	-4.26743	1.70442
C	-3.12775	-1.12969	2.30353
H	-3.73659	-0.22123	2.26840
H	-3.74498	-1.94059	2.71208
H	-2.28114	-0.94852	2.97459

Frequencies

-94.5563	-6.3405	29.5193
35.8061	38.8691	44.2705
56.3409	61.5427	67.0396
70.9504	73.8285	87.9900
92.2416	113.2214	126.7725
136.0119	137.1696	146.2300
155.6419	163.6579	173.7998
177.8316	190.9376	194.0429
202.9965	205.6287	216.0798
220.5922	228.4965	231.8111
238.1556	244.1257	248.3810
253.7594	258.0476	264.3764
283.5898	295.5979	301.2078
304.7651	307.5791	308.5897
315.1028	317.1836	318.6504
322.8475	329.8960	340.2888
372.7951	377.2068	390.1455
400.6970	414.4405	416.3444
422.1033	426.7818	434.9411
443.7264	450.0202	456.7643
467.2577	533.2030	538.5422
543.4606	550.1872	553.2242
565.1764	576.9420	581.4457
586.6424	602.4214	618.0344
631.2238	666.7450	727.0662
765.8947	778.5252	784.9396
794.5321	810.2893	811.1739
813.5802	825.6262	848.7459
883.0187	913.6844	925.6456
942.4202	944.0491	944.3407
950.2502	952.8239	954.3824
955.5247	965.5453	973.5103
984.1420	1032.0057	1033.7870
1035.0735	1039.6513	1041.4438

C	0.86574	-0.19863	2.21284	1041.7052	1047.6484	1048.6419
O	0.81145	-0.13227	0.92309	1050.2861	1052.1348	1070.4635
O	0.00140	-0.67158	2.94801	1095.6384	1098.2873	1112.1116
C	2.13815	0.45158	2.77757	1126.4872	1160.1607	1185.2276
O	0.74364	-0.54101	-2.14265	1187.0081	1187.8190	1236.4975
C	3.36682	-0.29508	2.25896	1240.8318	1241.9520	1249.3806
H	3.35988	-0.34674	1.16508	1258.0385	1264.4817	1268.6125
H	4.28678	0.21619	2.57540	1319.9462	1338.4289	1360.0797
H	3.39933	-1.31951	2.65345	1363.2593	1369.8445	1374.2994
C	2.11159	0.42195	4.29906	1377.3840	1385.5705	1391.2725
H	3.02981	0.87129	4.70110	1392.0217	1392.8915	1394.3823
H	1.25146	0.97738	4.68873	1406.3915	1407.7428	1408.5865
H	2.03262	-0.60521	4.67142	1418.0594	1427.9105	1434.7222
C	2.16471	1.90216	2.28461	1439.1252	1445.8914	1447.2941
H	1.22996	2.42131	2.53991	1448.4589	1449.5306	1456.2801
H	2.99983	2.44656	2.74642	1456.7557	1458.2095	1463.1133
H	2.28105	1.94052	1.19534	1463.3639	1465.6240	1470.9341
C	0.07471	4.15513	-0.91988	1471.2608	1471.4528	1473.9866
H	0.37916	3.75031	-1.89301	1474.9803	1477.3748	1480.9273
H	0.10292	5.25107	-0.97721	1483.0720	1484.6969	1492.0128
H	0.80502	3.83603	-0.16234	1492.6643	1500.1893	1501.9721
C	-1.74161	4.27897	0.79313	1510.1160	1521.2842	1534.5134
H	-1.77353	5.37407	0.71994	1542.0298	1653.9056	1669.8186
H	-2.73379	3.92677	1.09976	1676.7113	1761.6272	1803.1446
H	-1.03527	4.00186	1.58291	2911.5556	3016.6987	3019.1599
C	-2.32621	4.08966	-1.63482	3021.7130	3026.2472	3032.1403
H	-3.33650	3.72934	-1.39753	3032.6661	3033.3664	3036.5119
H	-2.36865	5.18338	-1.71790	3037.4066	3038.0364	3045.1778
H	-2.03891	3.67384	-2.60555	3099.4400	3100.6059	3104.7280
Ir	-1.05066	-0.45967	-0.01907	3106.3245	3114.8240	3115.5248
H	1.20710	1.36395	-1.67567	3116.1147	3118.4061	3118.9559
C	2.98692	0.13944	-1.59879	3119.7479	3124.0443	3134.2611
C	3.72384	1.29008	-1.29533	3136.8581	3138.0396	3138.3394
C	3.65066	-1.10306	-1.61888	3139.4990	3144.4176	3145.3847
C	5.08046	1.24182	-1.02000	3147.2048	3161.0779	3167.3221
H	3.19134	2.24160	-1.27332	3168.9197	3169.6262	3185.2490
C	5.01784	-1.15327	-1.34093	3191.6668	3210.3913	3874.4997
C	5.72278	0.00596	-1.04519			
H	5.63154	2.14724	-0.78348			
H	5.52785	-2.11677	-1.35326			
H	6.78650	-0.06107	-0.82875			
O	2.94897	-2.21814	-1.89895			
H	3.54242	-2.97685	-1.85652			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.611128 Electronic Energy = -1607.48183694
Internal Energy (E)= -1606.83266894 Enthalpy (H)= -1606.83172494
Gibbs Free Energy (G)=-1606.93791494 Gibbs Free Energy of Solvation=-1607.00434548

St.Pt.	General Structure	Ball & Stick model

II-1

Cartesian co-ordinate

Atoms	X	Y	Z
C	2.73969	-0.32568	-1.68545
C	3.19309	-0.37210	-0.30356
C	2.71209	-1.61790	0.27215
C	1.91415	-2.28659	-0.70581
C	1.93208	-1.48277	-1.92561
C	-1.97719	-0.21510	-0.34076
C	-0.72184	-0.24450	3.67072
C	-0.13171	-0.78341	2.35634
O	0.25185	0.16244	1.55181
O	-0.09223	-1.98956	2.12397
C	2.99839	-2.08868	1.65277
H	3.06409	-1.24513	2.34904
H	2.21089	-2.75226	2.01659
H	3.96029	-2.61745	1.67736
C	1.16900	-3.55943	-0.50999
H	0.36844	-3.66256	-1.25019
H	1.83590	-4.42593	-0.60628
H	0.70358	-3.56809	0.48073
C	1.19698	-1.82877	-3.17311
H	0.16479	-2.11858	-2.94333
H	1.15687	-0.97639	-3.85803
H	1.68005	-2.66441	-3.69571
C	3.02999	0.77990	-2.63649
H	2.30088	0.80421	-3.45266
H	2.98507	1.74232	-2.11622
H	4.02903	0.65705	-3.07467
C	4.12530	0.59127	0.33871
H	4.02103	0.56837	1.42808
H	5.16705	0.34550	0.09093
H	3.90167	1.61097	0.01547
C	0.74482	2.64159	-0.51648
O	0.15880	1.50758	-0.74299
O	1.94260	2.81145	-0.30898
C	-0.24107	3.82162	-0.46067
O	-1.05083	-0.90487	-0.76507
C	-1.31303	3.70818	-1.54124
H	-1.88568	2.77930	-1.44178
H	-2.00943	4.55519	-1.47145
H	-0.86903	3.72178	-2.54481
C	0.51394	5.13663	-0.60933
H	-0.18142	5.98331	-0.53237
H	1.28129	5.23780	0.16399
H	1.01781	5.19433	-1.58173
C	-0.89700	3.75964	0.92264
H	-0.13955	3.78037	1.71672
H	-1.57219	4.61421	1.06593
H	-1.47925	2.83596	1.03810
C	-2.06800	0.40588	3.33981
H	-2.74597	-0.31397	2.85876
H	-2.55478	0.76326	4.25720
H	-1.93371	1.26448	2.66930
C	0.21449	0.79812	4.27867

Frequencies

25.6819	33.9567	42.5079
48.9673	54.7676	62.7568
65.1787	69.8904	79.0759
86.0182	92.4632	101.0144
104.6365	109.4845	127.2894
127.8212	139.9305	146.4854
152.4300	160.4619	170.1158
182.4481	183.2002	190.6190
197.4257	202.0868	209.5726
211.3699	215.0792	227.4945
240.5175	248.6071	251.7469
257.7432	266.4630	279.3661
284.5309	297.5479	304.2879
309.5885	320.4401	321.6689
329.2066	330.3472	342.8320
343.8055	352.3223	355.6910
373.0855	380.4777	390.3786
395.9521	403.6340	421.8493
435.1567	439.9502	445.4121
446.6257	453.6105	466.9499
469.0927	539.1810	540.1785
546.9708	557.0592	568.3104
571.2206	578.5912	587.1231
590.6853	603.4695	631.2107
641.5555	677.2759	732.8758
771.8376	786.0539	789.7489
796.4619	807.8858	813.7681
814.4450	818.5577	855.3506
889.3399	911.5808	917.2984
938.7896	941.2100	946.8171
949.0946	949.9413	963.1525
964.3736	967.2878	983.9322
992.2253	1027.4454	1030.6335
1040.0463	1040.7621	1042.5313
1045.2240	1047.0412	1047.3104
1049.4304	1051.7400	1074.1819
1095.3504	1102.6148	1112.0784
1132.0748	1166.9321	1188.2171
1189.1776	1190.3178	1238.3543
1241.1373	1245.4222	1246.8453
1251.5259	1263.0745	1267.9281
1329.6130	1343.4874	1360.7627
1367.5642	1373.0533	1376.7473
1378.0051	1381.5725	1385.8935
1390.0724	1395.1802	1396.3848
1397.2553	1400.6910	1404.6183
1414.3533	1419.1664	1428.4444
1435.8315	1443.5694	1443.6485
1444.7297	1451.2768	1451.5370
1455.7094	1457.7389	1459.2987
1467.3730	1468.0947	1469.2642
1471.0408	1475.0593	1476.1995
1476.3416	1483.9050	1486.5871
1487.7774	1491.0003	1492.9049
1498.5737	1503.1755	1504.3497
1512.9469	1527.4808	1542.6040

H	-0.19951	1.17451	5.22399	1544.3574	1649.7657	1678.3313
H	1.19972	0.36359	4.49450	1743.9937	1759.2441	1769.1310
H	0.36051	1.64285	3.59804	3013.6585	3023.3567	3025.7998
C	-0.93612	-1.39176	4.64952	3027.7650	3031.5131	3032.4764
H	0.01207	-1.88805	4.88687	3033.4115	3036.1492	3037.9207
H	-1.37192	-1.01392	5.58417	3039.5214	3043.5087	3047.7040
H	-1.60493	-2.14965	4.22902	3094.8480	3103.1730	3103.8775
Ir	1.06614	-0.33518	-0.31907	3110.7379	3113.5132	3118.1821
H	-1.75239	0.62648	0.33798	3118.7789	3118.9411	3121.5255
C	-3.38056	-0.40976	-0.65861	3122.1582	3124.1569	3125.0712
C	-4.28232	0.51666	-0.11329	3130.8641	3134.3948	3139.9882
C	-3.88073	-1.44938	-1.47227	3142.4500	3143.7412	3149.8210
C	-5.64238	0.43691	-0.35231	3151.3885	3156.3600	3160.7245
H	-3.87904	1.31567	0.50901	3169.5246	3176.6909	3179.1725
C	-5.25399	-1.52911	-1.70883	3194.9775	3212.9284	3873.5753
C	-6.12101	-0.59710	-1.15552			
H	-6.32438	1.16466	0.07673			
H	-5.63954	-2.33280	-2.33587			
H	-7.18654	-0.68124	-1.35624			
O	-3.02148	-2.33912	-1.99749			
H	-3.51662	-2.99637	-2.50049			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.612808 Electronic Energy = -1607.49674518
Internal Energy (E)= -1606.84466718 Enthalpy (H)= -1606.84372318
Gibbs Free Energy (G)=-1606.95292018 Gibbs Free Energy of Solvation=-1607.0142557

St.Pt.	General Structure	Ball & Stick model
II'-1A		

Cartesian co-ordinate

Atoms	X	Y	Z
C	0.52406	-2.57454	-0.92698
C	1.78302	-1.83866	-0.93174
C	2.17124	-1.61483	0.44632
C	1.11872	-2.11805	1.28852
C	0.11316	-2.73707	0.42921
O	0.70430	1.35583	0.56264
C	1.61556	2.04636	-0.10188
O	2.37971	1.53479	-0.90238
C	1.58748	3.54185	0.20420

Frequencies

27.0405	32.1404	48.3983
60.9181	71.7062	80.8490
85.2810	111.8879	124.4122
129.2484	133.1331	143.5626
152.4694	157.9309	166.4776
169.0885	174.6427	178.0839
183.9164	191.0722	196.5740
201.3699	218.7208	225.0404
255.7144	275.7023	292.1449
297.0939	305.6913	309.2657
314.0918	317.8557	332.5171
347.6848	357.8245	362.2338
391.2476	420.0072	427.7647

C	-2.71546	0.54209	0.61242	435.0407	442.0240	452.2622
H	-0.92348	1.19615	1.14623	458.9354	467.0711	471.3449
C	2.57483	-1.46078	-2.12879	532.4854	534.7027	537.2354
H	3.01562	-0.46857	-1.99758	545.1852	575.3151	584.1371
H	3.37562	-2.19149	-2.29900	589.5562	592.1815	601.4295
H	1.94949	-1.43180	-3.02592	636.3532	664.9746	720.7866
C	3.40265	-0.91855	0.89427	772.9352	778.1594	785.2192
H	3.70993	-0.16089	0.16824	799.0389	805.2719	810.3758
H	3.24960	-0.42030	1.85672	819.5331	888.5804	892.6433
H	4.21437	-1.64686	1.01545	919.9161	948.2160	950.7974
C	-1.13171	-3.38273	0.92095	953.0452	966.5671	969.2203
H	-1.88974	-3.45750	0.13591	969.8307	1012.2984	1017.9824
H	-0.91788	-4.39785	1.27818	1024.2276	1032.4747	1034.8469
H	-1.56492	-2.82404	1.75816	1035.7190	1036.8247	1040.0447
C	-0.20962	-3.00854	-2.14473	1048.3656	1061.1161	1085.8906
H	-1.26702	-3.19538	-1.93574	1096.2402	1107.6223	1134.4225
H	-0.14993	-2.24737	-2.92947	1166.7247	1187.1283	1189.5128
H	0.22280	-3.93381	-2.54430	1205.2361	1240.8682	1243.9076
C	1.07567	-2.10079	2.77396	1258.2562	1260.8741	1266.7574
H	1.41643	-3.06193	3.17900	1313.9579	1349.5530	1377.5010
H	1.71641	-1.31670	3.18634	1378.4222	1381.7867	1386.8694
H	0.05765	-1.92621	3.13811	1391.0175	1394.3372	1396.3994
Ir	0.30805	-0.61748	-0.00033	1401.0524	1416.9590	1423.0851
C	0.24748	4.08725	-0.30193	1425.5691	1432.9967	1434.9492
H	-0.59843	3.65675	0.24930	1438.9213	1443.2032	1448.3659
H	0.21134	5.17526	-0.17043	1454.6472	1456.2632	1462.1098
H	0.11435	3.87484	-1.37130	1463.0702	1465.2135	1472.1022
C	1.70961	3.77604	1.71083	1478.5508	1480.2321	1484.6904
H	2.65561	3.37872	2.09908	1485.9702	1489.7629	1490.7787
H	1.69272	4.85266	1.91948	1499.7629	1515.4964	1522.3580
H	0.88867	3.30974	2.26595	1523.9038	1540.6969	1627.1637
C	2.73234	4.23325	-0.52503	1669.0138	1723.9761	1791.8422
H	3.70205	3.84337	-0.19763	3009.0464	3026.3437	3034.7435
H	2.66472	4.08400	-1.60733	3044.8681	3045.7238	3046.6589
H	2.70692	5.30987	-0.31850	3046.9569	3047.1543	3048.8736
O	-1.46505	0.36402	1.15784	3118.5065	3121.2822	3126.0086
C	-3.80860	0.40381	1.44980	3126.5296	3128.5470	3131.6072
C	-5.09176	0.61569	0.95110	3133.1362	3133.4596	3133.9833
C	-2.89162	0.86231	-0.74901	3136.3047	3146.9017	3148.2140
C	-5.28928	0.97660	-0.38088	3150.0978	3155.1588	3159.5735
C	-4.19507	1.10271	-1.21896	3165.4434	3188.3093	3205.0826
H	-4.33360	1.36869	-2.26578	3216.1274	3223.6675	3394.5807
H	-6.29138	1.15492	-0.75846			
H	-5.94477	0.51417	1.61679			
C	-1.83523	0.86341	-1.73665			
H	-2.11646	1.27581	-2.72180			
O	-0.69076	0.40720	-1.63660			
H	-3.63680	0.15602	2.49366			
H	-1.37192	-1.01392	5.58417			
H	-1.60493	-2.14965	4.22902			
Ir	1.06614	-0.33518	-0.31907			
H	-1.75239	0.62648	0.33798			
C	-3.38056	-0.40976	-0.65861			
C	-4.28232	0.51666	-0.11329			
C	-3.88073	-1.44938	-1.47227			
C	-5.64238	0.43691	-0.35231			
H	-3.87904	1.31567	0.50901			
C	-5.25399	-1.52911	-1.70883			
C	-6.12101	-0.59710	-1.15552			
H	-6.32438	1.16466	0.07673			
H	-5.63954	-2.33280	-2.33587			

H	-7.18654	-0.68124	-1.35624
O	-3.02148	-2.33912	-1.99749
H	-3.51662	-2.99637	-2.50049

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.476260 Electronic Energy = -1261.05929992
Internal Energy (E)= -1260.55298992 Enthalpy (H)= -1260.55204592
Gibbs Free Energy (G)=-1260.64195592 Gibbs Free Energy of Solvation=-1260.74565242

St.Pt.	General Structure	Ball & Stick model
TS-2A		

Cartesian co-ordinate

Atoms	X	Y	Z
C	2.44985	-1.60550	-0.44592
C	2.77428	-0.20498	-0.41775
C	2.40977	0.31328	0.89318
C	1.84583	-0.76031	1.65438
C	1.84018	-1.95394	0.82130
O	-0.54412	1.32912	-0.76785
C	-0.07862	2.61478	-0.77407
O	0.98810	2.85822	-1.27576
C	-0.97735	3.61309	-0.06202
C	-2.52102	-0.76366	0.47465
H	-1.18752	1.05202	0.03866
C	3.40752	0.59158	-1.49858
H	2.91939	1.56631	-1.60286
H	4.46762	0.75635	-1.26636
H	3.35055	0.07946	-2.46256
C	2.65157	1.70524	1.34917
H	2.50759	2.41912	0.53186
H	1.98943	1.98345	2.17527
H	3.68521	1.80325	1.70466
C	1.38726	-3.30674	1.23786
H	1.04935	-3.89713	0.38096
H	2.20835	-3.85339	1.71825
H	0.56058	-3.25043	1.95238
C	2.62871	-2.52204	-1.59956
H	1.83276	-3.27133	-1.64171
H	2.61832	-1.97683	-2.54751
H	3.58763	-3.04796	-1.51841
C	1.29673	-0.67207	3.03086
H	2.04741	-0.99865	3.76118
H	1.00443	0.35224	3.28079
H	0.41402	-1.30808	3.14806
Ir	0.64611	-0.46963	-0.12065

Frequencies

-351.2302	26.9127	35.3682
57.5967	71.0291	71.8204
87.2523	100.7617	109.7481
110.8950	123.1601	127.5518
145.9438	157.7965	164.8568
169.6007	175.4713	184.1172
189.2100	194.4451	210.8230
216.6216	228.5139	235.6950
240.6177	248.3746	267.5089
301.6894	306.1195	312.5164
316.3051	319.1043	334.0977
344.9866	354.0852	373.3263
386.2315	390.2064	417.9581
436.5470	443.0998	449.8747
460.5373	467.2729	504.7214
517.0007	536.1363	537.2099
543.7229	549.4919	576.6943
585.0785	587.5468	596.0190
602.6678	671.5327	704.4276
748.9347	774.4215	776.7326
789.7261	807.4422	809.3702
835.9126	878.6953	897.0534
932.5319	944.4362	955.8782
956.8504	962.4162	963.2146
971.4991	1007.6387	1011.5720
1028.1649	1030.3397	1031.1358
1033.2910	1038.0098	1040.0185
1047.8636	1057.9873	1090.6604
1094.6671	1108.6207	1146.3455
1160.4563	1167.8266	1188.4817
1191.0238	1226.1568	1234.4434
1253.1062	1263.1280	1267.6814
1304.4403	1356.4099	1381.4189
1383.8945	1389.7075	1394.7058
1395.8373	1397.5004	1402.5789
1413.7787	1421.1422	1422.2974

C	-2.45545	3.37194	-0.37677	1430.6659	1433.4482	1435.2417
H	-2.82914	2.41284	0.00525	1437.0403	1441.5600	1444.6962
H	-3.05304	4.15857	0.09750	1453.0611	1456.4635	1459.2292
H	-2.64908	3.41018	-1.45468	1459.5153	1463.3374	1466.5077
C	-0.72011	3.42135	1.44270	1473.9583	1483.5601	1485.2966
H	0.32381	3.65028	1.69165	1485.9946	1492.1281	1494.6645
H	-1.35707	4.10968	2.01019	1499.0000	1502.0574	1507.4865
H	-0.94871	2.40160	1.78517	1517.1716	1533.7810	1594.5858
C	-0.57550	5.02382	-0.47562	1674.5099	1685.6704	1878.4396
H	0.48305	5.21165	-0.27262	2263.0833	3025.3646	3030.6111
H	-0.74498	5.18689	-1.54546	3034.6218	3044.7921	3046.9684
H	-1.17281	5.75441	0.08121	3047.9637	3051.2714	3051.5291
O	-1.41160	-0.12258	0.80035	3052.3990	3112.9967	3118.5918
C	-3.60346	-0.71836	1.36874	3126.4122	3130.2511	3132.1955
C	-4.81410	-1.30227	1.04770	3134.3815	3137.4459	3137.7586
C	-2.69965	-1.44981	-0.76303	3141.1705	3141.8922	3150.7898
C	-5.00542	-1.96250	-0.17676	3153.6693	3154.1986	3155.8251
C	-3.95862	-2.02880	-1.06279	3157.3489	3173.3641	3178.5259
H	-4.07868	-2.54080	-2.01668	3194.7583	3210.2339	3224.9423
H	-5.96367	-2.41334	-0.41455			
H	-5.63514	-1.24363	1.75855			
C	-1.67447	-1.64965	-1.72989			
H	-1.99594	-2.15394	-2.65643			
O	-0.45428	-1.37981	-1.67791			
H	-3.45693	-0.19756	2.31140			
H	-1.37192	-1.01392	5.58417			
H	-1.60493	-2.14965	4.22902			
Ir	1.06614	-0.33518	-0.31907			
H	-1.75239	0.62648	0.33798			
C	-3.38056	-0.40976	-0.65861			
C	-4.28232	0.51666	-0.11329			
C	-3.88073	-1.44938	-1.47227			
C	-5.64238	0.43691	-0.35231			
H	-3.87904	1.31567	0.50901			
C	-5.25399	-1.52911	-1.70883			
C	-6.12101	-0.59710	-1.15552			
H	-6.32438	1.16466	0.07673			
H	-5.63954	-2.33280	-2.33587			
H	-7.18654	-0.68124	-1.35624			
O	-3.02148	-2.33912	-1.99749			
H	-3.51662	-2.99637	-2.50049			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.473107 Electronic Energy = -1261.05756969
Internal Energy (E)= -1260.55503369 Enthalpy (H)= -1260.55408969
Gibbs Free Energy (G)=-1260.64235069 Gibbs Free Energy of Solvation=-1260.74324142

St.Pt.	General Structure	Ball & Stick model
III-1A		

Cartesian co-ordinate

Atoms	X	Y	Z
C	2.96311	-0.35813	-0.62630
C	2.60669	1.01147	-0.45195
C	2.12737	1.19133	0.91632
C	2.19739	-0.07214	1.58112
C	2.67379	-1.05678	0.61996
O	-0.97579	1.05502	-1.12785
C	-1.24931	2.33408	-0.69944
O	-0.37640	3.15563	-0.76600
C	-2.61790	2.55467	-0.07653
C	-1.83523	-1.50958	0.59140
H	-1.77581	0.50682	-1.06527
C	2.70148	2.09831	-1.45759
H	1.78844	2.70126	-1.46022
H	3.54565	2.75594	-1.21387
H	2.86033	1.70598	-2.46515
C	1.73081	2.48676	1.52518
H	1.29723	3.16712	0.78661
H	1.00336	2.34509	2.33078
H	2.61388	2.97318	1.95958
C	2.94359	-2.49098	0.89429
H	2.83844	-3.09596	-0.01134
H	3.96909	-2.61781	1.26420
H	2.26272	-2.89174	1.65095
C	3.48363	-0.99516	-1.86320
H	3.05712	-1.99290	-2.00732
H	3.24207	-0.40288	-2.74998
H	4.57416	-1.09834	-1.80989
C	1.79009	-0.35863	2.97968
H	2.65958	-0.31297	3.64660
H	1.05034	0.36476	3.33457
H	1.34457	-1.35398	3.06894
Ir	0.85738	-0.26895	-0.09665
C	-3.68794	1.60097	-0.61222
H	-3.53236	0.55266	-0.31034
H	-4.65871	1.88363	-0.19096
H	-3.78164	1.65526	-1.70390
C	-2.39751	2.31461	1.42762
H	-1.71893	3.07163	1.83787
H	-3.35635	2.39262	1.95351
H	-1.97221	1.31989	1.62423
C	-3.04203	3.99993	-0.32083
H	-2.27338	4.69987	0.01788
H	-3.22814	4.18779	-1.38438
H	-3.96773	4.20727	0.22761
O	-0.81538	-0.80643	0.98587
C	-2.91077	-1.67297	1.49979
C	-4.04294	-2.36801	1.14445
C	-1.96381	-2.12077	-0.70131
C	-4.17771	-2.96063	-0.12923
C	-3.14664	-2.84577	-1.02092
H	-3.21462	-3.30968	-2.00418
H	-5.07817	-3.50888	-0.38711
H	-4.85108	-2.46589	1.86595
C	-0.93621	-2.11332	-1.67725

Frequencies

34.2818	38.7300	58.3943
68.7443	77.9035	84.5790
90.5901	90.8994	104.6115
111.8129	126.2507	135.8139
149.7370	151.8869	164.8802
174.4676	184.6815	190.1946
198.2138	202.7142	216.2307
223.0672	232.1979	248.3508
251.9838	257.3167	276.6499
288.7662	305.5440	309.2117
315.2983	327.6247	336.4413
357.1340	359.1060	381.6984
390.9317	393.2592	404.6851
436.1983	443.1041	447.0029
459.6111	475.5075	512.1138
533.7121	535.7408	543.0596
546.3290	554.5821	577.3127
584.3062	588.4999	602.9179
619.2716	650.3018	676.1801
754.6339	766.1062	776.0889
777.6339	802.6236	806.3336
809.9699	876.8512	880.4778
906.4576	948.4846	954.9191
958.8636	967.7581	968.1597
971.6724	1009.1124	1009.9801
1020.9123	1026.2657	1032.3148
1034.2739	1037.4277	1043.2866
1046.0466	1054.0537	1089.9834
1097.9282	1109.2763	1111.7499
1154.3198	1167.9355	1187.8790
1189.4193	1223.1870	1244.1531
1246.1183	1262.8920	1264.7198
1323.7675	1370.0827	1378.7550
1380.9048	1390.2599	1391.1653
1392.0719	1399.9163	1402.0356
1409.4651	1420.6131	1427.3905
1430.9618	1434.3369	1434.9684
1439.9066	1443.6979	1447.8584
1451.0604	1454.5267	1458.8102
1463.3881	1465.7983	1470.4366
1474.0280	1483.4803	1485.5935
1490.2292	1491.3913	1493.4409
1496.8921	1499.0891	1512.4482
1521.7372	1543.8704	1584.9159
1672.9729	1685.6102	1903.7288
3017.3424	3032.8952	3036.4474
3045.7885	3046.4831	3049.7436
3049.9969	3051.1659	3051.4407
3102.3332	3120.0272	3127.8337
3129.2579	3133.0140	3134.6797
3134.9490	3136.6168	3137.1617
3140.7327	3151.1745	3153.8238
3157.6948	3160.0266	3166.0331
3175.6794	3180.5054	3189.7930
3203.9473	3220.7982	3760.9699

H	-1.11972	-2.72254	-2.57684
O	0.16097	-1.50451	-1.65800
H	-2.80335	-1.22132	2.48290
H	-1.37192	-1.01392	5.58417
H	-1.60493	-2.14965	4.22902
Ir	1.06614	-0.33518	-0.31907
H	-1.75239	0.62648	0.33798
C	-3.38056	-0.40976	-0.65861
C	-4.28232	0.51666	-0.11329
C	-3.88073	-1.44938	-1.47227
C	-5.64238	0.43691	-0.35231
H	-3.87904	1.31567	0.50901
C	-5.25399	-1.52911	-1.70883
C	-6.12101	-0.59710	-1.15552
H	-6.32438	1.16466	0.07673
H	-5.63954	-2.33280	-2.33587
H	-7.18654	-0.68124	-1.35624
O	-3.02148	-2.33912	-1.99749
H	-3.51662	-2.99637	-2.50049

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.476845 Electronic Energy = -1261.07148317
Internal Energy (E)= -1260.56462617 Enthalpy (H)= -1260.56368217
Gibbs Free Energy (G)=-1260.65295217 Gibbs Free Energy of Solvation=-1260.75252671

St.Pt.	General Structure	Ball & Stick model
III'-1A		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.81921	-2.44398	-0.92848
C	0.34475	-2.74183	-0.15693
C	0.07770	-2.34623	1.21916
C	-1.30124	-1.87617	1.28402
C	-1.84896	-1.92098	-0.03534
C	-1.82374	1.95580	-0.56892
Ir	-0.07594	-0.61663	0.01999
C	-2.85462	2.85797	-0.89533
C	-3.21954	3.85203	-0.01701

Frequencies

26.1426	36.0912	40.7567
51.7030	57.3238	65.1664
88.0946	94.8566	122.3750
135.5231	145.4921	151.7764
160.6126	164.0593	173.1818
180.9843	186.2838	194.3523
201.3308	210.3163	211.7506
226.2545	232.7383	234.8520
245.4983	256.7006	263.2800
278.3295	285.7333	303.2614
308.0613	311.2186	313.8637
324.2998	348.1144	374.7217
388.1531	415.4425	426.1663

C	-1.16692	2.02475	0.69065
C	-2.54055	3.95543	1.21255
C	-1.54064	3.07555	1.56325
H	-1.02558	3.14655	2.51820
H	-2.81545	4.74674	1.90806
H	-4.01024	4.55380	-0.26758
H	-0.26721	0.65704	-1.42036
O	1.90867	-0.06590	-0.01978
C	2.28866	1.04219	-0.60190
C	3.66686	1.51880	-0.13245
O	1.61695	1.69711	-1.38666
H	-3.33278	2.74952	-1.86700
C	-1.39207	0.98141	-1.54096
O	-1.96440	0.61198	-2.54852
O	-0.27167	1.16014	1.08162
C	4.30547	2.39847	-1.19995
H	3.64374	3.22570	-1.47242
H	5.25417	2.80952	-0.83005
H	4.51574	1.82607	-2.11193
C	3.38337	2.34870	1.12646
H	2.87925	1.74080	1.88769
H	4.32147	2.73527	1.54666
H	2.73253	3.19938	0.88905
C	4.58955	0.35383	0.21214
H	4.76763	-0.28501	-0.66281
H	5.56133	0.73470	0.55365
H	4.16428	-0.27045	1.00507
C	1.65451	-3.25821	-0.63838
H	2.46218	-2.57095	-0.35628
H	1.86771	-4.24224	-0.20282
H	1.66853	-3.35704	-1.72737
C	-0.99347	-2.59408	-2.39765
H	-0.04371	-2.81697	-2.89201
H	-1.69677	-3.40669	-2.61977
H	-1.39299	-1.66890	-2.83356
C	-3.23791	-1.56820	-0.43858
H	-3.26481	-1.16783	-1.45686
H	-3.88628	-2.45302	-0.39905
H	-3.66347	-0.80625	0.22302
C	-1.98213	-1.35961	2.50056
H	-2.71087	-0.58314	2.24584
H	-2.50932	-2.16725	3.02344
H	-1.26387	-0.91254	3.19482
C	1.03039	-2.50775	2.34930
H	0.75215	-1.88069	3.20142
H	1.06037	-3.55130	2.68953
H	2.04174	-2.21860	2.04322
H	-2.80335	-1.22132	2.48290
H	-1.37192	-1.01392	5.58417
H	-1.60493	-2.14965	4.22902
Ir	1.06614	-0.33518	-0.31907
H	-1.75239	0.62648	0.33798
C	-3.38056	-0.40976	-0.65861
C	-4.28232	0.51666	-0.11329
C	-3.88073	-1.44938	-1.47227
C	-5.64238	0.43691	-0.35231
H	-3.87904	1.31567	0.50901
C	-5.25399	-1.52911	-1.70883
C	-6.12101	-0.59710	-1.15552
H	-6.32438	1.16466	0.07673
H	-5.63954	-2.33280	-2.33587

431.8421	444.4151	457.9589
468.0659	530.7877	532.8995
536.3634	542.0544	547.3010
571.8879	583.5255	584.7920
595.2583	603.3916	619.9606
641.7659	652.3503	747.7033
764.1777	790.9007	802.9908
807.9301	816.1121	824.4970
861.2866	877.3374	914.7142
946.4611	952.9866	953.6033
954.5086	961.8969	962.2979
979.1721	1036.7718	1038.3196
1039.7383	1043.3286	1043.6827
1044.0355	1045.8542	1050.6201
1082.9737	1088.8483	1097.1529
1103.9013	1118.9666	1142.4889
1180.5967	1185.6503	1205.1460
1235.5520	1245.5773	1268.5154
1273.3959	1341.5494	1354.7659
1373.3033	1374.9698	1379.6177
1382.9655	1392.2546	1397.3656
1401.0917	1405.6029	1409.1644
1435.5646	1435.9276	1436.5137
1439.5491	1444.0995	1449.7306
1450.9281	1451.8865	1454.0150
1458.3473	1459.7093	1465.4409
1467.7208	1469.3971	1474.4286
1478.0092	1483.8030	1488.4576
1495.9945	1497.8916	1508.4595
1518.8678	1523.5907	1543.1374
1604.2579	1671.1504	1779.9995
1805.7272	2277.9465	3023.7688
3025.6906	3029.4207	3032.5410
3035.6126	3036.7398	3038.9883
3044.6089	3104.2203	3107.7278
3111.3802	3114.9325	3115.8425
3118.5280	3119.6986	3126.1848
3129.3354	3136.4608	3142.1952
3145.8014	3147.2195	3149.1518
3149.2106	3149.3228	3174.8601
3184.1272	3198.4756	3207.0416

H	-7.18654	-0.68124	-1.35624
O	-3.02148	-2.33912	-1.99749
H	-3.51662	-2.99637	-2.50049

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.462130 Electronic Energy = -1260.64913599
Internal Energy (E)= -1260.15718999 Enthalpy (H)= -1260.15624699
Gibbs Free Energy (G)=-1260.24605199 Gibbs Free Energy of Solvation=-1260.29408961

St.Pt.	General Structure	Ball & Stick model
TS-3A		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.95359	-1.76649	-0.89131
C	-0.97467	-2.53226	-0.18670
C	-1.00605	-2.13742	1.21911
C	-2.02351	-1.14434	1.36662
C	-2.58134	-0.87223	0.06660
C	-0.63507	2.52233	-0.48914
Ir	-0.41192	-0.41523	-0.03285
C	-0.96637	3.80971	-0.94348
C	-0.62833	4.91033	-0.18653
C	0.03241	2.32506	0.73908
C	0.05063	4.72139	1.03228
C	0.38186	3.46511	1.49610
H	0.90527	3.31981	2.43783
H	0.32289	5.59116	1.62796
H	-0.87355	5.91306	-0.52568
H	0.21619	0.44178	-1.33619
O	1.60306	-0.92193	0.05016
C	2.45998	-0.18335	-0.59853
C	3.90943	-0.41448	-0.15904
O	2.17428	0.67754	-1.42299
H	-1.47951	3.90495	-1.89804
C	-0.94457	1.33845	-1.26506
O	-1.61125	1.27029	-2.27379
O	0.30191	1.12189	1.16621
C	4.85879	-0.01710	-1.28189
H	4.64679	0.99794	-1.62899
H	5.89878	-0.06811	-0.93416
H	4.75602	-0.69165	-2.14090
C	4.10276	0.51173	1.04923
H	3.37671	0.27745	1.83740
H	5.11545	0.39409	1.45703
H	3.96414	1.56130	0.76152

Frequencies

-191.9673	15.7274	30.6674
39.6229	46.0375	55.8118
69.3879	86.5315	96.6943
133.0113	137.7155	146.4286
159.6379	162.5249	168.5527
172.1975	174.9609	177.8848
189.9071	192.0325	203.6136
209.7536	226.2221	247.9605
256.4651	261.4150	269.8632
274.2010	283.0996	288.9312
304.2119	307.0877	310.1645
321.2221	350.9059	351.9366
380.3235	391.1112	412.1395
426.1903	430.2801	440.1065
469.8418	495.5161	537.1969
540.9210	542.5178	552.6125
565.1215	568.8484	594.4048
596.7509	606.1040	626.2884
639.1099	653.4028	720.7664
762.1530	775.7061	791.6752
812.2329	817.0436	818.6954
843.6225	856.7250	881.2626
899.8172	922.2020	935.6541
944.8955	950.8802	951.6394
956.0720	965.1151	984.8029
1030.6651	1034.0292	1035.8324
1042.4097	1044.6116	1046.1131
1047.3934	1050.8617	1088.5628
1092.3082	1108.0654	1124.3908
1150.6662	1182.1816	1188.8914
1212.5258	1233.3184	1246.1850
1263.5094	1268.3532	1351.5455
1356.1392	1370.9465	1372.7688
1375.9575	1380.7405	1393.4935
1397.1577	1398.1652	1405.0858
1406.2422	1436.3866	1439.2234

C	4.15735	-1.86212	0.25316	1440.1730	1443.3579	1444.8811
H	3.97148	-2.54916	-0.58286	1445.1157	1449.3513	1453.8461
H	5.20316	-1.98751	0.56335	1460.1506	1461.8811	1465.3151
H	3.51199	-2.16061	1.08608	1466.6762	1467.0751	1473.8420
C	-0.04797	-3.55373	-0.74227	1475.7663	1484.5707	1485.2104
H	0.97766	-3.35822	-0.40547	1486.7514	1502.9242	1511.4942
H	-0.33575	-4.55957	-0.41066	1520.4088	1525.3637	1543.7429
H	-0.04660	-3.53914	-1.83598	1614.8406	1666.5367	1745.6099
C	-2.29814	-1.84276	-2.33773	1788.4156	1878.9342	3023.6673
H	-1.62189	-2.51600	-2.87258	3026.8917	3035.3066	3036.6602
H	-3.32190	-2.21591	-2.46766	3037.3877	3039.8155	3041.0055
H	-2.23135	-0.84983	-2.79919	3041.9344	3106.4527	3113.2483
C	-3.71253	0.04880	-0.22074	3116.2809	3116.4040	3116.6293
H	-3.68196	0.39619	-1.25717	3117.1752	3121.3848	3123.2180
H	-4.67406	-0.45099	-0.04598	3127.2208	3129.7330	3142.1375
H	-3.67207	0.93509	0.42262	3148.0833	3149.8626	3151.8305
C	-2.36442	-0.40690	2.61073	3154.0378	3166.0939	3168.9107
H	-2.64767	0.62799	2.39036	3191.4141	3201.5460	3209.2786
H	-3.20656	-0.88348	3.12824			
H	-1.51184	-0.37047	3.29515			
C	-0.13274	-2.71493	2.27695			
H	-0.13912	-2.10180	3.18275			
H	-0.45672	-3.72694	2.55259			
H	0.90424	-2.76976	1.92656			
H	-2.80335	-1.22132	2.48290			
H	-1.37192	-1.01392	5.58417			
H	-1.60493	-2.14965	4.22902			
Ir	1.06614	-0.33518	-0.31907			
H	-1.75239	0.62648	0.33798			
C	-3.38056	-0.40976	-0.65861			
C	-4.28232	0.51666	-0.11329			
C	-3.88073	-1.44938	-1.47227			
C	-5.64238	0.43691	-0.35231			
H	-3.87904	1.31567	0.50901			
C	-5.25399	-1.52911	-1.70883			
C	-6.12101	-0.59710	-1.15552			
H	-6.32438	1.16466	0.07673			
H	-5.63954	-2.33280	-2.33587			
H	-7.18654	-0.68124	-1.35624			
O	-3.02148	-2.33912	-1.99749			
H	-3.51662	-2.99637	-2.50049			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.458396 Electronic Energy = -1260.64392691
Internal Energy (E)= -1260.15595091 Enthalpy (H)= -1260.15500691
Gibbs Free Energy (G)=-1260.24495791 Gibbs Free Energy of Solvation=-1260.28520163

St.Pt.	General Structure	Ball & Stick model
IV-1A		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.56745	-2.49180	-0.67850
C	0.86979	-2.43177	-0.47523
C	1.13759	-2.28063	0.94454
C	-0.08968	-2.10913	1.59030
C	-1.16165	-2.17216	0.58226
C	-2.32904	1.36530	-0.60443
Ir	-0.08232	-0.42766	-0.16820
C	-3.37893	2.10035	-1.16918
C	-4.14342	2.92503	-0.36611
C	-2.03912	1.44072	0.76970
C	-3.85619	3.00336	1.00606
C	-2.82637	2.27932	1.57975
H	-2.60456	2.34287	2.64204
H	-4.45930	3.65215	1.63905
H	-4.95700	3.50922	-0.78758
H	0.60518	-0.41627	-1.59211
O	1.14070	1.24192	-0.06822
C	2.40892	1.12579	-0.32924
C	3.20083	2.40613	-0.02878
O	2.96869	0.10138	-0.71196
H	-3.56394	2.00292	-2.23677
C	-1.50427	0.44023	-1.38625
O	-1.67387	0.15997	-2.54951
O	-1.05754	0.71789	1.26513
C	2.50323	-2.22781	1.53159
H	3.00933	-3.19636	1.42488
H	3.10704	-1.47647	1.00944
H	2.47645	-1.97629	2.59561
C	1.90382	-2.77382	-1.48796
H	2.73966	-2.07147	-1.42608
H	2.27600	-3.79131	-1.30851
H	1.49329	-2.73248	-2.50155
C	-1.25060	-2.87576	-1.94396
H	-1.02893	-3.92128	-2.19089
H	-2.33542	-2.76960	-1.85595
H	-0.93833	-2.23874	-2.77838
C	-2.61343	-2.12914	0.91105
H	-3.22271	-1.95698	0.01840
H	-2.93633	-3.07298	1.36929
H	-2.82709	-1.31879	1.61660
C	-0.34375	-1.78210	3.01374
H	-0.75177	-0.76249	3.07987
H	-1.08491	-2.46548	3.44603
H	0.56755	-1.83205	3.61564
C	4.52514	2.37594	-0.78262
H	5.11517	3.26813	-0.53526
H	5.10658	1.48544	-0.52472
H	4.36327	2.36374	-1.86707
C	2.40958	3.65598	-0.40261
H	1.46445	3.70717	0.14554
H	2.99962	4.55246	-0.16991
H	2.17916	3.67369	-1.47497
C	3.46438	2.39312	1.48127
H	4.02366	1.49382	1.77222

Frequencies

22.2662	30.0753	36.2542
45.6310	57.7525	80.2531
94.1109	121.2146	128.4970
141.4676	157.8219	164.6265
169.8860	178.3314	181.7525
192.7819	206.2985	210.7402
218.9661	223.7833	240.6645
242.6141	247.2857	250.7498
259.6363	265.5475	276.3580
284.5940	290.4532	299.6233
301.1185	302.2028	314.5715
323.7881	335.9066	350.6608
378.8416	391.7167	414.0327
426.9393	444.5523	448.2749
473.5332	532.5571	534.1059
541.3901	552.5382	570.5422
572.3271	594.3947	604.3193
613.0662	621.6328	643.7646
649.5053	669.4126	756.3226
765.6532	782.1791	792.9702
810.8477	813.9814	820.4792
860.5346	866.7305	890.8890
921.0103	943.6655	944.9364
955.2137	955.7229	956.6887
958.5108	971.5986	982.4701
1021.3380	1031.3654	1041.4651
1042.9466	1043.7086	1045.5833
1049.0314	1052.3049	1087.7949
1093.4995	1110.4398	1117.0866
1147.7324	1176.8672	1189.0197
1205.4348	1239.4247	1249.1822
1266.2059	1266.7927	1341.0894
1361.7507	1363.0005	1370.8247
1380.2300	1385.2837	1390.3923
1392.3047	1393.8550	1401.4494
1417.8901	1423.6618	1430.8675
1440.7882	1444.4463	1450.1028
1451.0970	1452.3662	1458.7973
1461.9755	1462.7937	1464.2315
1465.7179	1469.2613	1476.1445
1478.3575	1482.6658	1486.3576
1487.3722	1489.5248	1502.2955
1518.0758	1531.1723	1586.4311
1628.3835	1662.1793	1756.8064
1816.8579	2205.5898	3018.4750
3023.6893	3030.4207	3035.9906
3037.2237	3039.3467	3043.4064
3043.9595	3098.2099	3109.8019
3110.9453	3118.6322	3120.4330
3122.4426	3128.6345	3129.3150
3132.1277	3143.1684	3144.0160
3146.9267	3150.6300	3150.6753
3154.4056	3173.0657	3191.6669
3194.9575	3202.0361	3209.7896

H	4.05947	3.27016	1.76784
H	2.52330	2.41529	2.04307
H	-2.80335	-1.22132	2.48290
H	-1.37192	-1.01392	5.58417
H	-1.60493	-2.14965	4.22902
Ir	1.06614	-0.33518	-0.31907
H	-1.75239	0.62648	0.33798
C	-3.38056	-0.40976	-0.65861
C	-4.28232	0.51666	-0.11329
C	-3.88073	-1.44938	-1.47227
C	-5.64238	0.43691	-0.35231
H	-3.87904	1.31567	0.50901
C	-5.25399	-1.52911	-1.70883
C	-6.12101	-0.59710	-1.15552
H	-6.32438	1.16466	0.07673
H	-5.63954	-2.33280	-2.33587
H	-7.18654	-0.68124	-1.35624
O	-3.02148	-2.33912	-1.99749
H	-3.51662	-2.99637	-2.50049

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.461420 Electronic Energy = -1260.65251733
Internal Energy (E)= -1260.16164433 Enthalpy (H)= -1260.16070133
Gibbs Free Energy (G)=-1260.24959133 Gibbs Free Energy of Solvation=-1260.28971302

St.Pt.	General Structure	Ball & Stick model
TS-4A		

Cartesian co-ordinate

Atoms	X	Y	Z
C	0.39251	-2.31520	1.10412
C	-0.95230	-2.30024	0.57542
C	-0.88448	-2.48402	-0.87118
C	0.46080	-2.47007	-1.24389
C	1.27406	-2.28214	-0.03251
C	2.12889	1.57762	0.56236
Ir	0.11191	-0.44987	0.01711
C	3.00617	2.47662	1.18044
C	3.87194	3.22778	0.40759
C	2.11262	1.41492	-0.83487
C	3.85776	3.06882	-0.98738
C	2.99999	2.18191	-1.61320
H	2.98834	2.06305	-2.69380
H	4.53834	3.66108	-1.59710
H	4.55567	3.93553	0.86881
H	-0.91295	-0.02257	1.25448
O	-1.31384	0.97468	-0.60761
C	-2.19065	1.29790	0.27648

Frequencies

-318.5904	24.8504	37.7195
44.5605	60.0966	80.4685
96.8214	109.2749	127.9629
135.9322	156.1192	161.8068
168.1338	172.6133	187.5000
197.0635	200.1854	205.6622
208.5358	209.8342	217.1976
233.5929	240.8037	246.2368
251.9776	264.4110	270.5701
275.4130	279.9711	290.4461
302.3124	305.8514	310.4537
329.1813	337.5722	353.8896
372.2321	394.1635	426.2561
427.9157	436.5972	445.5730
474.4309	510.2008	535.9878
538.1655	540.9596	554.0154
572.5412	595.8151	617.9012
618.4469	628.0600	633.1282
643.0311	656.1499	677.9615
760.5140	768.9191	791.4598
809.4649	815.9883	838.0814
860.8842	862.0313	881.3889

C	-3.30606	2.21614	-0.21480
O	-2.18589	0.86084	1.44295
H	2.97948	2.56272	2.26467
C	1.19450	0.73228	1.31375
O	1.11975	0.68556	2.52179
O	1.27975	0.55157	-1.37267
C	2.76436	-2.28992	-0.01725
H	3.15277	-1.91381	0.93466
H	3.16020	-3.30194	-0.17346
H	3.16202	-1.64358	-0.80781
C	0.75729	-2.37769	2.54542
H	0.44609	-3.33900	2.97266
H	1.83662	-2.27430	2.68701
H	0.28633	-1.56483	3.10914
C	-2.20470	-2.39608	1.37706
H	-2.50960	-3.44566	1.48396
H	-2.07314	-1.97045	2.37617
H	-3.02745	-1.85246	0.89987
C	-2.08730	-2.49965	-1.74797
H	-2.74687	-3.34206	-1.50405
H	-2.67005	-1.57711	-1.61543
H	-1.82002	-2.57131	-2.80584
C	1.03568	-2.45320	-2.61314
H	0.27764	-2.64348	-3.37808
H	1.48098	-1.46740	-2.81090
H	1.82761	-3.20480	-2.71729
C	-4.17959	1.37192	-1.14983
H	-5.02455	1.97038	-1.51327
H	-3.60420	1.02250	-2.01492
H	-4.58855	0.49834	-0.62338
C	-4.13611	2.71504	0.96130
H	-3.52377	3.29462	1.66093
H	-4.94514	3.35976	0.59518
H	-4.57650	1.88207	1.51882
C	-2.71209	3.39492	-0.98389
H	-3.52040	4.04439	-1.34374
H	-2.05811	3.99734	-0.34179
H	-2.12561	3.05576	-1.84261
H	-2.80335	-1.22132	2.48290
H	-1.37192	-1.01392	5.58417
H	-1.60493	-2.14965	4.22902
Ir	1.06614	-0.33518	-0.31907
H	-1.75239	0.62648	0.33798
C	-3.38056	-0.40976	-0.65861
C	-4.28232	0.51666	-0.11329
C	-3.88073	-1.44938	-1.47227
C	-5.64238	0.43691	-0.35231
H	-3.87904	1.31567	0.50901
C	-5.25399	-1.52911	-1.70883
C	-6.12101	-0.59710	-1.15552
H	-6.32438	1.16466	0.07673
H	-5.63954	-2.33280	-2.33587
H	-7.18654	-0.68124	-1.35624
O	-3.02148	-2.33912	-1.99749
H	-3.51662	-2.99637	-2.50049

931.2458	945.3855	948.2946
954.6126	957.3228	958.3429
958.8520	964.3589	977.0093
1031.0603	1039.7448	1040.1517
1044.4787	1047.4207	1047.9827
1050.2473	1052.8218	1087.3414
1088.4157	1107.9675	1117.2895
1147.8640	1177.0773	1186.4113
1205.9153	1239.4628	1253.0223
1265.5488	1269.6733	1344.4382
1368.8696	1374.8795	1378.8791
1384.8707	1390.0921	1390.6979
1398.5030	1399.3994	1407.4801
1427.9405	1428.9375	1435.8807
1438.3510	1447.1251	1451.5560
1452.6790	1454.3407	1455.8354
1457.8060	1460.3263	1460.9137
1462.7709	1468.6414	1470.8559
1479.0535	1480.9657	1483.3838
1489.4966	1497.5080	1506.6254
1511.6175	1518.1353	1580.4341
1593.6126	1627.0577	1662.1031
1764.8781	1816.6192	3022.9560
3024.2704	3030.3138	3034.5003
3036.5254	3038.5573	3040.5765
3040.9368	3099.6369	3101.2024
3110.0920	3117.9077	3118.4677
3122.0431	3125.2670	3128.2026
3131.6981	3139.2051	3140.7982
3142.9621	3146.9043	3149.8645
3150.2148	3151.0037	3172.2048
3189.9988	3200.3748	3205.3673

Statistical Thermodynamic Analysis

Temperature=298 K	Pressure=1 atm
Zero-point correction= 0.459311	Electronic Energy = -1260.65072759
Internal Energy (E)= -1260.16259359	Enthalpy (H)= -1260.16164959
Gibbs Free Energy (G)=-1260.24823559	Gibbs Free Energy of Solvation=-1260.28946675

St.Pt.	General Structure	Ball & Stick model
V-1A		

Cartesian co-ordinate

Atoms	X	Y	Z
C	0.45931	-2.06640	1.35480
C	-0.89018	-2.08753	0.87420
C	-0.86450	-2.52356	-0.52957
C	0.46645	-2.65221	-0.93036
C	1.32161	-2.27695	0.20656
C	2.07282	1.68668	0.47114
Ir	0.24007	-0.48109	-0.09100
C	2.85259	2.65965	1.11153
C	3.85194	3.30670	0.41142
C	2.26138	1.37305	-0.89744
C	4.05081	2.99134	-0.94520
C	3.27647	2.05463	-1.60285
H	3.42769	1.82560	-2.65515
H	4.83634	3.50544	-1.49759
H	4.47611	4.05425	0.89415
H	-1.17183	1.21512	1.72965
O	-1.37357	0.91623	-0.67482
C	-2.21966	1.37855	0.10051
C	-3.54724	1.89904	-0.41747
O	-2.09835	1.43010	1.39923
H	2.64910	2.87987	2.15809
C	0.95039	0.98730	1.07622
O	0.43766	1.30034	2.16356
O	1.48415	0.48984	-1.46900
C	2.80953	-2.36301	0.20307
H	3.23983	-1.81615	1.04902
H	3.15439	-3.40434	0.25783
H	3.21625	-1.91573	-0.71104
C	0.87715	-1.83238	2.76372
H	0.76938	-2.74852	3.35807
H	1.92215	-1.51090	2.82059
H	0.27582	-1.04113	3.22455
C	-2.11950	-1.96880	1.70926
H	-2.40751	-2.93929	2.13670
H	-1.97288	-1.26739	2.53796
H	-2.97109	-1.60896	1.11910
C	-2.09002	-2.64775	-1.36592
H	-2.74743	-3.44455	-0.99372
H	-2.67018	-1.71373	-1.35261
H	-1.84913	-2.86778	-2.41006

Frequencies

18.8734	33.7064	59.5472
66.8916	79.1068	83.5237
104.6253	126.3718	129.6155
147.2791	152.3271	159.4640
169.6575	176.3475	180.8473
188.4529	197.1381	203.8278
211.5721	223.3910	227.6976
241.8458	252.7322	264.1363
265.9221	273.7274	276.3723
284.9809	296.2581	303.9757
309.9674	314.0410	324.4384
341.2129	368.9662	392.7757
396.5847	414.6553	419.6139
426.2533	445.6882	465.2976
486.4019	533.2305	537.1900
539.7705	547.7797	556.9302
568.9918	592.8122	601.9229
612.7471	623.9673	630.4002
660.2375	689.3923	761.6765
765.2527	781.4966	788.6964
802.3910	812.0628	856.6815
868.3538	896.3997	912.7404
947.9381	950.9288	951.3281
954.1202	957.9773	959.5241
965.5937	977.3441	1034.4842
1039.5182	1041.1113	1042.3330
1046.6632	1049.8433	1052.2790
1056.7546	1086.7959	1089.2490
1104.8876	1115.2311	1144.5643
1179.5468	1182.1943	1208.1185
1239.0748	1248.4011	1263.7369
1276.8931	1339.7961	1350.2689
1366.6126	1374.3936	1380.4945
1391.5894	1393.7598	1394.6950
1396.3521	1399.9691	1417.3470
1428.5177	1434.1931	1440.9895
1448.5724	1450.8282	1453.2953
1456.2571	1458.0668	1459.7786
1462.1979	1463.5180	1469.6024
1470.3223	1474.7453	1481.6574
1485.1453	1488.3064	1495.8551
1505.1630	1510.9514	1520.4603
1521.5694	1533.9806	1589.8440
1613.2034	1657.8868	1668.8237

C	1.00250	-2.93281	-2.28977	1742.2187	3018.3892	3021.9813
H	0.20253	-3.09303	-3.01880	3026.3916	3028.9060	3031.7469
H	1.60833	-2.08647	-2.63874	3039.9485	3040.0483	3045.5617
H	1.64248	-3.82457	-2.28702	3084.2274	3088.4227	3098.7110
C	-4.62993	0.92749	0.07145	3103.5935	3109.1884	3113.9169
H	-5.60939	1.26266	-0.29081	3123.6733	3124.4879	3134.0904
H	-4.45904	-0.08570	-0.31933	3134.7103	3136.0598	3137.4713
H	-4.66282	0.87918	1.16519	3140.2030	3140.3013	3144.2242
C	-3.80767	3.29563	0.15022	3144.4847	3152.4007	3165.8787
H	-3.03093	4.00259	-0.16491	3183.3405	3197.7228	3203.5312
H	-4.77014	3.66664	-0.22270			
H	-3.84005	3.28599	1.24369			
C	-3.53762	1.93911	-1.94040			
H	-4.50272	2.31477	-2.30106			
H	-2.74749	2.59662	-2.31846			
H	-3.37186	0.94438	-2.36815			
H	-2.80335	-1.22132	2.48290			
H	-1.37192	-1.01392	5.58417			
H	-1.60493	-2.14965	4.22902			
Ir	1.06614	-0.33518	-0.31907			
H	-1.75239	0.62648	0.33798			
C	-3.38056	-0.40976	-0.65861			
C	-4.28232	0.51666	-0.11329			
C	-3.88073	-1.44938	-1.47227			
C	-5.64238	0.43691	-0.35231			
H	-3.87904	1.31567	0.50901			
C	-5.25399	-1.52911	-1.70883			
C	-6.12101	-0.59710	-1.15552			
H	-6.32438	1.16466	0.07673			
H	-5.63954	-2.33280	-2.33587			
H	-7.18654	-0.68124	-1.35624			
O	-3.02148	-2.33912	-1.99749			
H	-3.51662	-2.99637	-2.50049			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.465016 Electronic Energy = -1260.68475717
Internal Energy (E)= -1260.19071417 Enthalpy (H)= -1260.18977117
Gibbs Free Energy (G)=-1260.27702417 Gibbs Free Energy of Solvation=-1260.31539033

St.Pt.	General Structure	Ball & Stick model
V'-1A		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.30892	2.52206	0.81999
C	1.06986	2.12582	0.86410

Frequencies

21.0600	33.7471	43.4017
59.0822	76.6690	81.6615
84.2892	95.3306	100.5417
106.7825	117.1470	121.0116
137.6476	142.9207	149.5028
152.5925	159.1690	169.8884

C	1.57254	2.10696	-0.51289
C	0.49391	2.30824	-1.37895
C	-0.71056	2.50313	-0.56428
C	-2.74545	-0.69597	0.52002
Ir	-0.15003	0.49523	-0.01022
C	-2.54139	-0.84387	-0.86998
C	-3.57583	-1.41344	-1.64298
C	-3.93305	-1.11873	1.12967
C	-4.74726	-1.81045	-1.02444
C	-4.94096	-1.67097	0.36096
H	-4.02922	-1.00537	2.20819
H	-5.87220	-1.99814	0.81647
H	-5.53916	-2.25015	-1.62913
H	-3.42104	-1.53892	-2.71197
C	1.01441	-1.40696	0.13917
C	2.39886	-1.22088	-0.42624
C	0.22474	-2.57975	-0.48993
O	0.48564	-2.92874	-1.60950
N	1.04011	-1.48133	1.52319
N	0.99149	-1.53516	2.64525
C	2.99838	1.92508	-0.89473
H	3.10760	1.34534	-1.81663
H	3.47521	2.90254	-1.04627
H	3.56098	1.41494	-0.10495
C	1.88469	2.02944	2.10889
H	2.71998	1.32886	1.99410
H	2.30403	3.00150	2.40305
H	1.26580	1.66526	2.93794
C	-1.14352	2.87884	1.99845
H	-0.99282	2.17095	2.82019
H	-0.88620	3.88592	2.35110
H	-2.21057	2.86790	1.75380
C	-2.05331	2.84131	-1.11374
H	-2.84346	2.64158	-0.38242
H	-2.11141	3.89894	-1.40374
H	-2.27280	2.23534	-1.99957
C	0.49523	2.25669	-2.86589
H	0.30667	3.24734	-3.30118
H	1.44993	1.88923	-3.25439
H	-0.28733	1.57943	-3.22852
C	-1.58156	-0.18778	1.25396
O	-1.39068	-0.50301	-1.39398
O	-1.48729	-0.17395	2.47477
O	2.63335	-1.09181	-1.59729
C	4.70197	-1.15550	0.12877
H	5.22162	-0.66620	0.95893
H	4.76788	-0.51995	-0.76043
O	3.32568	-1.22534	0.55144
C	5.23656	-2.53913	-0.14208
H	4.70472	-2.99914	-0.98106
H	6.29943	-2.49025	-0.39995
H	5.12610	-3.17939	0.73892
C	-0.79366	-3.28475	0.36342
H	-1.63014	-3.57605	-0.27860
H	-0.33118	-4.20125	0.75134
H	-1.17930	-2.70089	1.20152
H	-1.60493	-2.14965	4.22902
Ir	1.06614	-0.33518	-0.31907
H	-1.75239	0.62648	0.33798
C	-3.38056	-0.40976	-0.65861
C	-4.28232	0.51666	-0.11329

184.7294	201.2578	207.3761
211.5672	218.4531	225.9389
230.1074	237.7014	244.7480
257.3906	263.6032	268.2277
276.3404	286.9720	305.1066
313.3393	321.6549	329.2075
333.0640	347.6185	370.4230
373.3087	385.6452	402.5573
413.2698	434.1066	445.7118
458.7948	481.0342	499.4317
502.9285	533.9865	537.1687
538.5612	542.4743	555.3004
567.5770	589.8533	595.5364
601.7262	607.7158	619.1292
626.0199	666.9880	676.8730
758.2027	765.6245	766.1471
774.1926	806.7707	818.2850
822.0220	859.1919	865.3192
876.0169	892.2524	952.6699
957.6405	959.4790	973.9472
977.8677	986.8847	1029.9120
1032.8362	1041.6897	1042.7574
1045.7582	1049.7075	1053.2239
1060.4056	1091.0818	1092.5436
1094.5836	1111.8106	1112.9165
1118.1292	1143.5525	1169.5956
1181.6950	1187.7428	1189.3326
1202.0243	1262.1572	1267.3238
1313.4313	1348.4048	1374.3937
1376.7151	1378.0166	1382.1134
1388.0169	1394.6763	1401.1068
1408.4013	1410.2887	1432.2167
1437.3075	1444.3444	1448.9242
1449.1830	1454.4104	1458.8678
1461.4355	1463.6637	1467.3257
1473.3923	1474.7443	1475.2889
1480.3772	1485.8599	1493.7920
1504.4804	1510.9001	1518.3384
1519.0681	1522.5375	1582.3979
1616.3121	1660.9740	1740.7822
1854.0698	1898.3945	2259.7636
3027.1515	3029.6220	3032.2922
3039.4128	3039.9470	3051.8441
3053.0241	3071.6599	3103.4180
3103.6337	3113.9919	3120.2654
3122.0442	3123.7372	3130.2096
3135.8376	3140.6250	3141.3629
3143.0404	3145.2502	3153.2363
3156.2184	3171.5862	3181.1620
3191.2545	3196.7370	3202.1625

C	-3.88073	-1.44938	-1.47227
C	-5.64238	0.43691	-0.35231
H	-3.87904	1.31567	0.50901
C	-5.25399	-1.52911	-1.70883
C	-6.12101	-0.59710	-1.15552
H	-6.32438	1.16466	0.07673
H	-5.63954	-2.33280	-2.33587
H	-7.18654	-0.68124	-1.35624
O	-3.02148	-2.33912	-1.99749
H	-3.51662	-2.99637	-2.50049

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.461151 Electronic Energy = -1482.11200971
Internal Energy (E)= -1481.61818971 Enthalpy (H)= -1481.61724571
Gibbs Free Energy (G)=-1481.71265471 Gibbs Free Energy of Solvation=-1481.75542602

St.Pt.	General Structure	Ball & Stick model
TS-5A		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.88254	2.51139	0.52458
C	0.43802	2.27857	1.05521
C	1.35076	2.20252	-0.07214
C	0.60098	2.28760	-1.27584
C	-0.79269	2.43086	-0.90037
C	-2.66524	-0.87864	0.53503
Ir	-0.14699	0.44978	-0.05224
C	-2.46904	-1.03965	-0.85512
C	-3.49988	-1.63636	-1.61159
C	-3.84721	-1.30057	1.15881
C	-4.66465	-2.03173	-0.98050
C	-4.85471	-1.86951	0.40326
H	-3.94030	-1.16866	2.23538
H	-5.78266	-2.19334	0.86757
H	-5.45599	-2.48735	-1.57393
H	-3.35103	-1.77588	-2.67958
C	1.10653	-1.17428	0.05260
C	2.54516	-0.92544	-0.32988
C	0.59473	-2.46242	-0.62013
O	0.97215	-2.71427	-1.73798
N	1.18594	-1.54129	1.65894
N	0.90503	-1.45177	2.73798
C	2.83402	2.16581	0.04315
H	3.29906	1.76768	-0.86331
H	3.21891	3.18045	0.20871
H	3.16064	1.55303	0.89219
C	0.79863	2.28541	2.50119

Frequencies

-406.2881	33.1976	36.2252
40.2585	58.0581	73.6964
84.6705	88.2114	101.1761
108.9350	118.8533	127.6333
136.7210	142.7227	145.8577
151.9946	171.1844	179.4424
185.6951	192.7917	203.5537
205.5448	221.1938	226.4721
229.1707	233.6912	238.7243
247.8004	256.1284	264.1308
266.8661	280.4115	286.8752
291.0814	296.8022	308.6201
316.1617	319.4512	329.9280
342.5102	358.8468	377.8200
401.8443	409.5265	415.1575
428.5488	435.3686	443.6902
480.5247	507.4253	534.3979
540.1587	541.8406	549.1093
564.6993	570.6738	589.3022
591.7130	601.4871	609.1775
624.5211	661.3057	673.2572
708.2319	747.7614	762.2591
765.1758	799.8081	813.5128
815.1294	858.5430	865.1094
877.7168	887.8854	899.1641
950.5668	952.8835	956.7803
969.0307	975.9346	1006.8921
1035.5488	1041.4364	1043.5021
1045.1792	1049.4754	1051.4912
1056.2587	1085.9030	1089.4858
1093.6688	1110.4244	1113.7482

H	1.80819	1.88850	2.65824	1119.4477	1144.9938	1179.9677
H	0.76805	3.29748	2.92628	1182.6374	1186.6478	1201.4841
H	0.10736	1.64941	3.06864	1207.7652	1267.3393	1278.6695
C	-2.10184	2.77290	1.33900	1315.7693	1347.1313	1378.9814
H	-2.06673	2.22493	2.28630	1381.5144	1382.5854	1385.7437
H	-2.18561	3.84294	1.56952	1389.8100	1397.2183	1399.7253
H	-3.01447	2.47031	0.81422	1406.4575	1414.2765	1441.9590
C	-1.91767	2.51761	-1.87173	1444.4419	1450.2703	1454.4043
H	-2.88858	2.42595	-1.37464	1454.9616	1457.3605	1460.2529
H	-1.89854	3.47423	-2.40924	1463.5356	1466.0717	1467.6223
H	-1.84780	1.71006	-2.60967	1470.2368	1473.1141	1479.9313
C	1.11542	2.23978	-2.67278	1480.1056	1484.7727	1487.4858
H	1.29160	3.24699	-3.07539	1492.3237	1499.4371	1509.1142
H	2.05055	1.67451	-2.73381	1517.0306	1521.6517	1547.1297
H	0.39798	1.73965	-3.33270	1614.9391	1660.9124	1731.5516
C	-1.50920	-0.33009	1.24712	1837.8838	1877.8333	2265.4697
O	-1.33259	-0.67678	-1.39523	3028.4144	3032.3077	3035.9123
O	-1.40701	-0.28079	2.46628	3036.3069	3038.7763	3047.3945
O	2.85949	-0.57164	-1.43752	3055.1572	3075.0802	3107.0931
C	4.80858	-1.00178	0.34043	3109.7230	3115.0836	3115.4334
H	5.29608	-0.78152	1.29476	3119.7607	3126.5530	3133.5551
H	4.92919	-0.14433	-0.33020	3139.2385	3142.2411	3143.2938
O	3.41275	-1.14221	0.67327	3146.5988	3150.2669	3161.7155
C	5.33292	-2.26837	-0.28839	3171.7103	3174.2864	3181.0540
H	4.83061	-2.45756	-1.24196	3183.2872	3198.2653	3203.3735
H	6.40726	-2.17787	-0.47908			
H	5.17256	-3.12607	0.37262			
C	-0.32585	-3.36935	0.14655			
H	-0.85931	-3.99306	-0.57459			
H	0.27224	-4.02458	0.79339			
H	-1.04764	-2.83706	0.77308			
H	-1.60493	-2.14965	4.22902			
Ir	1.06614	-0.33518	-0.31907			
H	-1.75239	0.62648	0.33798			
C	-3.38056	-0.40976	-0.65861			
C	-4.28232	0.51666	-0.11329			
C	-3.88073	-1.44938	-1.47227			
C	-5.64238	0.43691	-0.35231			
H	-3.87904	1.31567	0.50901			
C	-5.25399	-1.52911	-1.70883			
C	-6.12101	-0.59710	-1.15552			
H	-6.32438	1.16466	0.07673			
H	-5.63954	-2.33280	-2.33587			
H	-7.18654	-0.68124	-1.35624			
O	-3.02148	-2.33912	-1.99749			
H	-3.51662	-2.99637	-2.50049			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.459126 Electronic Energy = -1482.10456030
Internal Energy (E)= -1481.6129093 Enthalpy (H)= -1481.6119653
Gibbs Free Energy (G)=-1481.7063383 Gibbs Free Energy of Solvation=-1481.74581038

St.Pt.	General Structure	Ball & Stick model
VI-1A		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.19843	2.26442	0.73011
C	0.08697	2.03453	1.34587
C	1.10081	2.19999	0.32785
C	0.44021	2.52278	-0.90721
C	-0.97185	2.54177	-0.65170
C	-2.58472	-1.15821	0.44832
Ir	-0.17672	0.38158	-0.14111
C	-2.59742	-0.92115	-0.93830
C	-3.72199	-1.32724	-1.68267
C	-3.65115	-1.80179	1.08881
C	-4.77055	-1.95438	-1.03385
C	-4.74982	-2.19755	0.34976
H	-3.58648	-1.97268	2.16141
H	-5.59074	-2.69183	0.82884
H	-5.63457	-2.27078	-1.61576
H	-3.73378	-1.15241	-2.75548
C	1.12627	-0.95329	-0.49858
C	2.55429	-0.55042	-0.70312
C	0.99153	-2.40394	-0.87489
O	1.85435	-2.86685	-1.60582
N	1.55570	-1.96420	2.73418
N	1.98230	-1.05920	3.20310
C	2.56839	2.26343	0.57900
H	3.13748	2.07118	-0.33603
H	2.84147	3.25910	0.95183
H	2.88235	1.52806	1.32972
C	0.32416	1.85336	2.80541
H	1.39360	1.81378	3.03283
H	-0.10868	2.69119	3.36641
H	-0.13195	0.92404	3.16613
C	-2.50649	2.26432	1.44709
H	-2.46360	1.63131	2.33995
H	-2.77858	3.27854	1.76732
H	-3.31802	1.88252	0.81780
C	-2.01917	2.74089	-1.69005
H	-3.00862	2.45640	-1.31930
H	-2.06175	3.78949	-2.00928
H	-1.81205	2.12036	-2.56942
C	1.10790	2.80473	-2.20732
H	1.48730	3.83533	-2.23600
H	1.94876	2.12126	-2.36956
H	0.41016	2.68444	-3.04193
C	-1.37576	-0.71512	1.14696
O	-1.55626	-0.35849	-1.50824
O	-1.16399	-0.86842	2.33022
O	2.94733	0.12127	-1.63225
C	4.75601	-0.83174	0.10467
H	5.16669	-0.90171	1.11654
H	4.94357	0.17475	-0.28709
O	3.33814	-1.01182	0.27818

Frequencies

28.0312	45.6353	49.2787
58.7207	64.5846	81.6042
81.8076	95.8969	100.3461
106.9527	112.2438	126.3521
137.7107	144.8851	147.0569
155.5978	157.9459	162.3309
165.5779	177.2892	178.1968
184.5961	191.9687	196.3478
199.6785	217.8602	231.1888
238.5820	247.7208	259.6876
263.0844	276.2404	296.4705
301.6673	304.3796	312.9875
319.1313	322.3723	333.5463
353.3167	356.5731	360.6405
373.7619	389.5600	401.5038
424.7526	432.1348	458.3085
476.4102	490.8312	531.1299
539.5613	541.1442	550.2710
568.9257	579.7993	590.9778
600.1854	603.7469	626.7316
644.4911	670.6856	680.6179
736.3746	754.2317	758.5172
769.1941	812.7267	815.9757
817.2886	858.4135	861.0819
881.4906	888.5856	950.3014
956.0298	959.0043	962.2208
981.8622	1010.6251	1023.7681
1032.1492	1035.8592	1041.5030
1043.7075	1047.7125	1050.8874
1053.6311	1084.4382	1090.5408
1111.8534	1112.4911	1117.3549
1128.0007	1149.0700	1177.8319
1185.9804	1190.1569	1204.3479
1245.5977	1264.4979	1291.1551
1324.4635	1341.9443	1376.9401
1380.8446	1384.8388	1387.2416
1390.7016	1393.2451	1395.6669
1404.7549	1419.8582	1436.6760
1438.7802	1442.5738	1443.8862
1453.9256	1457.2532	1462.1949
1464.1267	1467.0139	1469.5671
1477.2904	1478.5522	1481.4781
1485.2156	1487.8491	1488.4251
1493.8846	1501.1933	1510.8163
1514.5322	1524.1082	1532.2203
1624.2392	1660.1349	1777.0023
1795.2841	1820.7440	2466.3705
3035.8459	3037.1273	3041.5567
3041.9289	3044.0837	3053.5509
3057.0916	3065.6424	3116.5759
3117.2098	3119.8553	3122.9165
3125.6652	3127.4197	3137.9829
3145.0340	3145.1078	3146.4989
3151.4154	3155.6001	3159.1372

C	5.31066	-1.89607	-0.80942	3169.9501	3171.0664	3171.5824
H	4.90408	-1.78628	-1.81905	3190.9190	3203.0741	3206.9298
H	6.40174	-1.81897	-0.86399			
H	5.04818	-2.89235	-0.43993			
C	-0.14463	-3.24058	-0.37972			
H	-1.07484	-2.95602	-0.88450			
H	0.07527	-4.28728	-0.60147			
H	-0.30384	-3.10739	0.69612			
H	-1.60493	-2.14965	4.22902			
Ir	1.06614	-0.33518	-0.31907			
H	-1.75239	0.62648	0.33798			
C	-3.38056	-0.40976	-0.65861			
C	-4.28232	0.51666	-0.11329			
C	-3.88073	-1.44938	-1.47227			
C	-5.64238	0.43691	-0.35231			
H	-3.87904	1.31567	0.50901			
C	-5.25399	-1.52911	-1.70883			
C	-6.12101	-0.59710	-1.15552			
H	-6.32438	1.16466	0.07673			
H	-5.63954	-2.33280	-2.33587			
H	-7.18654	-0.68124	-1.35624			
O	-3.02148	-2.33912	-1.99749			
H	-3.51662	-2.99637	-2.50049			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.459950 Electronic Energy = -1482.15533580
Internal Energy (E)= -1481.6617658 Enthalpy (H)= -1481.6608218
Gibbs Free Energy (G)=-1481.7579488 Gibbs Free Energy of Solvation=-1481.79183356

St.Pt.	General Structure	Ball & Stick model
VI'-1A		

Cartesian co-ordinate

Atoms	X	Y	Z
C	1.40660	-2.39486	-0.53404
C	2.27180	-1.32740	-1.00393
C	2.76877	-0.63268	0.15034
C	2.11982	-1.19854	1.31345
C	1.30495	-2.30268	0.87532
C	-2.22798	-1.11402	-0.45802
Ir	0.54583	-0.27986	0.00309
C	-2.15864	-0.68198	0.88306
C	-3.30473	-0.83535	1.69224
C	-3.40184	-1.66552	-0.99100
C	-4.44853	-1.39752	1.15641
C	-4.51274	-1.81794	-0.18431

Frequencies

-42.8306	-23.6871	24.3706
32.3683	40.7832	50.3152
58.4521	65.3812	80.5939
87.3917	102.0036	108.2722
115.2332	122.3005	127.3993
133.7333	137.0594	145.9494
152.3114	158.7015	167.0974
171.1667	180.2892	186.9837
189.3357	196.5312	209.4970
212.2970	217.7227	229.2541
240.6028	247.3633	257.4827
266.9274	271.7307	284.9682
289.0037	292.4830	297.6530
316.6163	317.6010	328.0172
369.4894	374.0938	395.5872
409.0958	412.3871	429.2227

H	-3.40561	-1.96586	-2.03682
H	-5.42653	-2.25748	-0.57516
H	-5.32458	-1.51496	1.79209
H	-3.25946	-0.50389	2.72702
C	0.23348	1.53143	-0.48203
C	1.10553	2.36701	-1.36258
C	-0.92269	2.25119	0.12663
C	-3.25105	2.53135	0.18225
H	-3.27253	2.17552	1.22100
H	-3.14819	3.62319	0.21022
C	-4.45433	2.07856	-0.59918
H	-5.36779	2.48721	-0.15497
H	-4.39524	2.41877	-1.63831
H	-4.52777	0.98498	-0.59728
O	-2.09059	1.97117	-0.45627
O	-0.78634	3.02928	1.04674
C	3.83769	0.40046	0.15454
H	3.90851	0.90306	1.12431
H	4.80901	-0.06911	-0.04906
H	3.65692	1.15556	-0.61800
C	2.69694	-1.14206	-2.41752
H	3.19798	-0.18129	-2.55079
H	3.37243	-1.94939	-2.73151
H	1.82282	-1.14913	-3.07807
C	0.80044	-3.43191	-1.41058
H	0.53243	-3.01764	-2.38673
H	1.51879	-4.24644	-1.57129
H	-0.10615	-3.86219	-0.97144
C	0.46144	-3.12987	1.78229
H	-0.22840	-3.77047	1.22422
H	1.08229	-3.77509	2.41709
H	-0.13780	-2.49055	2.44256
C	2.29916	-0.81260	2.74059
H	2.92690	-1.54028	3.27241
H	2.76253	0.17248	2.84177
H	1.32862	-0.76925	3.24852
C	-1.02665	-0.90789	-1.25680
O	-1.05816	-0.14556	1.34882
O	-0.88960	-1.10623	-2.43693
N	2.24084	3.30904	1.54001
N	2.32992	2.70467	2.46082
C	0.69149	3.79270	-1.61721
H	0.64765	4.35740	-0.68002
H	1.40003	4.25595	-2.30635
H	-0.31595	3.82068	-2.05293
O	2.09856	1.90166	-1.90307
H	-1.60493	-2.14965	4.22902
Ir	1.06614	-0.33518	-0.31907
H	-1.75239	0.62648	0.33798
C	-3.38056	-0.40976	-0.65861
C	-4.28232	0.51666	-0.11329
C	-3.88073	-1.44938	-1.47227
C	-5.64238	0.43691	-0.35231
H	-3.87904	1.31567	0.50901
C	-5.25399	-1.52911	-1.70883
C	-6.12101	-0.59710	-1.15552
H	-6.32438	1.16466	0.07673
H	-5.63954	-2.33280	-2.33587
H	-7.18654	-0.68124	-1.35624
O	-3.02148	-2.33912	-1.99749
H	-3.51662	-2.99637	-2.50049

464.0558	475.8741	535.5765
539.0818	539.7949	551.7352
561.8272	580.8556	584.1392
598.3950	604.3529	621.3699
631.5526	653.9414	666.5036
732.0769	759.9849	765.2603
807.0766	809.7169	810.0065
820.6133	846.9797	862.6757
876.8082	886.4561	930.2553
948.3453	958.3333	963.2800
974.6599	1019.8291	1023.9300
1031.3751	1035.7876	1041.1087
1043.2129	1043.5901	1048.5211
1059.3504	1086.4367	1087.9809
1109.7218	1110.5376	1119.4667
1142.0494	1142.1285	1170.9492
1180.6637	1186.5986	1206.3127
1236.7854	1266.7879	1279.5513
1316.5326	1343.8962	1364.5812
1375.3053	1377.4791	1383.2113
1387.7237	1391.2564	1394.6997
1397.4498	1421.5483	1431.1367
1437.9106	1438.8282	1442.3851
1445.3216	1447.4841	1451.4813
1456.8766	1459.2563	1462.3894
1464.7210	1466.3375	1468.1306
1472.2749	1482.3678	1486.8779
1489.9260	1497.4418	1499.5712
1511.9151	1517.1029	1552.6910
1618.1850	1657.7555	1770.8050
1821.6465	1828.6582	2465.5694
3034.6870	3037.4249	3038.0025
3038.7032	3044.0553	3044.7858
3045.3126	3048.5078	3097.6363
3111.9555	3117.7037	3117.9587
3122.6745	3129.4750	3134.9866
3142.0190	3142.1673	3142.6984
3149.1838	3163.9195	3166.4995
3174.2036	3178.8421	3179.5178
3186.3767	3196.6739	3204.6018

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.456606 Electronic Energy = -1482.16011681
Internal Energy (E)= -1481.66997981 Enthalpy (H)= -1481.66903581
Gibbs Free Energy (G)=-1481.76731481 Gibbs Free Energy of Solvation=-1481.79952183

St.Pt.	General Structure	Ball & Stick model
TS-6A		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.66722	-2.15707	0.56558
C	-2.32292	-0.99202	1.15814
C	-2.88683	-0.22301	0.09775
C	-2.53756	-0.88528	-1.15415
C	-1.84519	-2.10912	-0.84005
C	2.03409	-1.04834	0.67411
Ir	-0.70644	-0.25657	-0.16118
C	1.97130	-1.09532	-0.74230
C	3.03328	-1.72725	-1.42475
C	3.09590	-1.63674	1.37681
C	4.07040	-2.30196	-0.71393
C	4.11405	-2.26896	0.69073
H	3.09346	-1.57259	2.46295
H	4.93755	-2.73500	1.22478
H	4.87247	-2.79704	-1.25918
H	3.00003	-1.75413	-2.51130
C	0.24819	1.34104	0.41364
C	-0.26643	2.23668	1.49041
C	1.32077	1.92719	-0.45613
C	3.61765	2.05074	-0.94390
H	3.40478	1.62501	-1.93401

Frequencies

-253.5910	-100.1113	33.3010
36.0907	49.1167	56.6910
79.6683	88.4806	90.6722
93.5775	98.9754	100.9239
111.9843	118.2653	123.8773
134.5307	139.2509	151.6981
159.4533	164.7969	167.7695
177.4192	179.6663	195.1765
202.3899	215.7729	223.4796
230.3061	236.0879	243.4707
247.2506	258.9213	282.7912
290.4765	299.4287	305.4860
314.5274	317.4774	320.8251
328.1096	356.0855	360.4947
380.6048	392.7605	399.4849
410.9347	419.6852	446.4920
458.1337	468.2061	526.7610
535.7414	542.4206	548.1323
555.6978	559.7568	580.7189
591.0881	597.2764	608.0271
616.4501	640.8050	683.2689
723.0976	754.7360	767.4792
799.2835	809.1232	810.2546
818.5773	820.9161	861.2414
875.1778	889.3430	932.8747

H	3.60682	3.14266	-1.04810	957.5790	964.5660	972.8329
C	4.90801	1.53462	-0.36498	982.1556	1022.4781	1028.1358
H	5.75062	1.81676	-1.00450	1032.7043	1033.6350	1038.2119
H	5.07954	1.95057	0.63341	1041.1512	1043.4635	1044.9025
H	4.88555	0.44166	-0.28211	1047.8725	1093.1233	1095.5352
O	2.56604	1.65518	-0.05006	1108.9906	1113.1813	1118.5022
O	1.06769	2.64644	-1.39729	1137.0665	1145.6109	1180.6760
C	-3.71733	1.00144	0.25782	1183.8416	1186.7690	1199.8456
H	-3.85026	1.52641	-0.69362	1240.5002	1260.4190	1291.8354
H	-4.71460	0.74116	0.63591	1306.7510	1345.9091	1371.8501
H	-3.24989	1.69091	0.97101	1376.4130	1379.4511	1380.9751
C	-2.47819	-0.76033	2.61978	1390.3267	1393.5467	1394.4156
H	-3.04392	0.15210	2.81715	1401.4496	1419.2956	1429.1289
H	-3.00156	-1.61011	3.07760	1437.9661	1440.5978	1447.3752
H	-1.50586	-0.64099	3.10853	1451.1233	1456.2016	1457.8778
C	-0.95249	-3.20936	1.34016	1458.1322	1459.8772	1464.8658
H	-0.63307	-2.82695	2.31430	1472.7670	1474.9366	1477.4117
H	-1.60445	-4.07478	1.51629	1481.5926	1486.3260	1493.0364
H	-0.05824	-3.55897	0.81258	1499.4776	1514.1015	1517.1449
C	-1.26506	-3.04214	-1.84492	1522.1142	1532.9635	1553.4895
H	-0.53631	-3.71871	-1.38722	1609.6051	1660.2344	1775.9316
H	-2.04514	-3.65246	-2.31700	1827.3603	1843.7514	2468.5217
H	-0.74333	-2.48794	-2.63409	3036.1499	3038.4437	3038.7445
C	-2.93515	-0.44932	-2.52066	3040.0755	3040.5383	3041.0847
H	-3.90041	-0.88975	-2.80591	3041.7286	3046.4009	3095.4862
H	-3.02939	0.63950	-2.58728	3118.2873	3118.6204	3120.3454
H	-2.19234	-0.75952	-3.26289	3120.7705	3124.0564	3131.1401
C	0.99534	-0.32364	1.39204	3139.7867	3140.8249	3140.8622
O	0.97744	-0.55141	-1.39532	3151.2131	3151.7290	3156.0015
O	0.82966	-0.24709	2.57910	3169.6759	3171.7895	3176.2120
N	-1.78088	3.64820	-1.02772	3189.6289	3200.1149	3205.5520
N	-2.17239	3.17939	-1.94849			
C	0.44769	3.54164	1.72250			
H	0.48508	4.13987	0.80498			
H	-0.06207	4.10002	2.50996			
H	1.48492	3.34404	2.02279			
O	-1.22272	1.91066	2.17577			
H	-1.60493	-2.14965	4.22902			
Ir	1.06614	-0.33518	-0.31907			
H	-1.75239	0.62648	0.33798			
C	-3.38056	-0.40976	-0.65861			
C	-4.28232	0.51666	-0.11329			
C	-3.88073	-1.44938	-1.47227			
C	-5.64238	0.43691	-0.35231			
H	-3.87904	1.31567	0.50901			
C	-5.25399	-1.52911	-1.70883			
C	-6.12101	-0.59710	-1.15552			
H	-6.32438	1.16466	0.07673			
H	-5.63954	-2.33280	-2.33587			
H	-7.18654	-0.68124	-1.35624			
O	-3.02148	-2.33912	-1.99749			
H	-3.51662	-2.99637	-2.50049			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.457899 Electronic Energy = -1482.14232105
Internal Energy (E)= -1481.65156905 Enthalpy (H)= -1481.65062605

Gibbs Free Energy (G)=-1481.74632805 Gibbs Free Energy of Solvation=-1481.78260657

St.Pt.	General Structure	Ball & Stick model
VII-1A		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.32683	-2.17580	0.62696
C	-2.05518	-1.10938	1.28687
C	-2.84827	-0.44630	0.29157
C	-2.66708	-1.16493	-0.96605
C	-1.77534	-2.24637	-0.75935
C	2.48208	-0.49172	0.91371
Ir	-0.71449	-0.35593	-0.22708
C	2.25048	-1.07066	-0.36068
C	3.28661	-1.84253	-0.93004
C	3.68324	-0.74851	1.58793
C	4.47572	-2.05334	-0.25462
C	4.68522	-1.51258	1.01864
H	3.80215	-0.30528	2.57481
H	5.61816	-1.68736	1.54801
H	5.25137	-2.65942	-0.72031
H	3.10365	-2.27931	-1.91003
C	0.49398	1.11043	0.73840
C	-0.22693	2.18198	1.56198
C	0.85656	1.61061	-0.61082
C	2.52325	2.13948	-2.19960
H	2.04274	1.33196	-2.76304
H	2.17964	3.09634	-2.61019
C	4.02256	2.01516	-2.17149
H	4.42409	2.06004	-3.18870
H	4.47455	2.82181	-1.58585
H	4.31341	1.05785	-1.72372
O	2.07535	2.04759	-0.82671
O	-0.01738	1.52547	-1.49111
C	-3.83475	0.64088	0.53407
H	-4.07760	1.17496	-0.39034
H	-4.77103	0.22915	0.93452
H	-3.43705	1.36662	1.24877
C	-1.98013	-0.80892	2.74254
H	-2.44819	0.14916	2.97536
H	-2.47923	-1.60413	3.31194
H	-0.93925	-0.74812	3.08428
C	-0.39087	-3.12927	1.28159
H	0.12853	-2.65253	2.11993
H	-0.92990	-4.00549	1.66613
H	0.37019	-3.47856	0.57533
C	-1.22240	-3.19606	-1.76241
H	-0.13024	-3.09230	-1.81790
H	-1.45437	-4.23409	-1.49283

Frequencies

32.9226	45.9883	52.1026
60.8856	69.4049	79.0231
85.4475	93.3594	100.2119
112.5803	115.3773	121.2333
129.3164	136.4440	144.3268
153.6977	169.2125	172.9024
173.7195	179.0331	181.9636
183.4226	193.3201	205.7237
209.2869	212.8617	219.1870
237.9086	240.9467	253.0480
263.8302	265.2256	277.6383
287.6441	291.2347	304.1437
308.0246	312.8177	321.6370
330.4828	358.6962	391.8000
401.8250	410.8301	420.8034
426.4884	445.1245	483.1059
499.4335	528.7436	538.0116
540.3095	542.7468	554.1090
558.1760	578.0268	588.2995
598.5206	611.8683	629.3832
654.8196	669.1315	729.1341
746.5298	761.1292	801.1565
811.7403	816.8622	817.8821
838.1501	858.3966	865.9204
882.0066	897.4200	959.4946
959.6428	972.2318	977.1009
996.9524	1018.4816	1036.9169
1040.2503	1044.9077	1046.3106
1052.2219	1053.9895	1061.5660
1085.5421	1093.9717	1101.5570
1116.9253	1125.6886	1131.7584
1151.6478	1164.2441	1181.1484
1183.9682	1191.3685	1212.3251
1255.2874	1283.6706	1291.6956
1344.2801	1352.4005	1367.4741
1377.2336	1378.2702	1382.5596
1392.8887	1398.2412	1398.6898
1404.7825	1428.0976	1437.9359
1443.6063	1444.7076	1445.2042
1448.0603	1451.7064	1456.9313
1458.0177	1460.6540	1462.2759
1468.7267	1474.8250	1476.2498
1478.6779	1488.4282	1492.0952
1504.5597	1509.4774	1516.5770
1522.5321	1544.7114	1555.5251
1612.7688	1662.5418	1678.4588
1734.7546	1846.6699	2465.2595

H	-1.62586	-3.00986	-2.76202	3026.4063	3035.1635	3036.6532
C	-3.28410	-0.74486	-2.25371	3038.7577	3040.5319	3045.4371
H	-4.35104	-1.00100	-2.27801	3047.8080	3057.1623	3102.4564
H	-3.19921	0.34038	-2.38632	3113.6734	3113.7583	3115.6172
H	-2.79729	-1.22256	-3.10884	3118.2748	3130.8814	3136.4239
C	1.51683	0.40944	1.57153	3139.8381	3141.1537	3144.0716
O	1.13023	-0.94451	-1.04373	3145.4625	3149.4030	3168.7409
O	1.50818	0.57357	2.79135	3172.0694	3173.7483	3183.4953
N	-1.92067	3.64607	-0.64067	3187.5824	3189.6272	3202.4203
N	-2.73715	3.18200	-1.22292			
C	0.58601	3.41429	1.84261			
H	0.91038	3.87719	0.90185			
H	-0.00656	4.12688	2.42052			
H	1.48656	3.13246	2.39935			
O	-1.36416	2.06523	1.96140			
H	-1.60493	-2.14965	4.22902			
Ir	1.06614	-0.33518	-0.31907			
H	-1.75239	0.62648	0.33798			
C	-3.38056	-0.40976	-0.65861			
C	-4.28232	0.51666	-0.11329			
C	-3.88073	-1.44938	-1.47227			
C	-5.64238	0.43691	-0.35231			
H	-3.87904	1.31567	0.50901			
C	-5.25399	-1.52911	-1.70883			
C	-6.12101	-0.59710	-1.15552			
H	-6.32438	1.16466	0.07673			
H	-5.63954	-2.33280	-2.33587			
H	-7.18654	-0.68124	-1.35624			
O	-3.02148	-2.33912	-1.99749			
H	-3.51662	-2.99637	-2.50049			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.460870 Electronic Energy = -1482.18057354
Internal Energy (E)= -1481.68625754 Enthalpy (H)= -1481.68531354
Gibbs Free Energy (G)=-1481.78190754 Gibbs Free Energy of Solvation=-1481.82000879

St.Pt.	General Structure	Ball & Stick model
VII'-1A		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-2.60729	-0.30363	-1.97467
C	-1.87526	-1.50863	-1.76791
C	-2.03982	-1.93757	-0.38547
C	-2.87172	-0.97586	0.27112
C	-3.16516	0.07995	-0.69446

Frequencies

24.5292	41.6572	51.9283
63.1790	70.1069	74.2288
84.5747	88.6479	98.6768
102.3586	107.1075	114.5796
124.0636	133.2972	135.9009
137.8007	141.9224	150.9620
155.6876	161.8620	167.7159
174.2866	176.2305	188.3813
188.7501	198.7297	213.6105

O	1.40877	-0.33037	-1.31351	222.9102	231.4393	240.5303
C	2.29693	-1.34983	-1.22253	248.6516	249.5914	255.9153
O	1.88375	-2.48303	-1.20476	260.2246	266.3550	274.1767
C	3.78609	-1.00493	-1.21651	282.6026	285.9378	298.2980
C	0.43540	2.66790	-0.56910	301.0337	306.7761	309.1161
H	1.83866	0.54051	-1.27845	315.7370	328.9717	341.9788
C	-1.05686	-2.24011	-2.76818	345.8123	364.8196	370.9779
H	-0.13135	-2.61189	-2.31430	380.1096	389.7340	393.3131
H	-1.61984	-3.09962	-3.15632	396.3517	416.1437	426.4432
H	-0.78461	-1.60052	-3.61345	439.5374	444.6911	448.6299
C	-1.52676	-3.21494	0.17790	455.9749	468.5219	494.8612
H	-2.08119	-4.07047	-0.22976	515.7713	531.9065	535.6083
H	-0.46346	-3.35026	-0.05441	540.9749	542.6156	551.0848
H	-1.63927	-3.22761	1.26692	552.2782	576.6549	583.5532
C	-3.98605	1.28938	-0.42928	592.6480	594.5482	606.5665
H	-3.80797	2.05423	-1.19173	632.0201	652.0069	693.4734
H	-5.05514	1.03814	-0.43475	721.0860	757.9443	766.4267
H	-3.72522	1.71527	0.54499	771.2210	772.6932	787.0270
C	-2.67582	0.51734	-3.21469	812.6909	815.4355	819.6433
H	-2.08960	0.06718	-4.02135	857.7892	873.0222	879.2186
H	-3.70992	0.61651	-3.56703	885.6776	902.6585	919.1582
H	-2.27745	1.52393	-3.03659	947.8066	952.5251	961.2206
C	-3.43067	-1.05997	1.64386	964.3508	970.9058	978.4283
H	-4.35264	-1.65643	1.62761	983.5973	994.4335	1011.5085
H	-2.72858	-1.52131	2.34335	1020.6912	1034.0177	1034.8100
H	-3.66405	-0.06554	2.03191	1043.5617	1046.1488	1046.2551
Ir	-1.07379	0.01767	-0.39230	1047.4295	1056.4343	1062.9844
C	4.38248	-1.66730	-2.46326	1096.9979	1098.1112	1104.6304
H	3.98031	-1.22654	-3.38454	1114.0476	1115.8109	1137.7809
H	5.47004	-1.52601	-2.46880	1138.7289	1146.2899	1153.0985
H	4.16769	-2.74055	-2.47195	1173.9671	1185.8903	1188.0512
C	4.08092	0.49267	-1.22858	1191.9548	1222.1836	1232.5543
H	3.73362	0.97975	-0.30821	1241.5530	1268.4052	1271.9805
H	5.16534	0.64265	-1.28253	1288.0929	1304.9133	1335.4136
H	3.65486	1.00284	-2.10520	1344.7749	1372.7810	1377.5186
C	4.38987	-1.62833	0.04380	1380.3291	1383.9123	1384.4754
H	3.95116	-1.18200	0.94561	1387.6863	1390.2396	1392.9569
H	4.21634	-2.70947	0.05835	1397.8983	1407.8641	1415.1368
H	5.47175	-1.44686	0.05676	1426.0863	1432.4243	1433.7016
O	-0.45821	1.85120	-1.07787	1440.6213	1442.6149	1449.1382
C	1.35416	2.32790	0.45783	1452.5751	1454.9932	1458.7040
C	2.35405	3.24784	0.82612	1463.4618	1464.8998	1468.2943
C	0.55067	3.94974	-1.15579	1468.9439	1473.2367	1476.4231
C	2.44861	4.49420	0.24182	1477.9675	1483.2466	1483.7285
C	1.52732	4.83824	-0.75699	1485.6730	1491.8547	1494.0367
C	1.32141	1.04920	1.20857	1499.6088	1502.6485	1506.3627
O	2.35734	0.59283	1.68261	1511.6186	1521.8473	1537.2391
H	-0.15546	4.19820	-1.94469	1541.2430	1551.6237	1608.3311
H	1.58293	5.81688	-1.23066	1665.9593	1745.7567	1783.4384
H	3.21554	5.19742	0.55496	1832.4248	1871.5961	3022.2178
H	3.04641	2.93782	1.60761	3033.9884	3034.4021	3035.8905
C	-0.03206	0.42800	1.45869	3039.3357	3039.6411	3042.9925
C	-0.84586	1.41966	2.32686	3045.8807	3046.1321	3058.4824
C	0.03392	-0.85229	2.22671	3061.6777	3107.4978	3109.3453
C	1.02868	-2.95202	2.50635	3113.2610	3119.8115	3120.0440
H	0.07331	-3.49258	2.53106	3123.1785	3126.3289	3135.2464
H	1.25356	-2.66374	3.54018	3136.1742	3138.0684	3138.9486
C	2.12489	-3.78231	1.89547	3142.0708	3144.4882	3146.7023
H	2.19730	-4.74454	2.41336	3148.2778	3148.6826	3157.6860
H	1.93529	-3.96450	0.83162	3163.9246	3164.6751	3172.1972
H	3.08996	-3.27367	1.98308	3177.6457	3184.2329	3189.1691

O	0.87486	-1.76478	1.71599	3198.0426	3205.3057	3759.6760
O	-0.64598	-1.07940	3.21403			
O	-1.98777	1.74505	2.07936			
C	-0.12379	1.98076	3.52396			
H	-0.84497	2.42988	4.20998			
H	0.46360	1.21125	4.03331			
H	0.57311	2.75865	3.18474			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.603275 Electronic Energy = -1719.55036718
Internal Energy (E)= -1718.90807518 Enthalpy (H)= -1718.90713118
Gibbs Free Energy (G)=-1719.01395018 Gibbs Free Energy of Solvation=-1719.06719524

St.Pt.	General Structure	Ball & Stick model
TS-7A		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-2.17627	-1.19446	-1.98761
C	-1.40387	-2.26771	-1.47764
C	-1.63449	-2.36414	-0.03897
C	-2.63229	-1.38238	0.31332
C	-2.90176	-0.59845	-0.86884
O	1.33238	-0.26604	-0.99174
C	2.47605	-0.94660	-1.07735
O	2.49930	-2.14391	-0.89514
C	3.72777	-0.11256	-1.33646
C	-0.07009	2.60189	-0.90244
H	0.98629	0.68646	-1.40249
C	-0.43419	-3.11914	-2.21548
H	0.53443	-3.13529	-1.70080
H	-0.80761	-4.14950	-2.28078
H	-0.26821	-2.75393	-3.23324
C	-1.06818	-3.41872	0.84453
H	-1.62608	-4.35935	0.74272
H	-0.02138	-3.61626	0.58210
H	-1.10235	-3.10702	1.89456

Frequencies

-913.6295	-124.5750	-120.5385
28.1771	37.5527	38.3347
49.6200	65.1903	71.9455
76.2990	82.8660	90.3160
102.9983	105.7637	115.5011
117.7794	122.1947	126.9955
131.1749	133.6267	143.4092
149.1105	152.4253	160.1335
164.0605	182.2332	183.9067
195.3021	201.1863	206.4329
213.2327	217.3853	224.1447
238.8509	244.5397	251.0218
261.8928	266.9112	289.6281
294.0021	297.5075	300.7371
313.0966	319.8889	320.6903
337.2441	352.0940	367.4983
377.0914	380.2506	387.0538
401.8053	406.1322	412.9386
422.1966	428.1959	436.1814
443.2336	462.3076	491.4458
523.1559	534.8124	536.4730
549.3352	552.6602	559.7218
569.1636	578.1639	588.8285

C	-3.83855	0.55118	-0.97818	596.4607	602.9434	610.6794
H	-3.48241	1.26714	-1.72807	639.4447	648.7846	686.3567
H	-4.83652	0.20919	-1.28319	726.7045	766.3116	775.3723
H	-3.90912	1.08781	-0.02858	776.4384	793.4700	805.1068
C	-2.19647	-0.67727	-3.38257	808.5230	812.9273	826.5911
H	-1.34104	-1.04444	-3.95804	860.5303	873.2008	884.5467
H	-3.11243	-0.98243	-3.90443	891.4115	909.9073	938.8078
H	-2.15104	0.41727	-3.39283	946.8176	949.9677	952.8088
C	-3.30250	-1.26859	1.63486	957.9544	965.4606	975.3739
H	-4.02171	-2.09102	1.74405	977.0200	989.3014	1011.8820
H	-2.57961	-1.33518	2.45479	1026.4976	1030.8006	1032.3057
H	-3.84016	-0.32290	1.73231	1036.4793	1043.1955	1046.8108
Ir	-0.82649	-0.41500	-0.39656	1049.4766	1052.8617	1057.7117
C	4.59272	-0.84463	-2.36014	1088.2311	1090.9003	1101.4088
H	4.10912	-0.87703	-3.34480	1111.1766	1111.8102	1131.6553
H	5.55288	-0.32619	-2.47296	1146.9828	1155.7015	1169.9770
H	4.78522	-1.87310	-2.03991	1173.6754	1183.7475	1187.6620
C	3.41827	1.30327	-1.81392	1194.1334	1221.9041	1235.8314
H	2.88817	1.88548	-1.04853	1242.4493	1265.6373	1283.2669
H	4.35839	1.82719	-2.02418	1286.9966	1311.0586	1322.6255
H	2.82606	1.30987	-2.73897	1347.9226	1365.8555	1371.8102
C	4.45910	-0.04355	0.01113	1372.6533	1379.1990	1379.7229
H	3.81986	0.39548	0.78832	1380.7849	1383.3328	1391.3399
H	4.76418	-1.04533	0.33430	1395.5398	1401.4843	1410.6769
H	5.35668	0.57905	-0.09322	1420.7597	1429.3414	1429.9191
O	-0.16115	1.39455	-1.48986	1436.0075	1438.1529	1444.2880
C	0.54397	2.75582	0.35331	1446.3674	1446.9488	1451.1186
C	0.76902	4.04040	0.85782	1455.2948	1456.9962	1457.4809
C	-0.50063	3.73504	-1.59765	1460.5160	1466.5181	1467.2042
C	0.34052	5.16208	0.16396	1470.5324	1472.6373	1481.3010
C	-0.30426	5.00042	-1.06234	1482.8213	1484.2339	1486.5049
C	0.92552	1.60144	1.21012	1490.0528	1500.9777	1503.7263
O	1.97993	1.61480	1.82544	1508.1967	1512.8140	1514.4062
H	-0.96740	3.59220	-2.56997	1534.5388	1552.8945	1631.2222
H	-0.64627	5.87356	-1.61440	1663.9219	1770.0113	1779.8303
H	0.49930	6.15561	0.57506	1828.0218	1832.8426	2106.6288
H	1.26881	4.13153	1.82084	3025.3419	3027.4648	3033.4730
C	-0.15120	0.54840	1.43353	3034.0259	3035.4267	3036.7551
C	-1.28921	1.33608	2.11131	3037.3677	3037.7948	3041.3052
C	0.27696	-0.59537	2.29844	3049.4141	3049.7436	3095.4305
C	1.89556	-2.22248	2.78321	3105.9829	3111.1842	3111.7740
H	1.18278	-3.04709	2.65203	3115.6402	3115.7085	3117.5804
H	1.85933	-1.93472	3.84115	3121.4701	3126.1882	3128.4507
C	3.28303	-2.60350	2.34229	3135.3519	3136.6997	3137.7044
H	3.63301	-3.46617	2.91914	3139.6039	3139.6919	3143.2232
H	3.29503	-2.86056	1.27703	3145.3410	3149.0648	3160.6949
H	3.98025	-1.77503	2.50746	3166.7533	3168.3420	3173.9330
O	1.47162	-1.10788	1.98621	3181.3004	3189.6393	3201.3907
O	-0.42561	-1.08254	3.17292			
O	-2.30740	1.65452	1.53151			
C	-1.04872	1.77833	3.53195			
H	-1.65928	2.65917	3.74460			
H	-1.34522	0.96226	4.19961			
H	0.01034	1.98164	3.72842			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm

Zero-point correction= 0.595881	Electronic Energy = -1719.54118318
Internal Energy (E)= -1718.90713818	Enthalpy (H)= -1718.90619418
Gibbs Free Energy (G)=-1719.01262818	Gibbs Free Energy of Solvation=-1719.06090849

St.Pt.	General Structure	Ball & Stick model
VIII-1A		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.15583	-2.65519	-1.69809
C	1.14545	-2.55463	-1.14854
C	1.01994	-2.58621	0.30616
C	-0.37639	-2.84149	0.62838
C	-1.10673	-2.79828	-0.59707
O	0.90114	0.78859	-1.12692
C	2.16302	1.10884	-1.02211
O	3.02653	0.39958	-0.52401
C	2.50527	2.50055	-1.57369
C	-2.38680	1.41345	-1.09983
H	-0.66258	0.97583	-1.85729
C	2.42058	-2.40259	-1.89587
H	3.12501	-1.77907	-1.34061
H	2.87262	-3.38825	-2.06970
H	2.26021	-1.92867	-2.87030
C	2.14867	-2.59701	1.27246
H	2.58249	-3.60330	1.34912
H	2.93251	-1.90139	0.95430
H	1.80427	-2.29370	2.26790
C	-2.57472	-2.96204	-0.76992
H	-2.93986	-2.35227	-1.60380
H	-2.81849	-4.01014	-0.99009
H	-3.11654	-2.64554	0.12392
C	-0.53415	-2.60494	-3.13616
H	0.29614	-2.25590	-3.75723
H	-0.82964	-3.59931	-3.49588
H	-1.38171	-1.92994	-3.29883
C	-0.89814	-3.17653	1.97866
H	-0.63683	-4.21671	2.21570
H	-0.46315	-2.53300	2.75028
H	-1.98473	-3.07776	2.02587
Ir	-0.08686	-0.89920	-0.33530
C	3.61686	2.33456	-2.60938
H	3.26627	1.77165	-3.48522
H	3.96039	3.31725	-2.95804
H	4.46738	1.79842	-2.17579
C	1.30589	3.20643	-2.19617
H	0.51604	3.37615	-1.45347
H	1.61656	4.18534	-2.58449
H	0.88807	2.63515	-3.03562
C	3.01538	3.32928	-0.39179

Frequencies

37.9373	48.6949	58.3627
66.4677	73.5183	79.0521
86.1137	93.6694	100.5565
112.6316	114.8491	120.4616
126.7216	131.0284	136.0008
138.7447	144.6350	147.7879
154.1177	159.0827	167.0211
173.0165	177.6009	189.0136
199.7838	203.8885	205.8347
215.6621	219.3462	230.1049
233.7686	242.0851	252.8145
268.2971	272.5069	275.9035
291.1526	300.5601	306.9284
307.6344	315.8161	323.7750
336.5021	339.4050	346.0905
366.7456	370.8555	375.1094
384.5681	390.7996	400.9277
406.7933	416.9944	421.6374
425.7715	429.7604	443.5448
468.5070	473.2441	504.4156
530.8618	537.7933	541.0229
549.1485	557.6960	566.3032
576.9312	582.0462	584.2001
593.2176	602.6416	629.2158
646.4817	679.3152	716.0283
754.6580	778.0629	789.7875
794.4101	804.4319	806.2914
812.4207	820.0064	824.4932
854.4635	874.8023	885.0001
889.0608	913.3776	926.0993
946.0349	952.8075	957.3732
960.8350	966.7360	976.9296
988.0538	989.7705	1019.1567
1023.4307	1030.6672	1033.9886
1041.6882	1042.3685	1050.6793
1052.0148	1053.9465	1065.2409
1091.8209	1097.1984	1099.3840
1113.9222	1115.5560	1136.4964
1152.0246	1165.9449	1174.7157
1185.4752	1190.1099	1200.2817
1234.5205	1237.9694	1244.1857
1257.2037	1267.4887	1288.8215
1290.8308	1322.7155	1349.9277
1367.1910	1368.9303	1374.5544
1375.1854	1376.8311	1382.8422

H	2.26039	3.37390	0.40426	1385.1149	1387.8688	1390.0028
H	3.93013	2.89096	0.02121	1396.1373	1399.1590	1415.7313
H	3.23853	4.35212	-0.72313	1424.2816	1428.4195	1434.3586
O	-1.51587	0.51096	-1.68262	1438.7433	1443.6480	1451.2076
C	-2.00435	2.14097	0.02879	1452.6171	1454.8728	1457.6792
C	-2.87298	3.12345	0.50941	1460.7534	1463.1894	1466.1619
C	-3.62551	1.60470	-1.69343	1468.9903	1470.3934	1472.4658
C	-4.11645	3.32498	-0.07544	1477.2749	1483.0020	1484.3206
C	-4.49768	2.55199	-1.16845	1486.8535	1489.5112	1491.4865
C	-0.75680	1.87770	0.82415	1496.9994	1500.6748	1516.4327
O	-0.05377	2.81446	1.15356	1520.8073	1529.0540	1536.1157
H	-3.87892	1.01956	-2.57390	1543.8613	1557.3942	1644.6733
H	-5.47147	2.69948	-1.62931	1679.1265	1768.4045	1777.1267
H	-4.78996	4.07911	0.32337	1792.7084	1831.3031	3022.2333
H	-2.55739	3.71038	1.37000	3025.7154	3029.7735	3037.3487
C	-0.59557	0.45294	1.31287	3038.3990	3038.7761	3039.0772
C	-1.94710	0.07193	1.94279	3040.0445	3048.8036	3051.4424
C	0.49699	0.23850	2.31225	3053.7290	3103.7178	3104.4377
C	2.70886	0.62479	2.97115	3106.9641	3115.3880	3115.6314
H	2.90563	-0.45432	2.99553	3120.0700	3120.2311	3123.4512
H	2.39178	0.91492	3.98086	3126.2218	3131.0467	3137.8403
C	3.91192	1.39364	2.49907	3141.1055	3141.9896	3146.0561
H	4.76522	1.18748	3.15407	3147.8381	3156.9805	3165.8067
H	4.16254	1.09857	1.47448	3166.4686	3168.7038	3176.5492
H	3.71818	2.47122	2.51425	3180.3491	3185.6826	3186.8672
O	1.63220	0.88379	2.05777	3198.5236	3205.6986	3453.2357
O	0.37725	-0.52181	3.26454			
O	-2.74818	-0.66389	1.40270			
C	-2.28109	0.72330	3.26229			
H	-3.36626	0.81155	3.35829			
H	-1.89863	0.08419	4.06492			
H	-1.80125	1.70256	3.37723			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.604079 Electronic Energy = -1719.55421561
Internal Energy (E)= -1718.91154561 Enthalpy (H)= -1718.91060161
Gibbs Free Energy (G)=-1719.01583961 Gibbs Free Energy of Solvation=-1719.06773403

St.Pt.	General Structure	Ball & Stick model
VIII'-1		

Cartesian co-ordinate

Atoms	X	Y	Z
H	1.13122	1.21312	0.29858
C	-2.16797	-2.55799	-1.13049
C	-1.84210	-2.80565	0.23678

Frequencies

24.2498	30.7022	40.5669
50.2810	57.8804	59.8815
66.2967	71.6045	78.5479
85.8127	88.5451	94.6319
102.2510	110.1574	111.9561
118.8459	122.6341	126.1375
135.0109	141.6511	145.3428

C	-2.71810	-1.99656	1.07596	151.1605	163.3822	166.7267
C	-3.60262	-1.26000	0.21091	169.8357	176.8207	178.8205
C	-3.23426	-1.56182	-1.16431	187.7841	191.7137	194.5725
C	-2.34916	2.17556	-0.27196	199.8072	203.4460	205.9884
O	-1.57873	1.33007	0.34659	214.0899	215.0569	219.3205
O	-3.25660	1.88593	-1.04637	224.0405	232.6327	234.6693
C	-1.97122	3.64362	-0.01954	242.2564	246.1531	249.7244
O	0.09651	-0.47710	1.53411	257.8478	265.7738	281.1248
C	0.65242	0.52160	1.98992	289.5508	293.1813	298.1664
O	1.20157	1.45681	1.25439	301.6302	304.3131	309.8967
C	0.74738	0.75176	3.48727	313.1264	314.4471	315.2098
C	-4.69406	-0.34362	0.62996	327.5453	329.5162	341.0388
H	-5.64317	-0.89275	0.68798	342.5621	344.5464	350.8829
H	-4.49033	0.08917	1.61524	353.7725	378.6590	380.7488
H	-4.79361	0.48217	-0.08011	387.6831	389.2842	400.4232
C	-3.89513	-1.00076	-2.37112	406.0534	411.8104	420.8206
H	-4.88416	-1.45468	-2.51673	428.4833	434.3732	443.2857
H	-4.00534	0.08331	-2.25773	447.0509	450.3944	480.0197
H	-3.29765	-1.18606	-3.26809	503.6306	532.7124	535.5458
C	-2.74100	-2.02368	2.56205	536.6632	539.9077	544.8822
H	-1.72487	-1.97803	2.96867	555.2393	571.2058	578.7734
H	-3.30146	-1.17471	2.96637	586.8186	593.6626	598.6106
H	-3.21226	-2.94507	2.92828	601.1843	618.0827	626.6793
C	-0.76231	-3.69586	0.73872	631.9589	672.0249	721.1028
H	-0.43518	-3.38545	1.73656	764.8173	772.7286	780.2318
H	-1.11866	-4.73205	0.80289	787.6851	792.5138	796.7469
H	0.11221	-3.65195	0.08298	803.6106	808.1546	808.3428
C	-1.48953	-3.14401	-2.31546	819.0851	829.5886	850.4316
H	-0.44850	-3.38404	-2.08482	856.7847	881.8832	899.0566
H	-2.00602	-4.05428	-2.64540	905.8172	911.8160	942.3374
H	-1.47781	-2.43429	-3.14839	949.1434	949.3922	950.8744
C	-0.68191	1.02768	3.96859	954.4546	956.2716	958.4908
H	-0.68583	1.15646	5.05800	965.6236	970.0740	979.9316
H	-1.08305	1.93986	3.51029	1009.4131	1016.0840	1031.3626
H	-1.34857	0.19796	3.70902	1034.9084	1035.2086	1038.0412
C	1.65013	1.92874	3.83764	1041.7788	1043.0583	1044.3758
H	1.68707	2.04588	4.92783	1048.3684	1051.3948	1051.8168
H	2.67217	1.77305	3.47430	1056.8596	1075.6770	1093.3636
H	1.27745	2.86362	3.40515	1096.2453	1105.9179	1108.3851
C	1.28137	-0.52949	4.13104	1131.1469	1146.9312	1157.1720
H	0.65013	-1.39179	3.88848	1177.2999	1179.1109	1184.4417
H	2.30188	-0.74577	3.78848	1187.8072	1195.5169	1235.9170
H	1.30721	-0.41262	5.22125	1239.1133	1242.7904	1247.7581
C	-3.16175	4.54390	-0.32614	1267.5440	1271.4182	1284.4001
H	-3.99623	4.33953	0.35619	1294.7925	1310.0666	1316.6870
H	-2.87830	5.59837	-0.21078	1327.8658	1335.0777	1363.1211
H	-3.52296	4.38386	-1.34612	1366.6886	1372.9996	1373.6394
C	-0.82890	3.94907	-0.99471	1375.8222	1378.5323	1380.9138
H	-0.50149	4.99170	-0.88850	1383.6332	1384.8127	1386.3262
H	0.03712	3.29877	-0.80612	1389.7800	1396.0892	1403.4049
H	-1.15548	3.79417	-2.03103	1412.5221	1415.8660	1418.3857
C	-1.49739	3.87720	1.41200	1422.6237	1428.6194	1432.0673
H	-1.25392	4.93856	1.55557	1435.8241	1443.0391	1445.5804
H	-2.28108	3.61492	2.13587	1447.9552	1449.4855	1450.7072
H	-0.60352	3.28527	1.63817	1455.9405	1458.4955	1459.4045
Ir	-1.58208	-0.69805	-0.19296	1460.9495	1461.1944	1465.2680
C	1.62546	0.42885	-1.57356	1467.6021	1468.1117	1473.1088
C	1.82287	-0.88535	-0.98785	1473.6727	1476.0896	1478.3637
O	0.92639	-1.73798	-0.92496	1479.1358	1480.6833	1483.7192
C	3.15046	-1.31246	-0.41837	1487.4562	1490.7698	1491.1240
C	4.35657	-1.29482	-1.12896	1494.9079	1497.1890	1498.5010

C	3.14656	-1.84189	0.87030	1512.4132	1515.0409	1523.5085
C	5.52949	-1.75753	-0.53815	1524.7456	1535.9521	1543.3415
C	4.31762	-2.28631	1.47728	1576.7750	1655.7973	1671.1145
H	2.19179	-1.88782	1.39486	1703.0401	1763.0719	1766.2786
C	5.51151	-2.24132	0.76687	1831.0632	3024.4186	3027.7325
H	6.45912	-1.74074	-1.10808	3031.7375	3032.7874	3034.0314
H	4.29463	-2.67630	2.49215	3034.1528	3037.3527	3039.3541
H	6.43572	-2.59416	1.21910	3040.9988	3042.4847	3044.5766
O	4.33166	-0.81863	-2.40056	3045.1183	3046.6950	3058.5953
H	5.22114	-0.83249	-2.76934	3085.8928	3101.0654	3111.9040
C	0.40237	0.69806	-2.26795	3114.2589	3117.5762	3119.8589
C	2.74075	1.38186	-1.72137	3120.1695	3121.2721	3121.6133
C	4.70919	2.13835	-0.65194	3127.6689	3128.5541	3129.9321
H	4.47650	3.19915	-0.81128	3134.3386	3134.8044	3137.0870
H	5.30044	1.80936	-1.51918	3139.9645	3142.8339	3145.1914
C	5.42319	1.89183	0.65252	3147.6561	3148.3812	3149.1518
H	6.37391	2.43394	0.68488	3149.7323	3153.8492	3157.8536
H	4.80583	2.22398	1.49423	3158.3142	3160.7464	3162.0953
H	5.62302	0.82070	0.78040	3167.4983	3181.3668	3193.8419
O	3.50130	1.38732	-0.60050	3203.8185	3450.6212	3897.8361
O	2.96786	2.13459	-2.64676			
C	0.35189	1.65471	-3.42578			
H	-0.67907	1.70466	-3.78578			
H	0.69885	2.64989	-3.13246			
H	1.03243	1.33403	-4.22061			
O	-0.70647	0.16363	-1.98774			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.752645 Electronic Energy = -2066.37750321
Internal Energy (E)= -2065.57673121 Enthalpy (H)= -2065.57578821
Gibbs Free Energy (G)=-2065.70136221 Gibbs Free Energy of Solvation=-2065.76973842

St.Pt.	General Structure	Ball & Stick model
TS-8		

Cartesian co-ordinate

Atoms	X	Y	Z
H	1.07929	1.00825	0.03746
C	-2.11321	-2.53717	-1.18817
C	-1.78834	-2.84139	0.16620
C	-2.70305	-2.10116	1.03007
C	-3.60945	-1.36041	0.18725
C	-3.21458	-1.57930	-1.19171
C	-2.48912	2.13566	-0.26108
O	-1.73371	1.31602	0.40732
O	-3.35899	1.81620	-1.06619

Frequencies

-503.8774	-124.3086	-52.4024
28.3974	32.5365	45.4639
54.8176	58.4007	61.3644
68.3632	69.8057	75.7784
85.0527	86.4374	88.6082
96.1388	101.0903	106.1435
113.2459	116.6663	119.5992
133.7857	141.1487	144.8088
146.8825	156.1957	160.4856
168.6817	176.3357	181.0674
189.2440	194.0885	196.0473
204.3684	207.2024	210.3007
215.5625	222.7016	229.9137

C	-2.14141	3.61547	-0.03308	235.8118	236.8986	244.9676
O	0.01527	-0.50070	1.45128	259.9994	262.8677	269.6266
C	0.58628	0.52936	1.85969	273.7078	279.4782	284.3464
O	1.11777	1.41165	1.08644	294.5335	301.7473	304.5717
C	0.68447	0.77655	3.35487	307.1898	313.0570	314.9949
C	-4.71528	-0.48165	0.64788	320.5752	327.4219	333.5169
H	-5.66148	-1.03778	0.65888	341.9463	342.8372	348.2139
H	-4.52403	-0.11116	1.66060	354.8039	359.1784	370.7937
H	-4.80962	0.38674	-0.01007	386.9168	391.3406	393.1383
C	-3.86943	-1.01408	-2.39944	406.6017	410.5799	421.4869
H	-4.68851	-1.66084	-2.74032	426.2756	434.9698	446.2302
H	-4.24811	-0.01031	-2.19058	448.6439	457.9229	468.8873
H	-3.14394	-0.91792	-3.21334	478.9348	527.5910	530.1100
C	-2.72379	-2.18273	2.51421	536.3523	537.7733	544.8035
H	-1.70669	-2.12616	2.91799	551.6368	569.8256	572.8874
H	-3.30206	-1.36188	2.95010	586.7714	589.0640	596.4648
H	-3.17064	-3.12796	2.84859	602.5422	608.5777	625.2853
C	-0.68323	-3.71756	0.63845	632.4981	665.0499	703.1776
H	-0.35222	-3.41909	1.63898	743.3885	760.8559	777.3636
H	-1.01173	-4.76370	0.68746	790.6881	793.3174	801.6706
H	0.18339	-3.63947	-0.02491	802.6905	807.1166	808.4495
C	-1.43073	-3.06081	-2.39898	818.9859	827.8563	844.5522
H	-0.41020	-3.37522	-2.17144	853.5114	865.9667	899.9436
H	-1.98921	-3.91419	-2.80497	906.0213	912.9294	940.3156
H	-1.36925	-2.29537	-3.17827	944.5224	948.6675	951.5687
C	-0.74942	1.00223	3.84829	954.1501	958.5236	959.7018
H	-0.74386	1.19357	4.92856	960.6411	969.6548	981.9901
H	-1.21192	1.85850	3.34191	992.6839	1018.4064	1030.8869
H	-1.37068	0.12208	3.64889	1031.8805	1036.4310	1037.0452
C	1.55019	1.98855	3.67549	1041.6621	1043.3127	1045.6880
H	1.60058	2.12414	4.76317	1051.3232	1052.0435	1055.6572
H	2.57019	1.86059	3.29625	1056.6276	1071.6851	1092.2291
H	1.14203	2.90416	3.23418	1094.7511	1102.0152	1106.5782
C	1.27404	-0.47466	4.01046	1128.4467	1144.9126	1154.9661
H	0.67343	-1.36293	3.78309	1171.5595	1175.0124	1185.0439
H	2.30008	-0.65572	3.66284	1187.8423	1191.9553	1235.1210
H	1.30321	-0.34338	5.09920	1238.0093	1248.6341	1251.9508
C	-3.35472	4.48375	-0.34250	1271.5670	1274.3511	1278.4544
H	-4.17448	4.28002	0.35790	1282.9662	1292.6971	1312.2778
H	-3.09160	5.54631	-0.25690	1322.2655	1350.3627	1367.0116
H	-3.72657	4.29012	-1.35277	1370.5557	1376.0616	1376.4385
C	-1.01517	3.92710	-1.02548	1376.8194	1378.6717	1379.3185
H	-0.72178	4.98266	-0.95179	1380.8278	1384.2458	1389.1179
H	-0.12755	3.31313	-0.81679	1390.8757	1397.5307	1401.6072
H	-1.34115	3.73081	-2.05501	1407.1711	1411.3354	1415.1793
C	-1.65198	3.88522	1.38569	1419.1539	1420.5978	1427.8257
H	-1.42789	4.95374	1.50615	1429.5344	1432.2859	1439.8375
H	-2.41609	3.61893	2.12851	1444.7413	1446.3307	1447.1508
H	-0.74160	3.31585	1.60355	1451.1466	1454.2502	1455.3639
Ir	-1.59877	-0.70512	-0.14148	1459.9685	1461.7670	1462.4568
C	1.67053	0.50348	-1.41232	1465.9752	1467.9202	1471.5699
C	1.92583	-0.88229	-0.99446	1475.2498	1475.5093	1476.4762
O	1.07972	-1.77253	-1.07597	1478.3796	1480.7634	1483.9547
C	3.24982	-1.28848	-0.40564	1484.6034	1485.4917	1487.3390
C	4.45990	-1.21579	-1.10327	1490.6515	1497.8263	1499.4502
C	3.24171	-1.86385	0.86136	1500.4360	1506.3018	1512.4258
C	5.63785	-1.67142	-0.51880	1538.9648	1541.4030	1547.4796
C	4.41803	-2.30071	1.46453	1551.3991	1623.0774	1657.0579
H	2.28362	-1.95781	1.37293	1671.9875	1747.6293	1756.6687
C	5.61711	-2.20226	0.76843	1766.3081	1836.3744	3017.8264
H	6.57275	-1.61139	-1.07699	3023.6466	3026.9378	3032.4907

H	4.39391	-2.72694	2.46456	3035.7693	3036.7360	3037.7160
H	6.54457	-2.54972	1.21801	3038.8556	3039.6963	3040.9722
O	4.42648	-0.68915	-2.35528	3042.3900	3044.1572	3049.8598
H	5.31550	-0.67326	-2.72507	3057.8039	3090.7659	3100.7130
C	0.46328	0.73871	-2.18291	3101.8572	3110.3823	3110.7892
C	2.78615	1.46868	-1.55078	3112.7897	3120.8218	3123.4722
C	4.78099	2.19473	-0.52669	3124.3566	3126.1642	3127.7620
H	4.52670	3.25456	-0.65310	3129.0889	3129.7002	3133.1893
H	5.35385	1.89580	-1.41701	3139.1770	3140.5466	3141.7095
C	5.53606	1.92931	0.75025	3143.1265	3145.9267	3147.2028
H	6.48855	2.46929	0.75562	3148.6046	3149.1903	3151.7934
H	4.95144	2.25271	1.61767	3155.2271	3155.5977	3163.4043
H	5.73872	0.85671	0.85789	3168.6995	3170.0839	3171.5921
O	3.58563	1.42219	-0.46537	3185.0971	3200.3789	3898.8117
O	2.97243	2.26321	-2.44959			
C	0.45461	1.62214	-3.39437			
H	-0.55281	1.62123	-3.81812			
H	0.75804	2.64063	-3.13443			
H	1.19413	1.27937	-4.12499			
O	-0.64664	0.23623	-1.88648			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.745743 Electronic Energy = -2066.36815662
Internal Energy (E)= -2065.57552562 Enthalpy (H)= -2065.57458262
Gibbs Free Energy (G)=-2065.69798962 Gibbs Free Energy of Solvation=-2065.76616368

St.Pt.	General Structure	Ball & Stick model
IX-1		

Cartesian co-ordinate

Atoms	X	Y	Z
H	1.38140	0.82831	-0.26935
C	-2.10996	-2.13511	-1.61642
C	-1.86867	-2.72109	-0.33863
C	-2.83112	-2.14771	0.59447
C	-3.68681	-1.23436	-0.15044
C	-3.22261	-1.20020	-1.50732
C	-2.46357	2.26695	0.05411
O	-1.77498	1.32908	0.63722
O	-3.37829	2.09926	-0.74793
C	-1.94423	3.67138	0.39000
O	0.03033	-0.69323	1.15630
C	0.50468	0.25608	1.91553
O	1.04405	1.28177	1.50729
C	0.36136	0.00595	3.42426
C	-4.81761	-0.45329	0.41525

Frequencies

22.4475	31.0056	40.1175
45.2580	49.6974	52.4896
60.6852	66.8374	76.4786
79.1550	84.0113	90.2006
90.8618	99.6766	101.5965
106.8132	109.4689	115.9549
122.0259	139.2662	140.4628
146.7377	150.2664	160.4876
164.3740	167.2100	176.5195
181.9657	187.6955	189.3788
196.0109	198.3424	202.7506
207.1218	214.9296	221.6904
226.7206	228.6454	231.5379
232.1358	234.3435	246.5852
265.0790	276.1401	281.4546
286.4672	289.4792	294.2739
296.8542	303.5509	308.5448
310.8155	313.3661	316.0425
319.1851	330.6762	339.3172

H	-5.74156	-1.04580	0.39055	345.0015	363.3923	366.5528
H	-4.61632	-0.17711	1.45661	367.8350	375.5360	378.4540
H	-4.95711	0.47586	-0.14360	389.2262	390.6645	392.5010
C	-3.81099	-0.40071	-2.61422	401.0155	418.8965	419.6679
H	-4.76422	-0.83492	-2.94289	426.4441	429.9611	438.4607
H	-3.97609	0.62766	-2.27625	442.7908	459.9973	471.8350
H	-3.13887	-0.36805	-3.47720	510.8284	516.9891	536.8028
C	-3.00908	-2.55789	2.01180	538.0824	547.1468	551.9566
H	-2.04616	-2.75062	2.49595	555.6627	568.0170	574.0323
H	-3.52621	-1.78694	2.59148	577.7004	589.9033	596.2010
H	-3.60493	-3.47867	2.06782	599.0752	601.7678	623.4548
C	-0.76880	-3.65450	0.02685	642.0118	667.9102	689.5768
H	-0.38570	-3.40949	1.02440	753.0530	767.3086	790.9120
H	-1.10969	-4.69743	0.03237	797.9121	800.8798	806.6107
H	0.07272	-3.55641	-0.66745	809.4605	811.3282	812.4089
C	-1.37592	-2.41026	-2.87853	818.4704	848.9293	853.3424
H	-0.42694	-2.91815	-2.69651	857.1371	862.4360	902.3495
H	-1.99700	-3.03515	-3.53356	904.2761	915.6400	943.5322
H	-1.15779	-1.47881	-3.41154	945.2133	947.3502	951.0265
C	-1.09906	0.30842	3.77765	956.3648	956.7275	965.8110
H	-1.27180	0.13236	4.84812	971.1537	973.8697	992.9591
H	-1.35197	1.35130	3.55101	1000.8163	1011.2476	1025.8339
H	-1.78113	-0.32877	3.20100	1036.0156	1039.3592	1040.1941
C	1.28545	0.93361	4.20300	1041.4654	1042.2164	1043.8812
H	1.15539	0.77830	5.28249	1045.8953	1048.9470	1052.4554
H	2.33584	0.74103	3.95109	1066.0705	1070.6071	1093.4931
H	1.07904	1.98323	3.97124	1099.2827	1110.7264	1112.2429
C	0.68250	-1.44620	3.77096	1116.5989	1143.6245	1162.5458
H	0.03201	-2.14096	3.22800	1168.1631	1176.6936	1184.5316
H	1.72440	-1.69206	3.52256	1188.8992	1230.8956	1235.2593
H	0.54952	-1.61461	4.84802	1239.2528	1244.9339	1250.6225
C	-3.00588	4.71462	0.06828	1258.7839	1263.6611	1274.1102
H	-3.89656	4.57775	0.69406	1275.1538	1280.1712	1286.4303
H	-2.61035	5.72228	0.25296	1310.4437	1320.9511	1356.1601
H	-3.32274	4.64570	-0.97697	1366.1341	1368.5056	1370.3646
C	-0.71963	3.86990	-0.51385	1373.5773	1375.2847	1376.3494
H	-0.29714	4.87266	-0.36506	1379.2962	1384.3647	1387.4573
H	0.05094	3.12697	-0.27276	1388.0135	1389.7024	1394.9344
H	-0.99434	3.76572	-1.57246	1397.5300	1400.6658	1414.4749
C	-1.51100	3.78076	1.84943	1418.0819	1428.6994	1429.3395
H	-1.15857	4.80029	2.05692	1431.2433	1435.7649	1436.1648
H	-2.34796	3.57263	2.53005	1443.6398	1444.7505	1446.3289
H	-0.69777	3.07938	2.06538	1452.4594	1453.1636	1456.5098
Ir	-1.65369	-0.57476	-0.15076	1461.2382	1461.8303	1462.7417
C	1.77795	0.61040	-1.29125	1464.1938	1470.9285	1471.8346
C	2.13287	-0.87122	-1.20183	1473.5436	1475.7497	1476.9341
O	1.39391	-1.69704	-1.70103	1476.9518	1480.7793	1482.7724
C	3.31200	-1.29787	-0.39298	1488.7275	1488.9072	1490.7079
C	4.61290	-1.13362	-0.87133	1494.2714	1496.3528	1497.4648
C	3.09979	-1.92918	0.82720	1502.4597	1509.5583	1515.2521
C	5.69555	-1.57277	-0.11783	1536.3957	1540.0013	1542.4379
C	4.17990	-2.35729	1.59405	1659.8519	1677.6800	1738.8153
H	2.07171	-2.05536	1.16624	1758.1187	1773.9388	1813.5782
C	5.47363	-2.17627	1.11805	1863.8782	2838.3843	3018.3888
H	6.70834	-1.44603	-0.50070	3021.0664	3023.1597	3024.8510
H	4.01079	-2.83752	2.55464	3029.7777	3030.5034	3033.6703
H	6.32454	-2.51303	1.70552	3036.5111	3039.5816	3044.5422
O	4.74201	-0.54330	-2.09020	3044.9691	3045.3761	3047.8982
H	5.67274	-0.47492	-2.32853	3048.5180	3098.4162	3101.3915
C	0.63389	0.75102	-2.26539	3102.0659	3102.1534	3109.7430
C	2.92715	1.58077	-1.45499	3110.1666	3113.0057	3115.3134

C	4.85170	2.36254	-0.35019	3122.6614	3125.1117	3126.3384
H	4.58554	3.41370	-0.51439	3128.5137	3128.8730	3129.8595
H	5.46963	2.04686	-1.20246	3137.9818	3138.1090	3138.2199
C	5.53081	2.13074	0.97347	3142.0615	3142.6648	3146.7351
H	6.47248	2.68645	1.02514	3149.2178	3152.2288	3155.9342
H	4.88756	2.45610	1.79667	3159.8975	3163.0974	3163.2507
H	5.74242	1.06336	1.11047	3177.2617	3184.4674	3184.5867
O	3.65827	1.57347	-0.34098	3198.9052	3215.5124	3897.6641
O	3.14601	2.29349	-2.40703			
C	0.92000	0.94807	-3.71343			
H	-0.00533	0.88337	-4.29044			
H	1.41585	1.91119	-3.86642			
H	1.63737	0.18240	-4.03787			
O	-0.52197	0.63428	-1.87363			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.750727 Electronic Energy = -2066.37371265
Internal Energy (E)= -2065.57443165 Enthalpy (H)= -2065.57348765
Gibbs Free Energy (G)=-2065.70102765 Gibbs Free Energy of Solvation=-2065.77073137

St.Pt.	General Structure	Ball & Stick model
III-1A'		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.37318	1.77808	1.37375
C	0.87165	2.18711	0.75951
C	0.61974	2.35883	-0.63549
C	-0.80076	2.10180	-0.87076
C	-1.42238	1.79697	0.37892
O	1.66512	-1.00014	-0.19123
C	2.93126	-0.66717	-0.25860
O	3.35638	0.46282	-0.45686
C	3.86219	-1.86979	-0.06816
C	-2.87270	-1.63166	0.52633
H	-1.13403	-1.86347	1.82675
C	2.14714	2.41796	1.48825
H	2.08922	3.35518	2.05735
H	2.35151	1.60734	2.19712
H	2.99374	2.46111	0.80217
C	1.61049	2.77560	-1.66096
H	1.74320	3.86517	-1.63865
H	2.57148	2.28761	-1.47232
H	1.28136	2.49943	-2.66766
C	-2.87548	1.58772	0.61841
H	-3.06518	0.99364	1.51790

Frequencies

21.5850	30.3498	37.8055
48.9443	54.3443	60.2651
83.2318	86.9074	99.1462
108.6688	121.6373	130.5952
140.5421	146.9389	161.5570
165.0680	177.4193	181.3708
197.0403	201.1608	208.9105
224.8878	229.2426	237.2948
243.1618	254.7483	273.1599
276.2543	282.2224	292.5593
310.5394	316.0299	320.0518
336.5727	357.8256	367.5498
374.6668	386.6301	413.2678
426.2471	439.4774	451.8023
460.3225	463.8637	532.0391
534.9724	536.7545	539.0029
564.4487	570.8701	577.6278
580.4557	602.7043	608.3763
642.1536	652.4595	740.6259
781.4504	789.4002	804.2495
811.0691	814.4656	832.5698
868.2883	875.6412	915.6093
945.7825	949.3837	950.8991
956.7670	962.1937	975.8032
978.2523	1023.0740	1025.0718

H	-3.37115	2.55865	0.74777
H	-3.35604	1.07179	-0.21961
C	-0.55246	1.46543	2.81556
H	-1.33971	0.72270	2.98484
H	0.37443	1.07823	3.25000
H	-0.82459	2.37647	3.36519
C	-1.48544	2.17511	-2.18821
H	-1.77261	3.20914	-2.41886
H	-0.83265	1.82019	-2.99263
H	-2.39059	1.55808	-2.19912
Ir	0.13247	0.31141	-0.11855
C	3.58787	-2.48527	1.30635
H	2.55599	-2.84297	1.38119
H	4.26394	-3.33320	1.47724
H	3.76033	-1.75495	2.10850
C	3.57084	-2.90192	-1.15956
H	3.75707	-2.48366	-2.15712
H	4.22788	-3.77258	-1.03340
H	2.53045	-3.23892	-1.11738
C	5.31287	-1.41474	-0.15323
H	5.52647	-0.95531	-1.12443
H	5.53978	-0.67027	0.61800
H	5.98322	-2.27325	-0.01710
C	-2.09700	-1.49189	-0.64584
C	-2.75789	-1.44441	-1.88536
C	-4.26831	-1.70311	0.44338
C	-4.14045	-1.53367	-1.94582
C	-4.90868	-1.66293	-0.78248
H	-4.82209	-1.78962	1.37675
H	-5.99142	-1.73191	-0.84579
H	-4.63381	-1.49990	-2.91572
H	-2.15141	-1.33937	-2.78324
O	-0.77087	-1.40970	-0.58668
C	-2.22580	-1.65111	1.84116
O	-2.80887	-1.42994	2.88950
H	-2.34796	3.57263	2.53005
H	-0.69777	3.07938	2.06538
Ir	-1.65369	-0.57476	-0.15076
C	1.77795	0.61040	-1.29125
C	2.13287	-0.87122	-1.20183
O	1.39391	-1.69704	-1.70103
C	3.31200	-1.29787	-0.39298
C	4.61290	-1.13362	-0.87133
C	3.09979	-1.92918	0.82720
C	5.69555	-1.57277	-0.11783
C	4.17990	-2.35729	1.59405
H	2.07171	-2.05536	1.16624
C	5.47363	-2.17627	1.11805
H	6.70834	-1.44603	-0.50070
H	4.01079	-2.83752	2.55464
H	6.32454	-2.51303	1.70552
O	4.74201	-0.54330	-2.09020
H	5.67274	-0.47492	-2.32853
C	0.63389	0.75102	-2.26539
C	2.92715	1.58077	-1.45499
C	4.85170	2.36254	-0.35019
H	4.58554	3.41370	-0.51439
H	5.46963	2.04686	-1.20246
C	5.53081	2.13074	0.97347
H	6.47248	2.68645	1.02514
H	4.88756	2.45610	1.79667

1028.5237	1034.2856	1037.4078
1038.0687	1040.3132	1044.9263
1047.8412	1090.2146	1097.6082
1106.2524	1110.0960	1148.6876
1188.4233	1189.9852	1200.7115
1234.6070	1242.9466	1262.7045
1274.6190	1308.2543	1349.3001
1364.3418	1374.0706	1375.8490
1380.1488	1386.1165	1393.7772
1399.3439	1406.0948	1411.0984
1421.5410	1425.4670	1434.3725
1437.7047	1444.3326	1446.6891
1446.8914	1454.1955	1457.4815
1458.6464	1463.1339	1464.8205
1470.9702	1471.9397	1476.3428
1476.8727	1491.3959	1491.8411
1498.2010	1500.5180	1502.2039
1510.0718	1523.7558	1544.0446
1622.4986	1660.0543	1778.1280
1802.5600	2925.0446	3023.1599
3027.4730	3035.9176	3036.4248
3038.0408	3040.2638	3040.9891
3042.4103	3103.3996	3107.2998
3113.7615	3119.1349	3121.5238
3122.8977	3123.7604	3126.0720
3135.9973	3136.2187	3141.2804
3145.1473	3147.6743	3154.5152
3162.4960	3172.9859	3186.9189
3191.2477	3200.3369	3203.0339

H	5.74242	1.06336	1.11047
O	3.65827	1.57347	-0.34098
O	3.14601	2.29349	-2.40703
C	0.92000	0.94807	-3.71343
H	-0.00533	0.88337	-4.29044
H	1.41585	1.91119	-3.86642
H	1.63737	0.18240	-4.03787
O	-0.52197	0.63428	-1.87363

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.462498 Electronic Energy = -1260.66085688
Internal Energy (E)= -1260.16796788 Enthalpy (H)= -1260.16702388
Gibbs Free Energy (G)=-1260.25910088 Gibbs Free Energy of Solvation=-1261.32997517

St.Pt.	General Structure	Ball & Stick model
TS-3A’		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-2.64348	-0.61927	-0.82870
C	-2.40447	-1.42562	0.35634
C	-2.21009	-0.56254	1.47037
C	-2.32603	0.80910	0.98832
C	-2.66444	0.75916	-0.41543
O	0.90889	-1.33180	-0.94624
C	1.51818	-2.04920	0.00915
O	0.94278	-2.42977	1.00621
C	2.98254	-2.34220	-0.29696
C	1.24791	2.17899	-0.52457
H	0.68993	-0.03640	-1.19738
C	-2.27475	-2.90658	0.34711
H	-3.26619	-3.37613	0.30629
H	-1.70815	-3.24049	-0.52899
H	-1.74498	-3.26746	1.23164
C	-1.85976	-0.94107	2.86631
H	-2.69604	-0.74775	3.55056
H	-1.59371	-1.99890	2.93671
H	-0.99292	-0.36827	3.21586
C	-2.97056	1.91340	-1.29903
H	-2.50535	1.79065	-2.28218
H	-4.05616	2.00314	-1.43234
H	-2.59986	2.85303	-0.87789
C	-2.94031	-1.11891	-2.19945
H	-2.53877	-0.43365	-2.95436
H	-2.48300	-2.09880	-2.36993
H	-4.02108	-1.21749	-2.36725

Frequencies

-1368.0821	38.2268	40.5840
48.4325	58.6791	65.9437
99.2104	99.9722	120.3419
128.2405	139.6056	146.8736
151.5197	156.4889	162.4151
171.6865	176.4239	192.3402
197.7951	206.5586	212.4607
215.7771	227.1412	237.6000
240.4266	261.4878	273.3475
286.5085	296.3575	297.1148
303.5987	312.6312	319.8564
328.7242	337.0693	358.6192
384.3959	390.5166	410.9569
420.3946	421.6696	441.7303
449.5321	474.1755	528.2280
535.5930	537.5226	546.5642
553.3072	560.5647	571.5272
586.5100	591.9776	599.9941
603.7390	622.0788	668.3400
752.5205	764.0828	780.7560
797.4399	811.2505	815.5460
846.6782	859.8800	873.9696
900.6495	945.1909	952.2771
955.9089	963.4593	967.8447
972.1564	979.0862	981.0144
1033.7162	1037.1510	1037.5180
1038.3546	1039.2711	1044.6459
1048.0227	1050.9491	1091.3098
1098.9822	1110.4365	1117.6396
1144.7456	1182.2424	1186.7813
1198.4564	1212.3257	1242.0892

C	-2.20426	2.02402	1.83901	1266.1824	1268.1523	1321.2428
H	-3.14758	2.24534	2.35464	1345.2184	1377.3392	1379.1427
H	-1.42577	1.88298	2.59647	1383.2840	1388.4701	1397.3829
H	-1.92477	2.89944	1.24325	1398.6583	1399.8348	1406.6091
Ir	-0.67671	-0.06345	-0.05136	1412.4541	1434.2078	1436.8203
C	3.13885	-2.88617	-1.71674	1439.1843	1446.5650	1448.0541
H	2.76094	-2.17856	-2.46097	1451.4897	1453.9902	1455.9314
H	4.20032	-3.07399	-1.92363	1462.8337	1463.4569	1470.9605
H	2.60065	-3.83427	-1.84087	1473.9839	1474.4703	1481.5897
C	3.73118	-1.01018	-0.16465	1482.8468	1483.5009	1487.7418
H	3.60670	-0.58522	0.83965	1494.4949	1503.5842	1513.7426
H	4.80291	-1.17031	-0.33902	1519.5122	1527.1883	1543.7332
H	3.37278	-0.27149	-0.89203	1592.7762	1616.1527	1666.3264
C	3.52500	-3.34324	0.71434	1790.9678	1818.8555	3025.2626
H	3.41723	-2.96717	1.73683	3032.5979	3032.9007	3038.4696
H	2.98883	-4.29729	0.65412	3038.6623	3039.0967	3039.8224
H	4.58829	-3.53176	0.51886	3041.0542	3110.2086	3113.9467
C	1.52631	1.63363	0.75358	3114.3049	3117.1156	3119.2433
C	2.49887	2.27963	1.54998	3121.9924	3124.4662	3124.5996
C	1.88964	3.34413	-0.97695	3127.1704	3136.9958	3138.9110
C	3.11787	3.42189	1.08494	3142.6361	3145.1408	3147.1736
C	2.82025	3.97146	-0.17725	3153.8655	3175.8769	3177.5430
H	1.63505	3.71782	-1.96704	3190.3328	3199.8603	3207.1874
H	3.32655	4.87256	-0.51278			
H	3.85913	3.91190	1.71430			
H	2.72949	1.85951	2.52625			
O	0.90787	0.56276	1.17739			
C	0.31292	1.42734	-1.34397			
O	-0.08907	1.72355	-2.45466			
H	-2.34796	3.57263	2.53005			
H	-0.69777	3.07938	2.06538			
Ir	-1.65369	-0.57476	-0.15076			
C	1.77795	0.61040	-1.29125			
C	2.13287	-0.87122	-1.20183			
O	1.39391	-1.69704	-1.70103			
C	3.31200	-1.29787	-0.39298			
C	4.61290	-1.13362	-0.87133			
C	3.09979	-1.92918	0.82720			
C	5.69555	-1.57277	-0.11783			
C	4.17990	-2.35729	1.59405			
H	2.07171	-2.05536	1.16624			
C	5.47363	-2.17627	1.11805			
H	6.70834	-1.44603	-0.50070			
H	4.01079	-2.83752	2.55464			
H	6.32454	-2.51303	1.70552			
O	4.74201	-0.54330	-2.09020			
H	5.67274	-0.47492	-2.32853			
C	0.63389	0.75102	-2.26539			
C	2.92715	1.58077	-1.45499			
C	4.85170	2.36254	-0.35019			
H	4.58554	3.41370	-0.51439			
H	5.46963	2.04686	-1.20246			
C	5.53081	2.13074	0.97347			
H	6.47248	2.68645	1.02514			
H	4.88756	2.45610	1.79667			
H	5.74242	1.06336	1.11047			
O	3.65827	1.57347	-0.34098			
O	3.14601	2.29349	-2.40703			
C	0.92000	0.94807	-3.71343			
H	-0.00533	0.88337	-4.29044			
H	1.41585	1.91119	-3.86642			

H	1.63737	0.18240	-4.03787
O	-0.52197	0.63428	-1.87363

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.457910 Electronic Energy = -1260.60943938
Internal Energy (E)= -1260.12212038 Enthalpy (H)= -1260.12117638
Gibbs Free Energy (G)=-1260.20886438 Gibbs Free Energy of Solvation=-1261.27199892

St.Pt.	General Structure	Ball & Stick model
IV-1A'		

Cartesian co-ordinate

Atoms	X	Y	Z
C	2.62019	0.63158	-0.89256
C	2.46298	1.50742	0.27686
C	2.36789	0.71525	1.42059
C	2.44599	-0.69246	0.99488
C	2.76126	-0.71262	-0.42400
O	-0.99207	1.19410	-0.96969
C	-1.58822	2.11157	-0.12419
O	-0.88620	2.73446	0.61795
C	-3.09556	2.23980	-0.27435
C	-1.31249	-2.12874	-0.41067
H	-1.64015	0.63580	-1.42707
C	2.33481	2.98522	0.17475
H	3.31163	3.44150	-0.03643
H	1.65995	3.26468	-0.64261
H	1.93666	3.42715	1.09164
C	2.06097	1.14000	2.81340
H	2.89915	0.93342	3.49221
H	1.83458	2.20926	2.86596
H	1.18385	0.60063	3.19257
C	3.12813	-1.88952	-1.25487
H	2.53777	-1.90961	-2.17763
H	4.19469	-1.85831	-1.51164
H	2.93330	-2.82863	-0.72700
C	2.83339	1.08652	-2.29499
H	2.52395	0.30736	-3.00067
H	2.24159	1.98248	-2.51476
H	3.88783	1.32692	-2.49066
C	2.46191	-1.85074	1.93052
H	3.44460	-1.96752	2.40727
H	1.71399	-1.71441	2.71920
H	2.21862	-2.78231	1.40886
Ir	0.73394	-0.08534	-0.06010
C	-3.44416	2.61410	-1.71942
H	-3.16311	1.84047	-2.44469
H	-4.52867	2.75227	-1.80168

Frequencies

26.3715	33.7564	41.3834
49.5304	68.2301	73.0601
96.6619	99.1273	106.3511
119.5698	134.0411	139.1033
147.6048	151.5170	158.9772
168.4726	179.1288	186.2135
191.6916	206.5549	207.9375
216.5629	241.0144	245.2432
266.2383	269.7352	271.9967
285.4857	287.7071	299.5013
304.2191	308.6580	316.8548
327.5844	342.5579	355.8344
365.6087	390.1437	405.2841
415.4074	429.3265	469.5122
473.8081	521.6337	530.1466
537.0662	542.1055	548.3602
559.9824	571.4803	593.0447
600.4938	604.2482	618.8554
627.0489	654.9046	678.6222
756.2048	761.1396	764.0056
769.7617	803.9164	809.1158
862.3122	866.6785	880.4364
893.9358	942.5344	947.4171
957.5221	959.6301	961.5524
962.2958	972.8997	1031.0117
1034.6344	1039.6043	1043.3194
1043.8693	1044.4081	1046.1483
1050.6862	1087.0675	1088.4818
1097.8641	1104.7735	1113.2174
1147.5115	1176.2701	1186.1995
1197.8544	1225.7343	1238.9394
1255.6917	1263.7593	1318.1926
1345.2800	1365.8542	1375.4096
1383.0750	1386.1025	1392.2854
1393.3588	1394.7027	1400.2728
1424.0656	1427.3678	1430.9956
1438.3856	1443.8768	1447.3515
1449.7097	1450.8911	1455.1138
1457.6810	1459.1042	1460.2534

H	-2.96094	3.55158	-2.01885
C	-3.75180	0.90712	0.10617
H	-3.43148	0.57618	1.10067
H	-4.84083	1.03359	0.11149
H	-3.52623	0.09077	-0.59460
C	-3.57219	3.33541	0.67190
H	-3.33240	3.08801	1.71095
H	-3.09750	4.29472	0.43998
H	-4.65834	3.45217	0.58136
C	-1.58138	-1.53895	0.84484
C	-2.66890	-2.03475	1.59536
C	-2.11509	-3.15986	-0.91366
C	-3.45014	-3.05430	1.08047
C	-3.19078	-3.62295	-0.17724
H	-1.86260	-3.57688	-1.88725
H	-3.82294	-4.42209	-0.55605
H	-4.28848	-3.42445	1.66918
H	-2.87386	-1.59570	2.57013
O	-0.84779	-0.53392	1.26142
C	-0.15028	-1.57183	-1.12475
O	0.18261	-1.92738	-2.24669
H	-2.34796	3.57263	2.53005
H	-0.69777	3.07938	2.06538
Ir	-1.65369	-0.57476	-0.15076
C	1.77795	0.61040	-1.29125
C	2.13287	-0.87122	-1.20183
O	1.39391	-1.69704	-1.70103
C	3.31200	-1.29787	-0.39298
C	4.61290	-1.13362	-0.87133
C	3.09979	-1.92918	0.82720
C	5.69555	-1.57277	-0.11783
C	4.17990	-2.35729	1.59405
H	2.07171	-2.05536	1.16624
C	5.47363	-2.17627	1.11805
H	6.70834	-1.44603	-0.50070
H	4.01079	-2.83752	2.55464
H	6.32454	-2.51303	1.70552
O	4.74201	-0.54330	-2.09020
H	5.67274	-0.47492	-2.32853
C	0.63389	0.75102	-2.26539
C	2.92715	1.58077	-1.45499
C	4.85170	2.36254	-0.35019
H	4.58554	3.41370	-0.51439
H	5.46963	2.04686	-1.20246
C	5.53081	2.13074	0.97347
H	6.47248	2.68645	1.02514
H	4.88756	2.45610	1.79667
H	5.74242	1.06336	1.11047
O	3.65827	1.57347	-0.34098
O	3.14601	2.29349	-2.40703
C	0.92000	0.94807	-3.71343
H	-0.00533	0.88337	-4.29044
H	1.41585	1.91119	-3.86642
H	1.63737	0.18240	-4.03787
O	-0.52197	0.63428	-1.87363

1464.8916	1473.5364	1476.1460
1479.7523	1481.9966	1484.5345
1488.7681	1497.7748	1498.7264
1515.9853	1517.9062	1596.1358
1618.7554	1658.4051	1756.3180
1921.2389	3024.9812	3026.2262
3028.4821	3031.1635	3032.2014
3035.4587	3036.1816	3046.1486
3100.2076	3102.9205	3106.6021
3109.1856	3115.6829	3121.5832
3122.1049	3131.2546	3133.8119
3137.2607	3138.3297	3140.9260
3141.2070	3147.1031	3150.1378
3154.9796	3166.8270	3184.5151
3187.9314	3202.7188	3802.6555

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.463240 Electronic Energy = -1260.66090600
Internal Energy (E)= -1260.16748 Enthalpy (H)= -1260.166537
Gibbs Free Energy (G)=-1260.25706 Gibbs Free Energy of Solvation=-1261.31755767

St.Pt.	General Structure	Ball & Stick model
II'-1B		

Cartesian co-ordinate

Atoms	X	Y	Z
H	-0.65968	-2.08813	0.48507
C	-1.48505	1.86403	-0.96703
C	-0.90936	2.72525	0.03715
C	0.42124	3.03582	-0.39400
C	0.65216	2.39117	-1.69108
C	-0.53712	1.67969	-2.04400
C	1.59994	-1.30604	-1.57756
O	1.21412	-0.85557	-0.40049
O	1.57718	-0.65137	-2.60805
C	2.19562	-2.71591	-1.53369
O	0.55294	0.46971	1.79226
C	1.11668	-0.62021	2.28612
O	0.50472	-1.65572	2.49035
C	2.56503	-0.43879	2.75465
C	1.89251	2.48219	-2.50217
H	1.79908	3.26867	-3.26228
H	2.75907	2.71946	-1.87615
H	2.08353	1.52298	-2.99178
C	-0.82321	0.91038	-3.28525
H	-1.61182	1.41192	-3.86193
H	0.06794	0.80725	-3.90526
H	-1.16064	-0.10550	-3.04656
C	1.40951	3.85614	0.35495
H	1.30769	3.70365	1.43513
H	2.43551	3.59307	0.07775
H	1.26658	4.92360	0.14422
C	-1.56049	3.11805	1.31641
H	-0.81595	3.36552	2.07923
H	-2.21605	3.98730	1.18185
H	-2.16158	2.29092	1.71181
C	-2.86807	1.32997	-0.95740
H	-3.23287	1.14517	0.05805
H	-3.53697	2.06620	-1.42431
H	-2.95267	0.40110	-1.53058
O	-1.51124	-2.28526	-1.35277
C	3.22686	-1.80168	2.92134
H	4.23821	-1.68243	3.33147
H	2.64488	-2.43968	3.59306
H	3.30839	-2.32454	1.95928
C	2.47636	0.25871	4.11868

Frequencies

33.1256	41.3877	52.5753
55.1285	56.2166	65.7940
72.4723	85.4785	86.8041
89.7630	91.2174	100.9884
110.1391	115.0188	116.0093
148.6927	152.0504	161.5145
168.9975	170.8272	178.7985
184.9856	190.6609	196.3346
206.3588	213.3444	218.4978
224.2211	229.2739	245.9407
251.3122	253.0671	255.8636
261.9006	277.3728	281.2238
297.9413	306.5498	312.4895
316.1989	323.7414	325.4120
329.0222	332.5905	333.8509
345.3131	355.3526	375.2929
381.7347	393.7435	394.9869
410.4271	420.2169	428.0018
434.6924	445.0708	454.4335
456.4288	459.5110	469.3155
534.4982	540.4196	547.7522
551.0281	554.2763	569.6562
570.7009	575.6049	582.6774
595.3731	605.2577	649.4858
671.9661	741.1508	780.5852
790.9515	796.8612	798.3896
802.7991	811.9434	814.0479
817.7279	840.5553	877.6731
890.9894	898.2520	916.7625
941.2038	946.1342	947.8431
949.7136	954.1713	959.9942
963.9933	976.9271	980.9831
998.9365	1023.2969	1031.5148
1033.7010	1036.4495	1038.9416
1040.1296	1042.7625	1045.7837
1052.1062	1053.6533	1091.7737
1098.7321	1099.5937	1108.9598
1132.4496	1156.4642	1190.1860
1190.4877	1209.3694	1227.4058
1234.3181	1236.0724	1240.1114
1262.3983	1265.3746	1279.1840
1327.0117	1342.2901	1344.1874
1366.4762	1377.8111	1379.1075
1380.1048	1381.4830	1382.5333

H	3.48220	0.40298	4.53454	1386.6995	1392.4178	1401.0675
H	1.99616	1.24073	4.02786	1403.0613	1408.1206	1414.6416
H	1.89666	-0.34550	4.82743	1426.0858	1430.2053	1436.7554
C	3.37937	0.42747	1.79621	1437.7979	1443.7704	1445.3980
H	3.40981	-0.00911	0.78940	1446.5227	1452.2386	1453.6609
H	2.96198	1.43857	1.71755	1457.1870	1458.4786	1460.0032
H	4.41069	0.51381	2.16326	1463.3140	1465.5270	1466.6393
C	2.01950	-3.37501	-2.89790	1469.2203	1471.5590	1472.9264
H	2.48080	-2.77820	-3.69058	1475.9711	1477.8819	1480.2175
H	2.48089	-4.37098	-2.89190	1488.8441	1491.0319	1499.5259
H	0.95538	-3.49134	-3.13652	1505.1088	1507.4917	1508.3337
C	1.56499	-3.58945	-0.45339	1511.4095	1521.4082	1530.9068
H	2.07109	-4.56374	-0.43048	1541.1518	1643.7430	1685.6477
H	1.63692	-3.13870	0.54345	1743.1232	1782.1236	1782.8225
H	0.50517	-3.76860	-0.67360	3019.6623	3023.7337	3026.2537
C	3.68910	-2.52375	-1.24212	3030.6971	3032.9477	3033.9390
H	4.19709	-3.49686	-1.23375	3037.1641	3039.1265	3039.6130
H	4.16135	-1.89676	-2.00877	3040.1321	3040.6804	3043.3512
H	3.84500	-2.05117	-0.26311	3109.0974	3113.0509	3115.0733
Ir	0.28807	0.92257	-0.15499	3117.2247	3119.0636	3119.0751
C	-1.56910	-2.03456	-0.14328	3120.3156	3121.6700	3122.2716
C	-2.78693	-1.64713	0.54488	3122.5111	3123.6260	3128.7169
C	-2.72183	-1.26961	1.89671	3132.7011	3135.1011	3138.7440
C	-4.02152	-1.60625	-0.14227	3139.5622	3142.7951	3146.5087
C	-3.86338	-0.85511	2.56044	3146.9902	3148.9023	3153.9714
H	-1.74529	-1.30154	2.38425	3157.3713	3179.0403	3182.6250
C	-5.17282	-1.20552	0.54046	3200.8252	3208.0241	3461.5780
C	-5.08393	-0.83540	1.87381			
H	-3.81830	-0.56123	3.60552			
H	-6.11591	-1.18589	0.00069			
H	-5.98655	-0.52104	2.39458			
O	-4.11241	-1.90718	-1.44195			
H	-3.20840	-2.16333	-1.74260			
H	5.67274	-0.47492	-2.32853			
C	0.63389	0.75102	-2.26539			
C	2.92715	1.58077	-1.45499			
C	4.85170	2.36254	-0.35019			
H	4.58554	3.41370	-0.51439			
H	5.46963	2.04686	-1.20246			
C	5.53081	2.13074	0.97347			
H	6.47248	2.68645	1.02514			
H	4.88756	2.45610	1.79667			
H	5.74242	1.06336	1.11047			
O	3.65827	1.57347	-0.34098			
O	3.14601	2.29349	-2.40703			
C	0.92000	0.94807	-3.71343			
H	-0.00533	0.88337	-4.29044			
H	1.41585	1.91119	-3.86642			
H	1.63737	0.18240	-4.03787			
O	-0.52197	0.63428	-1.87363			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.613850 Electronic Energy = -1607.50556410
Internal Energy (E)= -1606.8532241 Enthalpy (H)= -1606.8522801
Gibbs Free Energy (G)=-1606.9586691 Gibbs Free Energy of Solvation=-1607.01657539

St.Pt.	General Structure	Ball & Stick model
TS-2B		

Cartesian co-ordinate

Atoms	X	Y	Z
H	-0.06985	0.88142	0.97364
C	-1.64940	-1.87116	-1.01219
C	-1.49761	-0.95895	-2.10477
C	-0.16903	-1.16908	-2.65630
C	0.48623	-2.18989	-1.88594
C	-0.41663	-2.60061	-0.82746
C	2.49716	-1.09707	1.00443
O	1.86752	-0.18083	0.32498
O	2.28932	-2.30259	0.95461
C	3.54315	-0.48649	1.94917
O	0.49121	1.55245	-1.14800
C	0.69510	2.40094	-0.21724
O	0.47105	2.16948	0.99526
C	1.13483	3.79734	-0.64139
C	1.85474	-2.71828	-2.12613
H	1.81973	-3.54369	-2.84894
H	2.51060	-1.94058	-2.53157
H	2.29784	-3.06707	-1.18988
C	-0.23076	-3.70128	0.15686
H	-0.85767	-4.56225	-0.11249
H	0.81327	-4.00975	0.21424
H	-0.50706	-3.36695	1.16234
C	0.39839	-0.44460	-3.82471
H	0.04145	0.58953	-3.86263
H	1.49128	-0.41342	-3.78145
H	0.10844	-0.93814	-4.76146
C	-2.51770	-0.02275	-2.65382
H	-2.05528	0.92468	-2.95590
H	-3.01245	-0.45018	-3.53557
H	-3.28713	0.21204	-1.91101
C	-2.88230	-2.11378	-0.21763
H	-3.57974	-1.27180	-0.25065
H	-3.39337	-2.99480	-0.62874
H	-2.65686	-2.33133	0.83195
O	-0.46893	-0.82553	2.30709
C	1.88910	4.47723	0.49669
H	2.18869	5.48754	0.19064
H	1.27107	4.55259	1.39631
H	2.79485	3.91713	0.76060
C	-0.15669	4.56582	-0.94774
H	0.08101	5.59328	-1.25087
H	-0.71306	4.08693	-1.76426
H	-0.80411	4.61132	-0.06273
C	2.01022	3.72460	-1.88838
H	2.92253	3.14714	-1.69474
H	1.48144	3.24890	-2.72058
H	2.30497	4.73693	-2.19252
C	4.48718	-1.57218	2.44825

Frequencies

-1631.7852	38.5202	44.7562
47.4974	53.1360	64.2222
69.9254	78.7677	82.2429
89.9772	95.8196	107.4682
125.5414	132.9452	146.7358
150.5946	154.9307	165.6088
166.7049	173.6567	182.1756
186.4920	188.4412	196.8360
200.1531	213.5267	225.6928
227.2490	231.7971	244.4833
251.0790	252.7193	265.1809
273.8361	276.7877	281.8752
289.2039	303.9163	306.4044
308.5334	313.2025	324.0578
325.2771	326.7706	335.0101
343.2537	363.9972	371.5323
394.5017	398.4850	401.2455
413.1108	423.2408	431.3892
435.8589	437.8198	444.9998
452.4976	462.9340	477.0186
525.0513	535.3282	541.8731
547.9612	564.5591	571.2324
577.6365	587.5783	589.5310
601.7567	612.4864	635.3338
645.5318	684.8555	750.0021
779.0890	794.0820	795.0825
806.4944	817.3022	818.9598
819.9984	826.0434	829.5518
881.3507	901.1511	919.4130
927.3154	949.9639	952.0582
955.8205	956.6901	959.0555
965.4844	967.2090	971.2879
981.7439	992.4446	1037.4311
1038.6624	1041.9130	1043.5436
1044.4973	1046.6772	1050.7133
1052.0291	1052.5783	1060.8086
1087.0110	1095.2740	1109.5644
1133.3581	1155.4642	1182.1547
1188.4283	1212.5717	1236.0059
1240.1424	1246.8955	1249.1040
1259.8795	1266.3095	1268.3168
1308.9943	1343.4811	1355.7857
1366.8405	1375.4999	1379.6614
1381.1539	1383.0348	1385.1543
1388.2574	1390.1031	1396.0691
1399.6861	1400.9124	1412.5110
1417.6177	1430.7761	1431.5842
1432.5689	1442.1123	1447.2044
1449.5414	1452.6021	1455.7917
1458.3190	1460.6354	1461.5156
1463.3258	1465.8600	1469.6227
1471.8863	1472.9989	1475.8123

H	5.03072	-2.03872	1.61764	1477.0160	1478.0881	1478.4196
H	5.22212	-1.14225	3.14174	1483.2772	1489.5415	1490.9857
H	3.93655	-2.36326	2.96683	1498.7547	1502.5803	1503.1239
C	2.76775	0.11511	3.12727	1513.3843	1520.7650	1525.6991
H	3.47019	0.52686	3.86481	1528.0030	1535.2595	1638.7526
H	2.10494	0.92134	2.79054	1673.1428	1691.5569	1703.7688
H	2.15366	-0.64659	3.62368	1778.4419	3022.4802	3023.0280
C	4.33292	0.61744	1.24830	3025.8446	3031.7158	3035.0648
H	5.06910	1.04721	1.94092	3036.4367	3038.6291	3039.9683
H	4.87723	0.23024	0.37695	3041.3367	3041.7067	3043.3095
H	3.66777	1.41867	0.90608	3104.6754	3107.8738	3113.5184
Ir	0.04871	-0.47580	-0.62134	3113.7208	3115.6876	3118.5342
C	-0.88996	-0.04959	1.43825	3119.6087	3119.6745	3122.5208
C	-2.26855	0.45693	1.46173	3124.7885	3125.9791	3132.8588
C	-2.70152	1.41057	0.52775	3133.1375	3136.9833	3141.5956
C	-3.19031	-0.03281	2.41696	3143.5624	3145.8207	3146.8350
C	-4.01026	1.85546	0.50819	3149.6272	3152.7753	3167.9155
H	-1.98564	1.77530	-0.20835	3179.1243	3185.3942	3185.7146
C	-4.51695	0.41487	2.39033	3200.1557	3206.6598	3427.0140
C	-4.91530	1.34601	1.44785			
H	-4.33163	2.59411	-0.22142			
H	-5.20754	0.01059	3.12584			
H	-5.94842	1.68709	1.44185			
O	-2.85274	-0.95011	3.32411			
H	-1.88297	-1.10893	3.22778			
H	5.67274	-0.47492	-2.32853			
C	0.63389	0.75102	-2.26539			
C	2.92715	1.58077	-1.45499			
C	4.85170	2.36254	-0.35019			
H	4.58554	3.41370	-0.51439			
H	5.46963	2.04686	-1.20246			
C	5.53081	2.13074	0.97347			
H	6.47248	2.68645	1.02514			
H	4.88756	2.45610	1.79667			
H	5.74242	1.06336	1.11047			
O	3.65827	1.57347	-0.34098			
O	3.14601	2.29349	-2.40703			
C	0.92000	0.94807	-3.71343			
H	-0.00533	0.88337	-4.29044			
H	1.41585	1.91119	-3.86642			
H	1.63737	0.18240	-4.03787			
O	-0.52197	0.63428	-1.87363			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.609519 Electronic Energy = -1607.47132519
Internal Energy (E)= -1606.82420719 Enthalpy (H)= -1606.82326419
Gibbs Free Energy (G)=-1606.92697119 Gibbs Free Energy of Solvation=-1606.97484527

St.Pt.	General Structure	Ball & Stick model
III-1B		

Cartesian co-ordinate

Atoms	X	Y	Z
H	0.10352	1.97114	0.74853
C	-0.82861	-2.63382	-0.81205
C	-0.42831	-2.81266	0.55278
C	-1.54813	-2.41939	1.41532
C	-2.56375	-1.90702	0.60181
C	-2.10070	-1.93820	-0.79413
C	-2.28057	1.85198	-0.23022
O	-1.23194	1.34520	0.37700
O	-3.15075	1.18340	-0.76194
C	-2.32649	3.38540	-0.22298
O	0.95613	-0.01443	1.58986
C	1.52997	1.08379	1.63332
O	1.04396	2.16657	1.10001
C	2.86799	1.25384	2.32457
C	-3.87266	-1.34642	1.02770
H	-4.68609	-2.01957	0.72553
H	-3.92580	-1.21831	2.11311
H	-4.04069	-0.37630	0.54780
C	-2.92947	-1.62765	-1.99049
H	-3.48463	-2.51654	-2.32147
H	-3.62858	-0.81826	-1.77218
H	-2.29894	-1.28532	-2.81811
C	-1.49594	-2.48192	2.90219
H	-0.59157	-1.98721	3.27892
H	-2.35893	-1.98712	3.35722
H	-1.47683	-3.52078	3.25777
C	0.79400	-3.49792	1.06079
H	1.28310	-2.90871	1.84768
H	0.53434	-4.47447	1.49090
H	1.52657	-3.67081	0.26622
C	-0.10968	-3.08514	-2.03554
H	0.96952	-3.17183	-1.87391
H	-0.48489	-4.06610	-2.35514
H	-0.26440	-2.38454	-2.86310
O	-0.14965	0.81197	-2.23567
C	2.67060	2.19922	3.51490
H	3.63056	2.34962	4.02375
H	2.29594	3.17488	3.18904
H	1.96423	1.78207	4.24364
C	3.85390	1.87420	1.32688
H	4.82692	2.00240	1.81729
H	3.99812	1.22852	0.45013
H	3.50854	2.85391	0.98253
C	3.38515	-0.09698	2.80343
H	2.68282	-0.57146	3.49851
H	3.54235	-0.77917	1.95878
H	4.34363	0.03955	3.31844
C	-3.67411	3.85251	-0.76069
H	-4.49848	3.48943	-0.13630
H	-3.70916	4.94956	-0.77622
H	-3.84306	3.48142	-1.77627
C	-1.21081	3.89766	-1.13976
H	-1.25030	4.99358	-1.19381
H	-0.21422	3.61476	-0.78161

Frequencies

17.4749	36.1898	37.1773
45.7714	55.7210	67.4460
71.9510	79.0937	83.5313
87.4317	96.8503	116.8214
134.3813	139.4658	145.5563
154.3377	156.2804	159.1911
166.7158	168.6314	173.2217
184.8167	188.0192	194.0854
198.6359	206.0558	213.5988
214.9871	221.5028	223.3290
233.3418	252.1426	256.2479
274.7657	283.9309	286.7616
292.8997	294.8958	309.4236
314.0551	319.7831	324.2793
332.0705	339.2324	339.6298
359.0122	369.6499	388.7591
395.2387	396.5888	403.8245
411.8410	427.3656	440.7800
448.6664	455.5928	459.4544
468.9831	486.3418	531.8555
536.0767	547.5967	548.2835
553.1139	570.0970	572.3785
593.3998	595.1632	608.7810
615.6021	630.2451	667.3907
681.5415	755.0906	774.8823
777.7149	780.7267	797.6113
807.3824	811.0591	825.1057
828.2728	836.1541	877.1069
909.5401	910.4717	922.7420
949.1204	949.5001	956.4951
958.4291	963.0780	964.1260
965.3139	973.3382	974.7890
1005.2320	1019.0084	1028.7629
1038.2647	1040.0222	1043.3890
1046.2170	1048.1612	1050.0209
1052.0324	1056.3592	1057.5310
1092.7049	1096.5707	1109.1298
1123.4683	1148.8136	1179.8832
1185.8706	1198.4577	1231.5500
1239.8671	1242.9703	1245.5936
1251.5781	1259.8602	1265.1859
1340.0279	1347.5918	1367.3621
1367.8059	1374.3983	1384.3408
1385.0869	1386.4198	1393.1119
1398.8778	1401.0315	1404.8278
1405.6789	1418.6724	1424.1888
1431.0614	1436.1315	1440.3465
1442.2153	1445.2958	1451.0762
1454.6213	1455.6432	1458.4247
1459.3893	1460.0950	1462.7307
1464.7095	1465.3925	1469.7513
1477.8316	1479.1348	1480.8188
1484.7126	1484.7895	1489.0925
1490.4354	1498.3548	1498.8002
1500.4560	1511.4769	1523.9497
1527.9437	1532.7367	1559.9898
1584.5852	1636.7364	1666.1568
1694.2450	1737.0597	1797.8011

H	-1.32795	3.49894	-2.15435	2744.0497	3026.0415	3027.3537
C	-2.13111	3.92364	1.19572	3031.0360	3031.1363	3032.1810
H	-2.21094	5.01854	1.18874	3032.5010	3033.4930	3037.1656
H	-2.90110	3.53746	1.87577	3038.6096	3039.5714	3040.3105
H	-1.15188	3.66418	1.61106	3096.5818	3102.8541	3106.3152
Ir	-0.62047	-0.70041	0.11904	3110.5443	3115.7208	3119.0493
C	0.44977	0.11053	-1.40954	3120.0196	3122.6439	3123.6508
C	1.90963	-0.11000	-1.58743	3123.8202	3127.5543	3134.5753
C	2.63591	-0.98942	-0.76992	3137.7306	3137.7683	3141.3999
C	2.60983	0.57889	-2.61199	3143.4635	3145.0552	3145.8602
C	3.99264	-1.20281	-0.93980	3146.4669	3147.9931	3149.2488
H	2.09836	-1.50184	0.02419	3177.8911	3182.4671	3193.2568
C	3.99050	0.38014	-2.76469	3204.5624	3225.0654	3376.4826
C	4.66835	-0.50261	-1.94534			
H	4.52578	-1.89788	-0.29505			
H	4.49374	0.93083	-3.55537			
H	5.73664	-0.65180	-2.08869			
O	2.01470	1.42121	-3.45268			
H	1.05248	1.40850	-3.22142			
H	5.67274	-0.47492	-2.32853			
C	0.63389	0.75102	-2.26539			
C	2.92715	1.58077	-1.45499			
C	4.85170	2.36254	-0.35019			
H	4.58554	3.41370	-0.51439			
H	5.46963	2.04686	-1.20246			
C	5.53081	2.13074	0.97347			
H	6.47248	2.68645	1.02514			
H	4.88756	2.45610	1.79667			
H	5.74242	1.06336	1.11047			
O	3.65827	1.57347	-0.34098			
O	3.14601	2.29349	-2.40703			
C	0.92000	0.94807	-3.71343			
H	-0.00533	0.88337	-4.29044			
H	1.41585	1.91119	-3.86642			
H	1.63737	0.18240	-4.03787			
O	-0.52197	0.63428	-1.87363			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.614433 Electronic Energy = -1607.52627565
Internal Energy (E)= -1606.87360765 Enthalpy (H)= -1606.87266365
Gibbs Free Energy (G)=-1606.97941465 Gibbs Free Energy of Solvation=-1607.02155333

St.Pt.	General Structure	Ball & Stick model
III'-1B		

Cartesian co-ordinate

Atoms	X	Y	Z

Frequencies

23.8941	38.0846	39.1661
58.8586	63.5136	75.2894
86.5407	88.3792	111.2408

C	2.77297	0.18142	-1.18543
C	2.55342	1.24483	-0.30639
C	2.28828	0.69361	1.03218
C	2.50460	-0.73683	0.96736
C	2.64840	-1.06598	-0.41954
O	-0.91900	1.11911	-0.55775
C	-1.25014	2.17360	0.14083
O	-0.52187	2.73170	0.94782
C	-2.68698	2.64015	-0.13378
C	-1.74882	-1.85668	-0.85784
H	-1.16433	-0.24857	-1.72144
C	2.45284	2.69419	-0.61919
H	1.51049	3.09109	-0.22169
H	3.27403	3.24738	-0.14464
H	2.48908	2.88559	-1.69584
C	2.12236	1.47333	2.28737
H	3.09261	1.64715	2.77337
H	1.63795	2.43117	2.08769
H	1.47628	0.92516	2.98204
C	2.84372	-2.42098	-1.00539
H	2.26821	-2.53029	-1.93210
H	3.90092	-2.60044	-1.24322
H	2.51255	-3.20454	-0.31707
C	3.00586	0.23303	-2.65524
H	2.30452	-0.41472	-3.19579
H	2.88682	1.24785	-3.04641
H	4.01989	-0.10617	-2.90662
C	2.53820	-1.64684	2.14228
H	3.47650	-1.51372	2.69592
H	1.70296	-1.43210	2.81883
H	2.46641	-2.69803	1.84444
Ir	0.70619	-0.16359	-0.08377
C	-2.85974	2.94770	-1.62174
H	-2.66120	2.06635	-2.24176
H	-3.88818	3.27784	-1.81945
H	-2.18335	3.75014	-1.94281
C	-3.63620	1.50811	0.27343
H	-3.47832	1.21976	1.32132
H	-4.67917	1.83415	0.16553
H	-3.49189	0.61405	-0.34621
C	-2.98759	3.88574	0.68906
H	-2.87108	3.68702	1.75947
H	-2.30435	4.70261	0.43226
H	-4.01675	4.21998	0.50317
O	-0.79158	-1.15122	-1.58941
C	-1.67043	-1.82629	0.53051
C	-2.63161	-2.51153	1.27360
C	-2.74971	-2.55161	-1.51882
C	-3.64435	-3.21078	0.63094
C	-3.69987	-3.23180	-0.76228
C	-0.57051	-1.04857	1.19345
O	-0.51872	-0.99448	2.41092
H	-2.77448	-2.55467	-2.60560
H	-4.49074	-3.78196	-1.26681
H	-4.39424	-3.74337	1.21071
H	-2.55634	-2.46981	2.35793
H	-2.21094	5.01854	1.18874
H	-2.90110	3.53746	1.87577
H	-1.15188	3.66418	1.61106

123.4282	130.9860	138.8976
145.3643	150.1157	152.4181
169.3669	178.8765	191.5268
203.0152	210.4114	217.1870
219.7765	239.5787	242.5713
245.3027	261.1779	262.0207
278.8402	283.6758	287.6607
298.6835	311.3791	321.8335
339.7828	349.2477	362.7055
378.5458	387.4357	417.3202
427.6652	430.8209	437.5720
462.9473	515.9437	528.6432
537.7867	546.9462	553.5397
561.7833	580.6604	592.4856
597.0958	613.4700	623.5370
648.4553	668.5275	724.5470
772.8783	780.0940	782.3715
805.4687	808.0540	817.4957
836.5620	881.2115	893.5185
919.0399	942.3407	943.1877
946.3684	959.2788	959.8985
964.5674	993.8425	1027.5585
1034.8468	1036.0551	1042.8104
1043.4610	1045.0571	1047.7528
1052.1183	1085.6436	1089.4666
1104.0953	1107.1266	1152.3486
1176.4931	1184.8488	1189.5599
1224.3221	1238.3511	1245.0160
1263.1254	1271.3850	1330.4685
1359.3779	1364.9943	1369.8207
1372.8697	1376.5990	1386.3480
1388.3228	1390.3915	1394.9828
1413.0841	1427.2103	1431.0159
1440.0635	1442.8299	1444.4673
1449.1127	1450.1663	1453.9455
1455.9092	1457.6251	1463.3760
1467.9010	1469.3146	1470.4002
1472.7667	1482.0544	1483.1503
1485.2952	1493.5980	1504.9249
1509.2123	1526.2793	1587.6420
1649.5802	1667.1922	1762.9892
1790.5752	3023.6803	3026.3195
3029.3196	3030.5984	3034.9861
3035.8522	3036.7279	3037.4289
3099.6558	3108.4605	3109.5045
3111.1655	3119.0912	3119.2260
3119.5278	3123.4514	3123.5422
3124.7022	3137.6262	3139.7458
3142.1212	3143.4350	3150.5070
3183.3693	3195.1912	3198.7017
3203.9094	3208.7058	3523.6442

Ir	-0.62047	-0.70041	0.11904
C	0.44977	0.11053	-1.40954
C	1.90963	-0.11000	-1.58743
C	2.63591	-0.98942	-0.76992
C	2.60983	0.57889	-2.61199
C	3.99264	-1.20281	-0.93980
H	2.09836	-1.50184	0.02419
C	3.99050	0.38014	-2.76469
C	4.66835	-0.50261	-1.94534
H	4.52578	-1.89788	-0.29505
H	4.49374	0.93083	-3.55537
H	5.73664	-0.65180	-2.08869
O	2.01470	1.42121	-3.45268
H	1.05248	1.40850	-3.22142
H	5.67274	-0.47492	-2.32853
C	0.63389	0.75102	-2.26539
C	2.92715	1.58077	-1.45499
C	4.85170	2.36254	-0.35019
H	4.58554	3.41370	-0.51439
H	5.46963	2.04686	-1.20246
C	5.53081	2.13074	0.97347
H	6.47248	2.68645	1.02514
H	4.88756	2.45610	1.79667
H	5.74242	1.06336	1.11047
O	3.65827	1.57347	-0.34098
O	3.14601	2.29349	-2.40703
C	0.92000	0.94807	-3.71343
H	-0.00533	0.88337	-4.29044
H	1.41585	1.91119	-3.86642
H	1.63737	0.18240	-4.03787
O	-0.52197	0.63428	-1.87363

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.463220 Electronic Energy = -1260.66897530
Internal Energy (E)= -1260.1756233 Enthalpy (H)= -1260.1746803
Gibbs Free Energy (G)=-1260.2652063 Gibbs Free Energy of Solvation=-1260.30562806

St.Pt.	General Structure	Ball & Stick model
TS-3B		

Cartesian co-ordinate

Atoms	X	Y	Z

Frequencies

-1604.1331	29.2376	39.0928
46.5399	54.9564	67.8800
76.0370	87.3531	112.1411

C	2.86057	0.11212	-1.18208
C	2.66614	1.27317	-0.43265
C	2.37215	0.89209	0.95967
C	2.54390	-0.53314	1.06920
C	2.67714	-1.03509	-0.27984
O	-0.85113	1.47994	-0.76537
C	-1.62132	2.01301	0.20625
O	-1.13359	2.40991	1.23838
C	-3.09050	2.20061	-0.16548
C	-1.58329	-1.77252	-0.85169
H	-0.97489	0.29567	-1.25890
C	2.60396	2.67944	-0.90944
H	1.65760	3.14465	-0.60699
H	3.41512	3.27252	-0.46720
H	2.68130	2.75028	-1.99804
C	2.16689	1.83439	2.09312
H	3.12367	2.20295	2.48817
H	1.55638	2.68907	1.78550
H	1.62047	1.33693	2.90137
C	2.85642	-2.45364	-0.69260
H	2.34621	-2.64819	-1.64278
H	3.92014	-2.69393	-0.82507
H	2.44038	-3.14149	0.04996
C	3.08976	-0.01815	-2.64718
H	2.33487	-0.66650	-3.10921
H	3.04462	0.95157	-3.15143
H	4.07334	-0.45974	-2.85614
C	2.54359	-1.31176	2.33384
H	3.47471	-1.13299	2.88591
H	1.69487	-1.02329	2.96458
H	2.46093	-2.38646	2.14268
Ir	0.78456	-0.07020	-0.08376
C	-3.14579	3.27176	-1.26123
H	-2.59518	2.95661	-2.15427
H	-4.19015	3.45564	-1.54430
H	-2.71938	4.21869	-0.90728
C	-3.70120	0.90118	-0.68926
H	-3.62745	0.09046	0.04775
H	-4.76541	1.06229	-0.90277
H	-3.22728	0.56719	-1.62002
C	-3.85606	2.67442	1.06402
H	-3.81672	1.92707	1.86442
H	-3.43187	3.60270	1.45951
H	-4.90758	2.84997	0.80400
O	-0.69690	-1.01571	-1.54624
C	-1.55161	-1.76553	0.54797
C	-2.48416	-2.51033	1.27443
C	-2.53533	-2.53976	-1.52412
C	-3.43446	-3.26994	0.60954
C	-3.44921	-3.28351	-0.78852
C	-0.50856	-0.93744	1.21269
O	-0.46620	-0.82465	2.42530
H	-2.54649	-2.53209	-2.61127
H	-4.19163	-3.88196	-1.31283
H	-4.16135	-3.85488	1.16752
H	-2.43197	-2.47198	2.36050
H	-2.21094	5.01854	1.18874
H	-2.90110	3.53746	1.87577
H	-1.15188	3.66418	1.61106

122.8483	133.8280	142.0566
145.6835	157.8893	166.1331
168.5495	175.3893	178.1777
186.8151	204.5591	209.2383
216.5261	228.3988	247.8660
250.7261	255.2657	267.4512
282.0052	287.6837	294.6480
307.6945	310.9268	324.9863
330.0857	339.6060	349.5635
367.0666	375.8724	386.6437
403.7613	427.8264	436.1723
449.1683	463.3227	528.3095
537.1099	539.0330	551.3647
554.5717	569.2048	580.2909
592.7544	599.2673	601.2696
615.8411	649.2517	672.3539
761.7770	770.9631	784.1217
798.6796	806.5914	810.5467
852.3832	873.2722	892.6786
900.6220	946.8221	950.7734
952.9699	959.3729	959.8823
962.8624	979.2857	1028.5479
1036.1973	1039.7976	1040.0099
1043.7585	1044.1261	1046.3693
1052.8861	1086.0676	1089.3188
1103.4091	1106.8108	1145.9993
1174.6527	1180.2074	1189.7444
1195.0782	1242.1303	1249.4012
1265.1503	1297.5160	1317.6825
1366.1596	1366.4118	1373.3371
1380.1617	1386.9654	1387.9034
1397.6368	1401.1695	1401.8438
1417.4773	1428.9964	1435.6118
1439.6937	1446.3298	1447.3230
1449.9409	1450.9948	1455.8427
1457.3292	1461.5353	1464.2238
1464.8996	1470.7132	1470.9979
1480.2443	1480.9829	1481.7380
1486.3865	1499.2640	1506.9005
1507.9833	1509.3645	1539.7227
1591.6670	1640.1793	1655.3485
1769.5926	1842.7938	3028.5450
3028.8316	3030.6574	3031.1168
3032.8425	3035.2886	3037.6684
3039.7178	3099.5755	3108.8400
3113.8548	3115.4836	3116.5712
3121.2823	3123.9703	3125.2789
3126.7947	3137.6894	3139.5126
3139.9699	3141.1070	3143.7233
3144.1218	3149.9475	3181.5491
3192.3543	3201.9860	3207.5958

Ir	-0.62047	-0.70041	0.11904
C	0.44977	0.11053	-1.40954
C	1.90963	-0.11000	-1.58743
C	2.63591	-0.98942	-0.76992
C	2.60983	0.57889	-2.61199
C	3.99264	-1.20281	-0.93980
H	2.09836	-1.50184	0.02419
C	3.99050	0.38014	-2.76469
C	4.66835	-0.50261	-1.94534
H	4.52578	-1.89788	-0.29505
H	4.49374	0.93083	-3.55537
H	5.73664	-0.65180	-2.08869
O	2.01470	1.42121	-3.45268
H	1.05248	1.40850	-3.22142
H	5.67274	-0.47492	-2.32853
C	0.63389	0.75102	-2.26539
C	2.92715	1.58077	-1.45499
C	4.85170	2.36254	-0.35019
H	4.58554	3.41370	-0.51439
H	5.46963	2.04686	-1.20246
C	5.53081	2.13074	0.97347
H	6.47248	2.68645	1.02514
H	4.88756	2.45610	1.79667
H	5.74242	1.06336	1.11047
O	3.65827	1.57347	-0.34098
O	3.14601	2.29349	-2.40703
C	0.92000	0.94807	-3.71343
H	-0.00533	0.88337	-4.29044
H	1.41585	1.91119	-3.86642
H	1.63737	0.18240	-4.03787
O	-0.52197	0.63428	-1.87363

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.457794 Electronic Energy = -1260.63840056
Internal Energy (E)= -1260.15098956 Enthalpy (H)= -1260.15004556
Gibbs Free Energy (G)=-1260.23886856 Gibbs Free Energy of Solvation=-1260.2833218

St.Pt.	General Structure	Ball & Stick model
IV-1B		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-2.85566	0.04965	-1.12180
C	-2.64518	-1.22582	-0.59455
C	-2.33729	-1.10197	0.83809
C	-2.48142	0.27308	1.20254
C	-2.64261	1.01785	-0.03278
O	0.93909	-1.30407	-0.82974

Frequencies

31.2463	38.2634	49.7780
52.5277	68.6763	73.7957
83.4397	98.8667	107.2791
122.4843	133.6506	150.5399
160.0928	163.8164	164.8486
177.6763	181.6404	186.8841
211.9659	214.0911	221.1845
234.1852	239.6161	242.8588
260.7249	270.0556	270.8021
293.9192	300.4950	306.4444

C	1.62529	-2.22387	-0.07071
O	0.98654	-3.01353	0.56562
C	3.14116	-2.16155	-0.17316
C	1.34749	1.93206	-0.79453
H	1.46724	-0.61836	-1.28596
C	-2.56831	-2.52216	-1.32042
H	-1.60095	-3.00482	-1.12846
H	-3.35005	-3.21249	-0.97754
H	-2.67505	-2.39562	-2.40187
C	-2.14595	-2.23513	1.78470
H	-3.10875	-2.61492	2.15452
H	-1.60801	-3.06022	1.30870
H	-1.54885	-1.91716	2.64664
C	-2.81888	2.48995	-0.17170
H	-2.39507	2.83897	-1.12019
H	-3.87998	2.77287	-0.14684
H	-2.30028	3.02390	0.63150
C	-3.08334	0.44456	-2.53864
H	-2.30010	1.13496	-2.87733
H	-3.07299	-0.42193	-3.20669
H	-4.04922	0.95224	-2.66094
C	-2.43128	0.81108	2.58730
H	-3.35038	0.55359	3.12882
H	-1.57109	0.40121	3.12897
H	-2.32893	1.90111	2.59109
Ir	-0.75475	0.07540	-0.07981
C	3.54806	-2.47637	-1.61836
H	3.17887	-1.73224	-2.33462
H	4.64218	-2.48316	-1.68965
H	3.18288	-3.46219	-1.93026
C	3.64858	-0.77212	0.22767
H	3.31122	-0.49367	1.23364
H	4.74496	-0.78377	0.22790
H	3.33686	0.02475	-0.46107
C	3.72284	-3.21101	0.76694
H	3.44026	-3.00866	1.80525
H	3.36613	-4.21442	0.51338
H	4.81674	-3.19936	0.69585
O	0.46035	1.17680	-1.42232
C	1.46099	1.84381	0.60755
C	2.42489	2.57933	1.30187
C	2.22820	2.78165	-1.48935
C	3.28386	3.41838	0.61139
C	3.17306	3.51010	-0.78318
C	0.56288	0.86039	1.24567
O	0.65317	0.54586	2.42313
H	2.14749	2.85194	-2.57190
H	3.84656	4.16883	-1.32946
H	4.03653	3.99947	1.13831
H	2.47995	2.46167	2.38293
H	-2.21094	5.01854	1.18874
H	-2.90110	3.53746	1.87577
H	-1.15188	3.66418	1.61106
Ir	-0.62047	-0.70041	0.11904
C	0.44977	0.11053	-1.40954
C	1.90963	-0.11000	-1.58743
C	2.63591	-0.98942	-0.76992
C	2.60983	0.57889	-2.61199
C	3.99264	-1.20281	-0.93980
H	2.09836	-1.50184	0.02419
C	3.99050	0.38014	-2.76469

308.8306	312.2158	326.4773
331.5040	360.1901	365.0938
377.7043	390.0248	405.5715
415.2039	430.1462	469.0828
476.8947	518.6518	532.1207
539.4540	542.4077	550.1257
568.2140	592.9767	596.5578
600.6726	614.4831	621.9767
656.1601	679.3639	731.3947
763.5199	766.8862	768.3145
805.7264	806.3872	814.4349
860.8479	866.0178	885.6295
896.5357	945.4776	954.7954
956.0165	956.5197	963.0114
969.8793	975.4485	1019.0461
1033.2179	1038.0740	1043.2539
1044.1783	1045.4544	1045.7880
1048.6775	1064.6844	1089.9282
1095.5309	1109.4992	1110.4655
1142.8474	1169.0779	1178.5605
1186.5199	1199.1188	1240.1696
1256.3403	1264.3189	1309.2936
1339.3091	1368.3572	1375.1554
1377.0111	1388.8889	1391.5315
1393.7020	1396.2091	1404.2432
1419.8370	1429.9830	1431.5872
1437.9708	1446.8910	1451.1002
1451.4721	1454.0944	1456.3922
1458.4543	1461.5120	1466.8445
1468.3521	1470.0260	1475.3705
1478.7909	1481.0399	1485.5284
1487.6830	1502.0556	1509.2451
1513.1991	1519.9300	1592.4143
1625.5594	1657.6871	1758.5093
1906.8469	3026.9558	3028.7500
3029.3511	3029.9234	3033.6109
3035.2456	3035.8581	3047.6665
3101.0879	3108.8462	3112.3725
3112.4005	3115.2208	3120.3111
3123.4815	3124.8772	3128.7773
3135.9414	3137.9814	3138.9482
3140.1954	3141.9371	3149.5517
3160.1756	3170.8989	3182.8520
3191.8713	3201.8709	3668.4880

C	4.66835	-0.50261	-1.94534
H	4.52578	-1.89788	-0.29505
H	4.49374	0.93083	-3.55537
H	5.73664	-0.65180	-2.08869
O	2.01470	1.42121	-3.45268
H	1.05248	1.40850	-3.22142
H	5.67274	-0.47492	-2.32853
C	0.63389	0.75102	-2.26539
C	2.92715	1.58077	-1.45499
C	4.85170	2.36254	-0.35019
H	4.58554	3.41370	-0.51439
H	5.46963	2.04686	-1.20246
C	5.53081	2.13074	0.97347
H	6.47248	2.68645	1.02514
H	4.88756	2.45610	1.79667
H	5.74242	1.06336	1.11047
O	3.65827	1.57347	-0.34098
O	3.14601	2.29349	-2.40703
C	0.92000	0.94807	-3.71343
H	-0.00533	0.88337	-4.29044
H	1.41585	1.91119	-3.86642
H	1.63737	0.18240	-4.03787
O	-0.52197	0.63428	-1.87363

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.463796 Electronic Energy = -1260.66460444
Internal Energy (E)= -1260.17101344 Enthalpy (H)= -1260.17007044
Gibbs Free Energy (G)=-1260.25932744 Gibbs Free Energy of Solvation=-1260.30312252

St.Pt.	General Structure	Ball & Stick model
IV'-1B		

Cartesian co-ordinate

Atoms	X	Y	Z
C	1.95563	-0.94866	-1.82951
C	2.72101	-0.03990	-1.08856
C	2.75985	-0.49745	0.30390
C	2.11256	-1.77201	0.36582
C	1.50285	-2.00738	-0.92186
C	-2.19731	-0.97647	-0.52153
Ir	0.55858	-0.27295	-0.07381
O	-1.22649	-0.36879	-1.17717
C	-1.99941	-1.33419	0.82569
C	-3.01152	-1.95669	1.56230
C	-3.43507	-1.26667	-1.12490
C	-4.22545	-2.24192	0.96163
C	-4.42312	-1.89360	-0.38221
C	-0.67857	-0.99272	1.37884

Frequencies

29.8390	44.6685	49.0532
70.4230	79.3493	87.5869
98.7655	115.1890	120.7431
127.5623	136.1849	137.2642
143.8936	146.3649	159.3389
163.9959	171.3314	182.2709
186.5728	197.4826	204.6165
212.8763	222.1235	230.9688
241.0884	243.0448	252.2572
265.4104	266.6130	275.9804
282.9288	291.0289	296.7348
301.3333	312.5464	324.8624
327.9908	341.9179	346.8041
355.5422	358.9179	390.4924
397.4950	436.9197	441.6137
461.4193	475.5960	485.5534
501.3034	530.5280	537.8120
542.3992	552.0927	565.1857

O	-0.36103	-1.19324	2.53955	570.4938	591.2502	594.7295
H	-3.58720	-1.00178	-2.17008	604.0757	616.2215	625.2705
H	-5.37636	-2.12066	-0.85725	636.8893	661.4608	673.4326
H	-5.02008	-2.72916	1.52064	678.5127	759.9024	766.7514
H	-2.81305	-2.20289	2.60355	769.7282	809.6433	815.9386
C	-0.09019	1.84432	0.46391	860.8625	865.8115	870.2572
C	1.05450	2.20449	1.43606	890.2492	914.6084	953.7634
C	-1.52552	2.00399	0.93917	957.6520	959.1027	969.8851
C	-2.50018	2.38651	-1.33100	974.5899	992.7029	1034.7328
H	-2.05652	3.33508	-1.66414	1037.6404	1043.6341	1046.3163
H	-1.92755	1.53278	-1.71540	1046.8029	1050.2470	1054.0050
C	-3.94503	2.29856	-1.75200	1059.4635	1088.6449	1091.9352
H	-4.02027	2.32125	-2.84403	1110.7887	1117.0030	1124.3936
H	-4.38178	1.36277	-1.38828	1146.0564	1147.6562	1173.0205
H	-4.52170	3.13451	-1.34401	1181.4011	1183.9265	1187.4685
O	-2.50437	2.35561	0.10857	1203.5325	1268.5242	1291.4342
O	-1.76823	1.85054	2.10792	1330.7918	1339.8891	1373.6825
N	0.21437	2.46407	-0.72350	1376.5523	1379.7173	1382.8779
N	0.64726	2.99905	-1.61221	1391.7396	1396.0773	1397.1268
C	3.63570	0.07394	1.36528	1403.0353	1421.9801	1429.9115
H	3.35421	-0.30987	2.35184	1431.4226	1437.4607	1440.5820
H	4.68340	-0.20647	1.18721	1443.9209	1453.4987	1455.2958
H	3.58476	1.16793	1.39652	1458.8351	1459.5076	1462.7645
C	3.37621	1.20526	-1.57058	1469.4966	1474.4027	1481.5964
H	3.12583	2.06184	-0.93201	1484.5413	1489.2536	1493.0858
H	4.46896	1.09712	-1.54309	1503.8956	1504.7269	1513.2758
H	3.09471	1.44402	-2.60159	1517.7187	1518.5421	1581.7039
C	1.53476	-0.85246	-3.25420	1626.9899	1659.0506	1762.5962
H	0.44606	-0.96273	-3.33726	1790.9383	1863.1594	2260.3759
H	1.80811	0.11335	-3.69196	3031.1707	3031.7395	3032.8199
H	1.99636	-1.64173	-3.86191	3033.7129	3037.3725	3037.8030
C	0.74502	-3.21703	-1.34782	3049.6242	3054.2180	3107.7720
H	-0.00799	-2.95885	-2.10036	3110.9685	3113.2549	3115.1265
H	1.41362	-3.97105	-1.78440	3123.5992	3136.2665	3137.1023
H	0.21779	-3.67428	-0.50406	3140.2298	3141.8310	3144.7127
C	2.09652	-2.67023	1.55008	3147.8082	3150.8088	3155.6842
H	3.08486	-3.12520	1.69394	3159.0753	3167.2476	3169.6053
H	1.82329	-2.11361	2.45286	3184.5315	3189.8071	3202.1352
H	1.36203	-3.47341	1.43637			
C	0.91139	1.81947	2.87275			
H	0.15466	2.44656	3.35339			
H	0.57544	0.78257	2.99026			
H	1.88393	1.98261	3.34471			
O	2.02823	2.78957	1.00040			
H	-1.15188	3.66418	1.61106			
Ir	-0.62047	-0.70041	0.11904			
C	0.44977	0.11053	-1.40954			
C	1.90963	-0.11000	-1.58743			
C	2.63591	-0.98942	-0.76992			
C	2.60983	0.57889	-2.61199			
C	3.99264	-1.20281	-0.93980			
H	2.09836	-1.50184	0.02419			
C	3.99050	0.38014	-2.76469			
C	4.66835	-0.50261	-1.94534			
H	4.52578	-1.89788	-0.29505			
H	4.49374	0.93083	-3.55537			
H	5.73664	-0.65180	-2.08869			
O	2.01470	1.42121	-3.45268			
H	1.05248	1.40850	-3.22142			
H	5.67274	-0.47492	-2.32853			
C	0.63389	0.75102	-2.26539			

C	2.92715	1.58077	-1.45499
C	4.85170	2.36254	-0.35019
H	4.58554	3.41370	-0.51439
H	5.46963	2.04686	-1.20246
C	5.53081	2.13074	0.97347
H	6.47248	2.68645	1.02514
H	4.88756	2.45610	1.79667
H	5.74242	1.06336	1.11047
O	3.65827	1.57347	-0.34098
O	3.14601	2.29349	-2.40703
C	0.92000	0.94807	-3.71343
H	-0.00533	0.88337	-4.29044
H	1.41585	1.91119	-3.86642
H	1.63737	0.18240	-4.03787
O	-0.52197	0.63428	-1.87363

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.461471 Electronic Energy = -1482.10866577
Internal Energy (E)= -1481.61485377 Enthalpy (H)= -1481.61391077
Gibbs Free Energy (G)=-1481.70715877 Gibbs Free Energy of Solvation=-1481.74347258

St.Pt.	General Structure	Ball & Stick model
TS-4B		

Cartesian co-ordinate

Atoms	X	Y	Z
C	1.71204	-1.20944	-1.82201
C	2.61857	-0.37695	-1.13237
C	2.65334	-0.80675	0.25969
C	1.85829	-1.99701	0.37176
C	1.20172	-2.20331	-0.88482
C	-2.31476	-0.79199	-0.50319
Ir	0.48716	-0.26415	-0.08596
O	-1.30848	-0.27507	-1.17618
C	-2.14219	-1.12546	0.85339
C	-3.19547	-1.65059	1.61115
C	-3.56990	-1.02078	-1.09994
C	-4.42587	-1.86646	1.01841
C	-4.59764	-1.55020	-0.33821
C	-0.80220	-0.88035	1.39492
O	-0.47646	-1.09230	2.54723
H	-3.70436	-0.77898	-2.15261
H	-5.56512	-1.72398	-0.80678
H	-5.25325	-2.27662	1.59131
H	-3.01335	-1.87902	2.65926
C	0.16506	1.70371	0.47428
C	1.32220	2.06735	1.42027
C	-1.22573	2.11076	0.90810

Frequencies

-406.4122	31.0707	44.7841
52.3251	62.2167	75.9145
93.5500	100.6851	111.2297
128.4945	133.8557	138.1901
142.5773	148.3876	156.0322
157.5878	172.9578	176.9778
180.2995	194.1270	197.4282
205.6004	214.5403	224.0500
235.0378	242.7889	246.9095
258.4799	259.4324	266.2807
277.2055	280.0401	287.1580
291.3855	298.3139	305.3536
308.7430	313.6185	327.9863
336.5771	345.4858	364.6073
395.5569	404.7527	409.4893
426.0381	433.2235	473.9496
488.4929	535.8159	536.9246
541.3501	549.3481	558.0904
570.5038	581.7421	595.0413
600.0795	608.6544	624.4499
628.9255	632.1751	645.0175
671.0989	732.5590	761.0845
765.2331	815.3830	820.8524
840.2863	844.1257	861.8269
864.0104	884.5200	907.5782
952.2940	956.9377	966.0925

C	-2.10006	2.62662	-1.38292
H	-1.60774	3.56544	-1.67194
H	-1.54966	1.77051	-1.78467
C	-3.53380	2.60020	-1.84784
H	-3.57779	2.67098	-2.93961
H	-4.00699	1.66292	-1.53566
H	-4.09936	3.43370	-1.41960
O	-2.14399	2.55786	0.05223
O	-1.51990	2.01754	2.07640
N	0.54872	2.68002	-0.81486
N	1.48635	3.12153	-1.24947
C	3.61727	-0.32722	1.28896
H	3.25445	-0.55041	2.29860
H	4.58848	-0.82662	1.16613
H	3.78408	0.75243	1.22136
C	3.42091	0.74333	-1.68095
H	3.31776	1.65017	-1.07061
H	4.48853	0.48526	-1.68160
H	3.13544	0.99029	-2.70855
C	1.27830	-1.11878	-3.24302
H	0.18576	-1.04344	-3.30731
H	1.70566	-0.24377	-3.74264
H	1.58356	-2.01076	-3.80554
C	0.26959	-3.30763	-1.24868
H	-0.51847	-2.94207	-1.91662
H	0.79538	-4.12432	-1.76071
H	-0.22341	-3.72108	-0.36265
C	1.77150	-2.84513	1.58980
H	2.73683	-3.33215	1.77803
H	1.49827	-2.24651	2.46659
H	1.01080	-3.62494	1.48544
C	1.13997	1.72328	2.87085
H	0.40911	2.40330	3.31794
H	0.73808	0.71249	3.00184
H	2.11364	1.83534	3.35461
O	2.36010	2.55915	1.01650
H	-1.15188	3.66418	1.61106
Ir	-0.62047	-0.70041	0.11904
C	0.44977	0.11053	-1.40954
C	1.90963	-0.11000	-1.58743
C	2.63591	-0.98942	-0.76992
C	2.60983	0.57889	-2.61199
C	3.99264	-1.20281	-0.93980
H	2.09836	-1.50184	0.02419
C	3.99050	0.38014	-2.76469
C	4.66835	-0.50261	-1.94534
H	4.52578	-1.89788	-0.29505
H	4.49374	0.93083	-3.55537
H	5.73664	-0.65180	-2.08869
O	2.01470	1.42121	-3.45268
H	1.05248	1.40850	-3.22142
H	5.67274	-0.47492	-2.32853
C	0.63389	0.75102	-2.26539
C	2.92715	1.58077	-1.45499
C	4.85170	2.36254	-0.35019
H	4.58554	3.41370	-0.51439
H	5.46963	2.04686	-1.20246
C	5.53081	2.13074	0.97347
H	6.47248	2.68645	1.02514
H	4.88756	2.45610	1.79667
H	5.74242	1.06336	1.11047

977.5415	993.3549	1010.3791
1032.3259	1037.3023	1040.5148
1041.5296	1044.9865	1048.5208
1052.6164	1087.8964	1093.4615
1112.6572	1112.7886	1118.2415
1141.5313	1148.5093	1162.2550
1180.4868	1183.5069	1190.3977
1206.0904	1266.5277	1301.1855
1326.2511	1339.5913	1374.0124
1378.9212	1380.3836	1384.1805
1388.4737	1392.6437	1396.3181
1399.5629	1422.0367	1428.6711
1438.3597	1440.8754	1447.5167
1450.2853	1452.3510	1459.7136
1460.6956	1461.2260	1467.0785
1468.6036	1471.2888	1471.9889
1473.9432	1484.5403	1485.4405
1487.8496	1490.1867	1506.7027
1512.9597	1519.9044	1563.6718
1624.2682	1657.7258	1776.0291
1776.6029	1838.7877	2212.3180
3030.0425	3032.2460	3033.7606
3034.3016	3034.9436	3039.2358
3051.5528	3057.8412	3105.9101
3111.8869	3112.2474	3116.1141
3123.5954	3123.7284	3140.3951
3141.6787	3144.7898	3145.2455
3146.3656	3151.0847	3154.6058
3157.2099	3168.4472	3171.2958
3190.2900	3193.3606	3207.1997

O	3.65827	1.57347	-0.34098
O	3.14601	2.29349	-2.40703
C	0.92000	0.94807	-3.71343
H	-0.00533	0.88337	-4.29044
H	1.41585	1.91119	-3.86642
H	1.63737	0.18240	-4.03787
O	-0.52197	0.63428	-1.87363

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.459023 Electronic Energy = -1482.10151968
Internal Energy (E)= -1481.61023768 Enthalpy (H)= -1481.60929368
Gibbs Free Energy (G)=-1481.70227968 Gibbs Free Energy of Solvation=-1481.73589712

St.Pt.	General Structure	Ball & Stick model
V-1B		

Cartesian co-ordinate

Atoms	X	Y	Z
C	0.47545	2.11894	-1.52651
C	-0.90653	1.71237	-1.55309
C	-1.50107	2.06699	-0.28158
C	-0.46127	2.60371	0.54960
C	0.74872	2.67338	-0.25244
C	2.20432	-1.24195	-0.77018
Ir	0.02774	0.45467	0.04265
O	0.93931	-1.06359	-1.07736
C	2.76274	-0.57778	0.33992
C	4.10228	-0.76891	0.71171
C	3.03368	-2.09386	-1.52525
C	4.90509	-1.59860	-0.04310
C	4.35583	-2.25539	-1.15838
C	1.86266	0.28194	1.09061
O	2.08398	0.87818	2.11173
H	2.60896	-2.61540	-2.37914
H	4.98865	-2.91446	-1.75039
H	5.94867	-1.74982	0.21919
H	4.47627	-0.24728	1.59000
C	-0.73191	-0.90819	1.12633
C	-1.69493	-0.68122	2.24970
C	-0.26693	-2.32472	0.98528
C	-2.07721	-2.72440	-0.57786
H	-2.88103	-3.45094	-0.40067
H	-2.42836	-1.74226	-0.22697
C	-1.69186	-2.66583	-2.03569
H	-2.55389	-2.37311	-2.64759
H	-0.87917	-1.94651	-2.18133
H	-1.34462	-3.64677	-2.37633
O	-0.97184	-3.16912	0.21046

Frequencies

20.8074	33.2824	37.0582
41.9100	47.4103	53.6751
68.8856	74.0482	84.6281
88.4159	104.4796	111.6069
114.9893	128.7511	146.2143
150.7227	155.4222	166.1243
173.7100	187.2636	190.7329
196.9793	198.5387	202.3193
206.8231	215.3108	227.0888
235.7233	240.7459	245.4130
255.6639	262.3443	268.5484
290.8550	294.2059	309.1886
314.2195	319.7226	335.3350
361.2731	368.2457	373.2984
377.1710	412.5197	414.2411
417.8928	421.4407	442.3889
471.7675	505.6278	533.7092
538.1920	540.4489	552.7446
568.7700	580.3991	589.3912
601.1426	607.4002	624.0480
631.2509	646.8292	658.6568
693.0748	722.3591	753.1491
762.2339	812.2526	816.3708
819.9088	843.7858	857.1354
877.8722	917.4574	941.3287
950.4869	962.6049	980.7452
981.5524	1002.0784	1024.1597
1034.2272	1037.3705	1038.1098
1041.7864	1045.2174	1049.6525
1055.4514	1094.2739	1097.6718
1112.2883	1119.2358	1123.0113
1146.5136	1147.0798	1178.7615
1185.7818	1187.3763	1208.4152
1230.7828	1261.2343	1282.7114

O	0.68070	-2.73654	1.61101	1341.6227	1353.2469	1374.7211
N	-5.34829	-1.56204	-1.05821	1379.3310	1383.5877	1394.4794
N	-4.83639	-0.80705	-1.68226	1398.7926	1400.4845	1402.0917
C	2.02801	3.28281	0.19878	1404.6398	1426.7661	1437.8140
H	2.00565	4.36668	0.02638	1439.9791	1447.6279	1450.0875
H	2.19450	3.11266	1.26634	1451.7122	1453.6584	1454.6891
H	2.88788	2.87305	-0.34212	1460.1937	1464.0555	1465.8458
C	1.43940	1.89493	-2.63975	1471.7804	1478.5655	1483.3135
H	1.23148	2.56362	-3.48471	1485.1834	1495.6903	1498.3282
H	2.47154	2.06667	-2.31899	1502.3810	1507.9621	1515.9808
H	1.37536	0.86256	-3.00468	1517.9314	1519.1699	1552.2476
C	-1.59831	1.13906	-2.74148	1623.1529	1660.8983	1777.7905
H	-1.89087	1.92786	-3.44805	1835.3120	1847.8454	2464.8003
H	-0.94056	0.44326	-3.27532	3017.6714	3032.2760	3036.7113
H	-2.50423	0.59057	-2.46157	3037.5473	3040.2389	3041.3469
C	-2.95045	2.00062	0.04444	3042.5045	3046.9164	3077.1247
H	-3.42924	2.96089	-0.18897	3109.8219	3114.0442	3120.9833
H	-3.45818	1.22952	-0.54561	3121.2128	3128.0203	3128.2132
H	-3.10885	1.77896	1.10301	3131.5315	3137.8911	3141.9976
C	-0.61044	3.17050	1.91696	3152.9933	3155.8097	3170.0977
H	-0.67770	4.26617	1.87847	3174.1288	3175.9400	3176.8912
H	-1.50222	2.77592	2.40913	3196.0693	3204.2831	3210.7723
H	0.25042	2.90320	2.53860			
O	-2.11875	0.43235	2.51880			
C	-2.09881	-1.87755	3.07164			
H	-1.21546	-2.30512	3.56121			
H	-2.82974	-1.57432	3.82342			
H	-2.51609	-2.67270	2.44087			
H	-1.15188	3.66418	1.61106			
Ir	-0.62047	-0.70041	0.11904			
C	0.44977	0.11053	-1.40954			
C	1.90963	-0.11000	-1.58743			
C	2.63591	-0.98942	-0.76992			
C	2.60983	0.57889	-2.61199			
C	3.99264	-1.20281	-0.93980			
H	2.09836	-1.50184	0.02419			
C	3.99050	0.38014	-2.76469			
C	4.66835	-0.50261	-1.94534			
H	4.52578	-1.89788	-0.29505			
H	4.49374	0.93083	-3.55537			
H	5.73664	-0.65180	-2.08869			
O	2.01470	1.42121	-3.45268			
H	1.05248	1.40850	-3.22142			
H	5.67274	-0.47492	-2.32853			
C	0.63389	0.75102	-2.26539			
C	2.92715	1.58077	-1.45499			
C	4.85170	2.36254	-0.35019			
H	4.58554	3.41370	-0.51439			
H	5.46963	2.04686	-1.20246			
C	5.53081	2.13074	0.97347			
H	6.47248	2.68645	1.02514			
H	4.88756	2.45610	1.79667			
H	5.74242	1.06336	1.11047			
O	3.65827	1.57347	-0.34098			
O	3.14601	2.29349	-2.40703			
C	0.92000	0.94807	-3.71343			
H	-0.00533	0.88337	-4.29044			
H	1.41585	1.91119	-3.86642			
H	1.63737	0.18240	-4.03787			
O	-0.52197	0.63428	-1.87363			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.459234 Electronic Energy = -1482.14652904
Internal Energy (E)= -1481.65317904 Enthalpy (H)= -1481.65223504
Gibbs Free Energy (G)=-1481.75243804 Gibbs Free Energy of Solvation=-1481.78883603

St.Pt.	General Structure	Ball & Stick model
TS-5B		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.04859	-2.54328	-1.04283
C	1.29695	-2.02928	-1.00942
C	1.70279	-1.89978	0.38610
C	0.57723	-2.24528	1.19111
C	-0.51131	-2.63238	0.29365
C	-2.33497	0.67975	-1.02167
Ir	0.09385	-0.48787	-0.06129
O	-1.10766	0.52613	-1.45805
C	-2.63713	0.62083	0.36199
C	-3.95548	0.76019	0.82634
C	-3.39898	0.90852	-1.91742
C	-4.98360	0.96372	-0.06948
C	-4.68829	1.04200	-1.44142
C	-1.55798	0.41026	1.30879
O	-1.60879	0.21412	2.49002
H	-3.17146	0.96987	-2.97868
H	-5.49679	1.20791	-2.15140
H	-6.00788	1.06804	0.27739
H	-4.13424	0.70507	1.89792
C	0.25773	1.26624	0.76312
C	0.98648	1.47952	2.05070
C	-0.16450	2.54398	0.08779
C	1.87506	2.46805	-1.26720
H	2.64873	3.24640	-1.25280
H	2.18309	1.66470	-0.58383
C	1.65872	1.93142	-2.66089
H	2.58652	1.49365	-3.04838
H	0.87495	1.16512	-2.65285
H	1.34214	2.73442	-3.33425
O	0.68609	3.10345	-0.79552
O	-1.17178	3.14416	0.37724
N	5.63639	1.37166	-0.34068
N	4.91713	1.06166	-1.12062
C	-1.86400	-3.06074	0.74547
H	-1.91342	-4.15303	0.84400
H	-2.10677	-2.62629	1.72020
H	-2.64205	-2.74897	0.04050

Frequencies

-235.1842	-17.0819	23.4387
27.0306	32.4427	35.9095
47.2275	57.5048	65.1597
88.0761	90.3639	94.5811
101.6127	104.1865	109.6818
133.4839	134.2155	144.7698
153.6594	167.9343	173.7572
176.0973	183.6277	192.2059
201.3334	204.6189	212.1934
223.9501	229.8711	235.6723
247.0556	249.2624	257.2234
275.8470	282.9552	291.7949
298.6458	306.6377	317.0160
324.0614	330.4055	349.3384
386.6048	399.6129	412.6562
416.2070	433.2779	444.5016
461.2635	499.7676	527.0492
532.5974	539.5196	546.7510
548.8539	560.8700	575.8531
586.1216	598.1222	605.6974
618.1381	638.4123	641.2960
687.2464	717.6288	750.7991
759.4963	792.1632	806.6185
810.9546	812.9233	857.9106
876.8786	915.5166	938.1586
950.4643	951.8072	958.7938
979.9933	1001.6198	1027.0930
1033.6940	1038.5884	1039.6826
1042.8191	1045.8309	1046.4030
1046.9489	1083.4096	1088.9576
1103.1406	1116.0682	1120.5314
1144.8109	1147.0492	1172.6107
1180.9444	1183.0744	1202.5467
1233.8523	1258.3591	1262.8944
1340.0945	1343.2043	1371.1375
1375.1379	1378.3787	1381.6955
1389.2908	1393.1299	1396.5458
1398.5908	1414.7722	1431.7313
1435.6880	1443.7121	1445.5778
1449.3609	1450.2536	1454.8481
1459.2330	1460.8426	1461.6054

C	-0.84215	-2.76505	-2.28242
H	-0.56504	-3.71080	-2.76521
H	-1.91570	-2.79558	-2.07066
H	-0.67594	-1.95668	-3.00384
C	2.15468	-1.80423	-2.20602
H	2.55020	-2.75527	-2.58842
H	1.58882	-1.32718	-3.01443
H	3.00961	-1.15756	-1.97651
C	3.05087	-1.51302	0.87712
H	3.64561	-2.39831	1.13717
H	3.60033	-0.95398	0.11275
H	2.95861	-0.87908	1.76412
C	0.51630	-2.33803	2.67539
H	0.30002	-3.37250	2.97364
H	1.45807	-2.02912	3.13286
H	-0.26360	-1.68553	3.08302
O	1.37470	0.53775	2.72345
C	1.22100	2.89827	2.49820
H	0.25603	3.38887	2.67505
H	1.81719	2.89857	3.41259
H	1.72660	3.48482	1.71948
H	-1.15188	3.66418	1.61106
Ir	-0.62047	-0.70041	0.11904
C	0.44977	0.11053	-1.40954
C	1.90963	-0.11000	-1.58743
C	2.63591	-0.98942	-0.76992
C	2.60983	0.57889	-2.61199
C	3.99264	-1.20281	-0.93980
H	2.09836	-1.50184	0.02419
C	3.99050	0.38014	-2.76469
C	4.66835	-0.50261	-1.94534
H	4.52578	-1.89788	-0.29505
H	4.49374	0.93083	-3.55537
H	5.73664	-0.65180	-2.08869
O	2.01470	1.42121	-3.45268
H	1.05248	1.40850	-3.22142
H	5.67274	-0.47492	-2.32853
C	0.63389	0.75102	-2.26539
C	2.92715	1.58077	-1.45499
C	4.85170	2.36254	-0.35019
H	4.58554	3.41370	-0.51439
H	5.46963	2.04686	-1.20246
C	5.53081	2.13074	0.97347
H	6.47248	2.68645	1.02514
H	4.88756	2.45610	1.79667
H	5.74242	1.06336	1.11047
O	3.65827	1.57347	-0.34098
O	3.14601	2.29349	-2.40703
C	0.92000	0.94807	-3.71343
H	-0.00533	0.88337	-4.29044
H	1.41585	1.91119	-3.86642
H	1.63737	0.18240	-4.03787
O	-0.52197	0.63428	-1.87363

1467.2392	1468.0183	1471.6795
1476.9450	1480.9180	1484.6095
1490.2222	1492.1243	1497.9690
1516.3651	1523.8035	1552.2037
1610.7668	1663.3914	1778.6853
1837.9132	1857.5058	2464.7591
3022.7485	3032.5236	3037.6306
3038.4877	3038.9749	3041.2710
3041.6191	3049.1408	3085.7989
3101.7491	3115.8031	3118.3553
3119.2400	3120.9619	3124.1073
3129.6674	3138.3858	3139.8052
3146.1088	3160.5401	3170.5493
3171.5470	3172.9914	3179.5395
3193.5820	3202.1694	3209.8152

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm

Zero-point correction= 0.456202 Electronic Energy = -1482.12927983

Internal Energy (E)= -1481.63951383 Enthalpy (H)= -1481.63856983
Gibbs Free Energy (G)=-1481.73810283 Gibbs Free Energy of Solvation=-1481.77733298

St.Pt.	General Structure	Ball & Stick model
VI-1B		

Cartesian co-ordinate

Atoms	X	Y	Z
C	0.46464	-2.67915	-0.03927
C	1.77667	-2.17846	-0.17572
C	2.07987	-1.33328	0.98484
C	0.94167	-1.31642	1.83444
C	-0.10819	-2.08313	1.16538
C	-2.36884	-0.13695	-1.13094
Ir	0.34558	-0.43424	-0.06366
O	-1.10103	-0.25855	-1.52022
C	-2.74888	0.39104	0.12631
C	-4.09400	0.38585	0.50620
C	-3.37814	-0.60673	-1.98706
C	-5.08025	-0.08253	-0.34620
C	-4.70891	-0.57159	-1.60027
C	-1.75688	0.94069	1.08210
O	-1.96645	0.91187	2.29471
H	-3.07670	-1.01062	-2.95139
H	-5.46956	-0.94632	-2.28311
H	-6.12449	-0.06614	-0.04589
H	-4.33923	0.77590	1.49188
C	-0.45433	1.43453	0.51308
C	0.44811	2.21793	1.46922
C	-0.71667	2.40267	-0.64176
C	1.36553	1.78516	-1.78282
H	2.25151	2.42038	-1.64999
H	1.48754	1.02285	-0.96583
C	1.31649	1.14940	-3.14750
H	2.20776	0.53008	-3.30721
H	0.42196	0.52615	-3.23683
H	1.28543	1.92110	-3.92307
O	0.23566	2.60095	-1.57706
O	-1.70348	3.09256	-0.67663
N	4.91376	1.85181	-0.83768
N	4.48134	1.01082	-1.40980
C	-1.45708	-2.38330	1.71361
H	-1.42227	-3.29897	2.31958
H	-1.82536	-1.56437	2.34138
H	-2.18593	-2.53445	0.90902
C	-0.30691	-3.51733	-0.99562
H	-0.63094	-4.45211	-0.52152
H	-1.20286	-2.98463	-1.33969
H	0.28576	-3.77349	-1.87820
C	2.70763	-2.41043	-1.31392

Frequencies

35.4976	40.6966	50.9289
62.4410	69.8747	73.9471
89.1487	92.7410	98.9091
100.0937	108.7539	110.4346
115.3284	126.3654	133.7208
141.7102	155.5138	158.9813
163.4935	168.9870	190.6685
196.2246	211.5746	215.1941
217.8074	221.1314	232.5653
233.7832	240.6802	258.6831
266.6086	272.5395	277.9095
279.2167	294.9694	302.7888
309.2104	319.9889	330.0036
340.8588	356.5126	375.0578
391.8967	400.7234	412.5147
433.4952	473.4456	479.7077
520.4019	529.4026	537.1452
539.4742	543.0173	550.1981
554.2398	579.6104	589.2726
595.4549	610.1223	632.8635
637.0163	668.3883	690.4314
719.1218	741.5636	762.8115
773.4666	806.6797	813.9185
847.5640	864.4532	877.5890
885.1715	912.2144	956.8862
961.4275	964.9379	968.3998
976.8773	1018.7323	1032.7070
1037.3989	1040.9117	1050.5669
1051.0354	1052.6322	1058.8136
1087.7981	1090.6507	1097.4731
1109.9626	1112.5783	1128.8426
1132.4487	1150.8720	1154.4089
1179.9881	1187.1045	1208.2781
1218.5682	1252.2845	1269.6407
1282.9875	1329.8735	1366.0182
1367.5522	1369.4308	1374.4478
1378.9979	1389.8565	1394.4037
1398.6488	1401.4430	1428.4103
1430.8601	1435.8085	1444.6149
1447.2736	1448.3938	1453.4656
1455.3746	1464.3372	1466.4235
1469.2528	1474.0319	1477.0810
1482.0912	1487.1084	1491.8585
1492.6807	1495.0332	1501.2458
1501.7131	1531.8000	1565.1837
1620.9497	1664.6673	1736.6263

H	3.43650	-3.19590	-1.07548	1803.0959	1855.4446	2464.6808
H	2.16477	-2.71103	-2.21556	2768.4586	3026.1407	3030.9367
H	3.27045	-1.50088	-1.55637	3036.5553	3036.9524	3042.0064
C	3.39049	-0.69342	1.28814	3045.3359	3049.6601	3073.0630
H	3.84374	-1.15234	2.17607	3101.6385	3111.5877	3114.8306
H	4.09612	-0.81525	0.46114	3120.0382	3123.8567	3130.4112
H	3.26268	0.37754	1.48115	3138.8936	3142.3143	3146.1485
C	0.82786	-0.67152	3.16961	3148.1987	3149.1367	3158.3282
H	0.93506	-1.42402	3.96181	3160.5467	3170.0272	3173.6722
H	1.60638	0.08511	3.30702	3189.1591	3194.4171	3205.6084
H	-0.14876	-0.18571	3.29325			
O	1.66132	2.09889	1.41761			
C	-0.20157	3.20532	2.38918			
H	-0.71422	2.65642	3.18633			
H	0.55294	3.87788	2.80319			
H	-0.98143	3.76512	1.85929			
H	-1.15188	3.66418	1.61106			
Ir	-0.62047	-0.70041	0.11904			
C	0.44977	0.11053	-1.40954			
C	1.90963	-0.11000	-1.58743			
C	2.63591	-0.98942	-0.76992			
C	2.60983	0.57889	-2.61199			
C	3.99264	-1.20281	-0.93980			
H	2.09836	-1.50184	0.02419			
C	3.99050	0.38014	-2.76469			
C	4.66835	-0.50261	-1.94534			
H	4.52578	-1.89788	-0.29505			
H	4.49374	0.93083	-3.55537			
H	5.73664	-0.65180	-2.08869			
O	2.01470	1.42121	-3.45268			
H	1.05248	1.40850	-3.22142			
H	5.67274	-0.47492	-2.32853			
C	0.63389	0.75102	-2.26539			
C	2.92715	1.58077	-1.45499			
C	4.85170	2.36254	-0.35019			
H	4.58554	3.41370	-0.51439			
H	5.46963	2.04686	-1.20246			
C	5.53081	2.13074	0.97347			
H	6.47248	2.68645	1.02514			
H	4.88756	2.45610	1.79667			
H	5.74242	1.06336	1.11047			
O	3.65827	1.57347	-0.34098			
O	3.14601	2.29349	-2.40703			
C	0.92000	0.94807	-3.71343			
H	-0.00533	0.88337	-4.29044			
H	1.41585	1.91119	-3.86642			
H	1.63737	0.18240	-4.03787			
O	-0.52197	0.63428	-1.87363			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.458819 Electronic Energy = -1482.16119943
Internal Energy (E)= -1481.66877143 Enthalpy (H)= -1481.66782843
Gibbs Free Energy (G)=-1481.76501043 Gibbs Free Energy of Solvation=-1481.81019707

St.Pt.	General Structure	Ball & Stick model
VI'-1B		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-2.43396	-0.57391	-2.10670
C	-1.74322	-1.74611	-1.72247
C	-2.01745	-2.00896	-0.30577
C	-2.92571	-1.01173	0.16446
C	-3.11679	-0.06595	-0.92601
O	1.43007	-1.06824	-1.35264
C	2.54875	-1.72149	-0.99905
O	2.46024	-2.89153	-0.70520
C	3.84421	-0.91807	-1.03108
C	0.70688	2.37587	-0.86781
H	1.50690	-0.10676	-1.50641
C	-0.88165	-2.60686	-2.57249
H	0.00547	-2.94531	-2.02810
H	-1.44813	-3.49118	-2.89410
H	-0.53807	-2.07701	-3.46597
C	-1.49583	-3.18976	0.43371
H	-2.06719	-4.09056	0.17272
H	-0.44423	-3.37222	0.17491
H	-1.55668	-3.03928	1.51590
C	-3.98184	1.13972	-0.87464
H	-3.79361	1.79765	-1.72820
H	-5.04067	0.84807	-0.89225
H	-3.78693	1.71052	0.03837
C	-2.37380	0.11955	-3.42172
H	-2.18412	1.19021	-3.28532
H	-1.56278	-0.27597	-4.04042
H	-3.31290	0.00762	-3.97780
C	-3.61496	-0.94844	1.48140
H	-4.57810	-1.47237	1.42501
H	-3.01185	-1.40393	2.27204
H	-3.81445	0.09040	1.76764
Ir	-1.06066	-0.06627	-0.40660
C	4.03296	-0.31008	-2.42630
H	3.25155	0.41746	-2.68183
H	4.99039	0.22366	-2.46095
H	4.04985	-1.08360	-3.20382
C	3.76937	0.20089	0.01248
H	3.52304	-0.18364	1.00941
H	4.73888	0.71079	0.06867
H	3.02176	0.96147	-0.24625
C	5.01261	-1.84594	-0.72046
H	4.93262	-2.26418	0.28854
H	5.05634	-2.68308	-1.42536
H	5.95313	-1.28538	-0.78387
O	0.14979	1.27432	-1.36453
C	1.11332	2.53331	0.47590
C	1.81863	3.68962	0.84756
C	0.99653	3.40770	-1.78015

Frequencies

31.5043	38.7628	48.8504
63.6136	68.2999	75.6113
77.1923	82.7923	85.0118
94.4967	101.4240	114.7698
117.6008	119.6885	134.2672
137.3327	141.4768	148.1925
163.0078	169.1491	176.0941
186.1667	194.8417	196.2958
199.0940	202.7968	216.7815
222.8668	229.5664	238.1154
242.7031	248.7281	254.5620
264.4836	268.9558	274.9080
280.1311	280.7424	289.2504
298.3559	308.1830	310.7201
315.2398	322.4383	324.2429
336.4824	340.8642	369.7131
375.5369	382.6916	385.5498
390.7050	394.3012	407.5360
422.1666	432.3763	438.3569
462.2172	479.9810	522.2401
532.3752	532.8127	539.6033
544.2865	551.1033	570.6105
574.0359	581.2197	585.6263
593.7536	603.5938	630.1441
657.3469	676.4481	691.3771
724.8660	761.6756	773.0967
775.5574	786.7849	793.8191
804.8362	807.1968	812.6023
861.8401	874.7168	880.0667
889.0489	904.0935	906.7710
946.4071	953.2704	955.8535
963.4068	972.5467	979.3693
981.1329	1001.9518	1009.9741
1032.7660	1034.4205	1036.0817
1036.9807	1039.9653	1043.3665
1046.0872	1049.5263	1062.0273
1085.9920	1088.2451	1091.6733
1098.6558	1113.1335	1115.4729
1129.1477	1140.1356	1149.6690
1174.4793	1183.3964	1187.3640
1192.4664	1212.4817	1235.3753
1240.7751	1261.8779	1272.6859
1282.7131	1296.6902	1332.0501
1347.9160	1369.5295	1375.7717
1376.8506	1382.4776	1383.4408
1387.9758	1392.7967	1394.3201
1398.6224	1409.5641	1415.5011
1421.1202	1430.1734	1433.7119
1442.4718	1443.3278	1444.9759
1449.4073	1450.9437	1454.0097
1457.7751	1459.5128	1459.7827
1462.0778	1469.8407	1470.0457

C	2.08949	4.69862	-0.05584	1475.2742	1477.0292	1482.5108
C	1.66844	4.54815	-1.38071	1484.8849	1486.5879	1487.4095
C	0.90958	1.51891	1.52619	1488.3554	1492.2749	1497.5798
O	1.63037	1.49406	2.51587	1503.4849	1508.9598	1510.5486
H	0.67917	3.26664	-2.81110	1531.3038	1559.3667	1620.7580
H	1.87303	5.33025	-2.10951	1666.7544	1752.1564	1793.6122
H	2.62075	5.59326	0.25776	1802.6704	1862.0817	3031.4812
H	2.14202	3.75902	1.88347	3034.2640	3039.3049	3039.5776
C	-0.30713	0.59250	1.48571	3041.7867	3042.8976	3045.5125
C	-1.36947	1.46445	2.17940	3048.9026	3049.3707	3055.2123
C	-0.03953	-0.68854	2.21454	3057.8767	3112.5849	3115.0031
C	1.47350	-2.44004	2.61324	3119.0921	3120.4249	3124.8621
H	1.15169	-2.31589	3.65263	3127.9249	3128.0579	3129.1427
H	0.89936	-3.27572	2.19026	3130.6056	3131.3837	3132.9138
C	2.95652	-2.67348	2.50692	3144.8285	3146.0793	3146.8456
H	3.50909	-1.79264	2.85465	3148.8985	3152.1245	3161.2838
H	3.24049	-3.52326	3.13691	3172.7644	3172.7815	3178.4135
H	3.24239	-2.90295	1.47551	3193.2719	3198.0153	3201.6534
O	-0.82120	-1.23881	2.97114	3205.2445	3209.1249	3667.9108
O	1.14224	-1.24268	1.88813			
C	-1.37626	1.50124	3.68208			
H	-1.89541	2.40466	4.01068			
H	-1.89608	0.61569	4.06077			
H	-0.35596	1.46529	4.07902			
O	-2.11766	2.17890	1.53726			
H	5.67274	-0.47492	-2.32853			
C	0.63389	0.75102	-2.26539			
C	2.92715	1.58077	-1.45499			
C	4.85170	2.36254	-0.35019			
H	4.58554	3.41370	-0.51439			
H	5.46963	2.04686	-1.20246			
C	5.53081	2.13074	0.97347			
H	6.47248	2.68645	1.02514			
H	4.88756	2.45610	1.79667			
H	5.74242	1.06336	1.11047			
O	3.65827	1.57347	-0.34098			
O	3.14601	2.29349	-2.40703			
C	0.92000	0.94807	-3.71343			
H	-0.00533	0.88337	-4.29044			
H	1.41585	1.91119	-3.86642			
H	1.63737	0.18240	-4.03787			
O	-0.52197	0.63428	-1.87363			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.602748 Electronic Energy = -1719.54899461
Internal Energy (E)= -1718.90715761 Enthalpy (H)= -1718.90621461
Gibbs Free Energy (G)=-1719.01333361 Gibbs Free Energy of Solvation=-1719.0699618

St.Pt.	General Structure	Ball & Stick model
TS-6B		
Cartesian co-ordinate		**Frequencies**

Atoms	X	Y	Z
C	-2.53848	-0.41682	-1.94745
C	-2.13050	-1.67816	-1.45000
C	-2.34383	-1.69825	-0.00357
C	-2.97742	-0.45229	0.36618
C	-3.01605	0.37630	-0.81826
O	1.00315	-0.98548	-1.30366
C	1.96541	-1.85563	-1.01507
O	1.68841	-2.93433	-0.53099
C	3.38260	-1.42730	-1.38565
C	0.93516	2.48290	-0.92052
H	0.81446	0.27448	-1.49933
C	-1.48364	-2.78526	-2.20053
H	-0.61543	-3.16682	-1.65050
H	-2.19354	-3.61029	-2.34389
H	-1.13431	-2.45608	-3.18353
C	-2.09462	-2.87591	0.87130
H	-2.89017	-3.62418	0.75757
H	-1.13956	-3.34669	0.60692
H	-2.03744	-2.58128	1.92389
C	-3.55828	1.75532	-0.92678
H	-2.99880	2.32738	-1.67501
H	-4.61156	1.72768	-1.23688
H	-3.47180	2.29124	0.02115
C	-2.41539	0.09700	-3.33870
H	-1.88377	1.05585	-3.35070
H	-1.85671	-0.59762	-3.97271
H	-3.40304	0.25183	-3.79133
C	-3.55057	-0.12891	1.69822
H	-4.54470	-0.58700	1.78373
H	-2.92216	-0.52070	2.50533
H	-3.65817	0.95009	1.83782
Ir	-0.97939	-0.11016	-0.38369
C	3.41883	-0.87689	-2.81286
H	2.80240	0.02275	-2.92208
H	4.45011	-0.60645	-3.07258
H	3.07344	-1.62170	-3.54091
C	3.81618	-0.33738	-0.40201
H	3.66773	-0.64815	0.63999
H	4.87956	-0.11028	-0.54983
H	3.25491	0.59182	-0.55952
C	4.31494	-2.62819	-1.27584
H	4.35928	-3.00817	-0.24992
H	3.98428	-3.45046	-1.92019
H	5.32884	-2.33596	-1.57664
O	0.20466	1.50232	-1.49062
C	1.53121	2.38909	0.34922
C	2.36243	3.43519	0.78091
C	1.13835	3.63252	-1.69279
C	2.56468	4.56686	0.01274
C	1.93712	4.66469	-1.22999
C	1.33790	1.27632	1.31374
O	2.20315	1.04152	2.14384
H	0.66468	3.67368	-2.67060
H	2.08127	5.54910	-1.84701
H	3.19887	5.37119	0.37595

-1640.1876	31.2332	43.2933
47.4948	58.2135	71.5914
75.0652	82.1126	87.5425
94.1025	102.4693	104.9111
111.2276	115.4342	120.2065
133.2689	137.3737	148.5347
151.2524	157.3249	163.0417
168.8998	177.2837	182.0654
192.3589	195.8082	200.0633
215.0711	218.0055	223.8164
228.6481	235.2307	241.4096
261.7717	271.2315	276.1855
294.6121	299.5262	300.8128
307.1561	315.2160	319.5326
320.1401	327.6925	331.4183
343.2593	346.5780	353.9866
367.7560	372.3143	382.8921
386.0867	387.0595	409.6541
415.1367	421.2457	435.0161
445.8006	467.4536	469.8834
531.3929	533.4070	537.0718
548.2665	552.5929	557.0938
563.5859	570.5505	592.3627
594.2871	599.4780	604.6854
605.5853	645.6818	689.2425
717.9295	763.5002	768.6919
777.3339	784.7282	801.6861
808.2837	811.4575	812.9790
858.5741	870.7597	884.7885
896.8921	903.2865	909.8784
945.0507	949.4891	956.1762
962.3070	971.0944	981.0393
984.3198	993.3024	1006.0032
1025.5814	1033.9202	1039.3000
1040.3569	1041.7636	1045.9179
1048.8152	1058.9409	1065.1934
1084.8671	1097.3304	1104.4024
1112.6033	1115.6528	1131.1909
1135.0693	1149.5395	1180.4535
1185.4454	1189.0734	1196.7898
1215.0618	1237.1580	1239.3367
1256.4087	1264.9786	1275.2996
1293.7903	1306.2335	1318.9370
1342.4839	1369.9288	1374.3054
1375.8546	1378.5312	1380.7654
1387.1396	1389.5055	1397.0793
1403.0517	1407.6266	1411.2276
1416.4833	1431.5115	1436.7840
1441.3057	1442.5453	1443.9241
1448.4270	1450.5694	1453.5883
1454.4595	1456.7873	1463.8425
1467.6006	1468.5146	1477.5855
1478.5100	1478.7745	1480.8868
1483.7441	1488.3722	1490.6408
1492.4671	1498.0406	1500.2670
1505.1838	1514.0459	1515.2550
1524.7409	1557.7749	1611.5146
1632.4604	1667.1614	1763.2832
1788.5846	1812.5167	1813.3275

H	2.83196	3.32652	1.75568	3029.5427	3034.3620	3034.5906
C	-0.02765	0.59665	1.42668	3035.3943	3037.8538	3038.6849
C	-0.87586	1.70416	2.07373	3039.9110	3040.3505	3041.3055
C	0.04902	-0.63877	2.27115	3045.2244	3055.8444	3110.6482
C	1.26072	-2.63114	2.67023	3114.9602	3116.6445	3116.8022
H	0.92365	-2.45952	3.69820	3119.7970	3120.9458	3121.9701
H	0.63308	-3.42032	2.23460	3124.7117	3126.7411	3128.2489
C	2.72400	-2.97737	2.59040	3132.5956	3137.9210	3142.2678
H	3.32927	-2.13822	2.95183	3147.6466	3148.1748	3148.2502
H	2.94269	-3.85629	3.20591	3148.7261	3151.6577	3164.5576
H	3.00110	-3.19918	1.55464	3170.1231	3177.3681	3180.7160
O	-0.75828	-0.94425	3.13504	3193.5898	3200.5072	3208.3310
O	1.06284	-1.42990	1.91388			
C	-0.71038	1.93810	3.55117			
H	-1.01569	2.96081	3.78498			
H	-1.34542	1.23214	4.09628			
H	0.31820	1.75251	3.87867			
O	-1.59139	2.42863	1.40879			
H	5.67274	-0.47492	-2.32853			
C	0.63389	0.75102	-2.26539			
C	2.92715	1.58077	-1.45499			
C	4.85170	2.36254	-0.35019			
H	4.58554	3.41370	-0.51439			
H	5.46963	2.04686	-1.20246			
C	5.53081	2.13074	0.97347			
H	6.47248	2.68645	1.02514			
H	4.88756	2.45610	1.79667			
H	5.74242	1.06336	1.11047			
O	3.65827	1.57347	-0.34098			
O	3.14601	2.29349	-2.40703			
C	0.92000	0.94807	-3.71343			
H	-0.00533	0.88337	-4.29044			
H	1.41585	1.91119	-3.86642			
H	1.63737	0.18240	-4.03787			
O	-0.52197	0.63428	-1.87363			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.596957 Electronic Energy = -1719.51583524
Internal Energy (E)= -1718.88013524 Enthalpy (H)= -1718.87919124
Gibbs Free Energy (G)=-1718.98556624 Gibbs Free Energy of Solvation=-1719.03827872

St.Pt.	General Structure	Ball & Stick model
VII-1B		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.28620	-2.64636	-1.62707
C	0.99836	-2.64419	-1.03561

Frequencies

23.1927	38.1870	59.4713
62.7886	70.2569	75.3685
79.0018	89.6360	93.0978
100.1008	108.7841	118.1650
128.0196	131.6295	134.5935
142.7793	146.2308	153.4553

C	0.82239	-2.62675	0.41596	159.4378	164.4357	169.8742
C	-0.60179	-2.76060	0.69219	170.6883	176.6246	183.4169
C	-1.28425	-2.68491	-0.56019	186.9337	194.8696	199.1738
O	1.06493	0.73495	-0.98227	204.2837	214.8405	218.5610
C	2.36152	0.85637	-0.87042	225.1307	238.3549	242.2164
O	3.09470	0.05124	-0.31147	248.3948	256.7492	266.7605
C	2.89314	2.12664	-1.55071	272.8408	278.9895	284.6537
C	-2.21434	1.54198	-1.25211	290.5650	308.4379	311.3441
H	-0.41992	1.05209	-1.81336	314.0446	320.0397	325.1682
C	2.30448	-2.61852	-1.74424	337.8138	365.3593	367.0008
H	3.02546	-1.99985	-1.20452	369.5573	376.7280	392.2142
H	2.70339	-3.63747	-1.83638	396.2780	397.6166	415.2334
H	2.20308	-2.20577	-2.75400	428.2746	435.9772	454.4683
C	1.92335	-2.68961	1.41289	464.1436	468.8863	503.0778
H	2.30177	-3.71603	1.51112	532.3645	535.5128	544.8313
H	2.74530	-2.03839	1.09718	548.5661	553.7451	563.8200
H	1.57941	-2.34836	2.39583	575.1534	583.7965	584.4326
C	-2.75184	-2.72571	-0.80118	590.3562	601.1181	627.3658
H	-3.04946	-1.92667	-1.49081	645.4473	681.5696	711.0015
H	-3.03985	-3.68679	-1.24776	753.2809	772.1668	776.4502
H	-3.31520	-2.57323	0.12109	789.4415	807.5005	809.3867
C	-0.61739	-2.59476	-3.07644	810.5632	824.6996	829.1934
H	-1.43759	-1.89376	-3.26696	859.9286	868.9515	880.7934
H	0.24114	-2.27794	-3.67646	887.3270	907.5519	925.4353
H	-0.93600	-3.58163	-3.43749	941.3211	947.4639	948.1877
C	-1.20839	-2.99077	2.02990	949.1121	971.9505	975.1472
H	-1.13971	-4.05716	2.28184	978.6750	982.1716	1009.1643
H	-0.68817	-2.42034	2.80674	1024.1084	1025.4266	1034.5418
H	-2.26253	-2.69932	2.04555	1041.9295	1045.1638	1048.0434
Ir	-0.12882	-0.87119	-0.29046	1051.2790	1055.1254	1058.9013
C	2.60419	2.02282	-3.05174	1089.5683	1092.6040	1097.2703
H	1.52858	1.96875	-3.25562	1112.0642	1113.3186	1132.9421
H	3.00167	2.90451	-3.57106	1147.6160	1156.6723	1182.3581
H	3.08117	1.13439	-3.48727	1185.5479	1187.3114	1200.6941
C	2.18937	3.35407	-0.97057	1226.6711	1238.5147	1242.2141
H	2.32720	3.42104	0.11614	1255.1797	1264.3784	1283.6066
H	2.60073	4.26634	-1.42303	1289.4213	1317.9642	1340.8084
H	1.11028	3.33498	-1.16134	1357.8157	1362.2482	1370.6986
C	4.39759	2.24378	-1.33963	1375.1750	1376.9771	1380.8303
H	4.64206	2.38137	-0.28035	1387.2105	1388.8973	1391.7642
H	4.91864	1.34562	-1.68757	1392.6940	1399.9310	1417.7585
H	4.78396	3.11083	-1.89096	1424.5574	1428.3883	1433.5979
O	-1.30656	0.62248	-1.74218	1433.9247	1435.5311	1442.4914
C	-1.95048	2.25559	-0.08252	1443.4619	1446.9516	1453.6194
C	-2.85465	3.24953	0.30226	1457.8077	1459.7392	1460.2239
C	-3.37168	1.76024	-1.98510	1461.4938	1463.0731	1468.0255
C	-4.01544	3.48103	-0.42338	1474.5821	1475.9654	1481.7532
C	-4.28089	2.72199	-1.55979	1486.9060	1487.9859	1490.6996
C	-0.82266	1.96636	0.86379	1494.8574	1497.2438	1507.7923
O	-0.23527	2.89476	1.38552	1516.9613	1519.9449	1527.9426
H	-3.53050	1.18303	-2.89260	1535.8550	1560.8794	1643.4133
H	-5.19090	2.89168	-2.13021	1674.0242	1771.6512	1774.9836
H	-4.71693	4.24509	-0.09860	1791.0048	1820.4418	3024.0699
H	-2.63059	3.81941	1.20197	3029.5542	3031.2665	3036.6409
C	-0.66400	0.51868	1.30601	3037.9375	3039.1014	3040.4403
C	-2.04375	0.16681	1.88661	3041.2550	3047.0840	3049.2865
C	0.42980	0.30815	2.30634	3052.7602	3100.9289	3107.2323
C	2.65568	0.71500	2.91114	3112.6649	3115.5968	3116.2392
H	2.32955	0.91778	3.93866	3118.4122	3118.6555	3124.4782
H	2.92774	-0.34753	2.85725	3127.0385	3128.1139	3128.6288
C	3.79449	1.59958	2.48075	3133.9014	3137.0525	3143.8561

H	3.48375	2.65056	2.46660	3144.6298	3148.2089	3169.1991
H	4.63320	1.49808	3.17760	3170.6818	3177.1319	3179.6752
H	4.13091	1.31161	1.47927	3182.8302	3184.9034	3192.5654
O	0.33368	-0.44917	3.26261	3201.7542	3209.3256	3446.5072
O	1.55723	0.95591	2.02270			
C	-2.36009	0.68610	3.26416			
H	-3.44394	0.72569	3.39627			
H	-1.92099	0.01076	4.00591			
H	-1.91041	1.67249	3.43323			
O	-2.88701	-0.42384	1.23902			
H	5.67274	-0.47492	-2.32853			
C	0.63389	0.75102	-2.26539			
C	2.92715	1.58077	-1.45499			
C	4.85170	2.36254	-0.35019			
H	4.58554	3.41370	-0.51439			
H	5.46963	2.04686	-1.20246			
C	5.53081	2.13074	0.97347			
H	6.47248	2.68645	1.02514			
H	4.88756	2.45610	1.79667			
H	5.74242	1.06336	1.11047			
O	3.65827	1.57347	-0.34098			
O	3.14601	2.29349	-2.40703			
C	0.92000	0.94807	-3.71343			
H	-0.00533	0.88337	-4.29044			
H	1.41585	1.91119	-3.86642			
H	1.63737	0.18240	-4.03787			
O	-0.52197	0.63428	-1.87363			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.602301 Electronic Energy = -1719.55373843
Internal Energy (E)= -1718.91220643 Enthalpy (H)= -1718.91126243
Gibbs Free Energy (G)=-1719.01869443 Gibbs Free Energy of Solvation=-1719.06928543

St.Pt.	General Structure	Ball & Stick model
V'-1C		

Cartesian co-ordinate

Atoms	X	Y	Z
C	1.15923	-1.12064	-2.03239

Frequencies

29.6845	49.8540	61.7984
72.4320	89.4290	98.0726
103.9949	109.7131	120.0544
128.3478	134.6485	137.8216
141.2319	145.8912	150.1735

C	2.05801	-0.13702	-1.49779	167.4609	181.0049	186.8502
C	2.71591	-0.72609	-0.33276	193.9241	200.2553	204.0528
C	2.13621	-1.97693	-0.06977	216.1227	219.3783	226.7288
C	1.10654	-2.20625	-1.08264	234.2142	246.9630	250.0487
C	-1.32336	0.28982	-1.04677	260.8293	264.6605	278.5240
C	-2.54417	-0.34151	-0.52208	283.1810	289.0071	298.1245
C	0.26994	1.18833	1.48800	305.2802	315.1474	319.0988
C	2.47378	1.10673	-2.20447	326.0543	342.5287	353.6944
H	3.26023	0.90021	-2.94416	355.3348	366.8513	379.7624
H	1.61913	1.54482	-2.73426	403.9120	414.9158	428.7746
H	2.85487	1.85451	-1.50309	440.5480	473.0996	504.5307
C	3.81426	-0.05092	0.40264	529.1990	534.6703	538.3576
H	4.69606	0.02176	-0.24864	542.0927	552.0823	554.8960
H	3.52428	0.96448	0.69609	569.2656	592.7747	593.6634
H	4.10050	-0.59098	1.30920	600.5103	605.7433	608.5115
C	2.43367	-2.91070	1.05227	621.3121	663.2783	674.3659
H	3.00958	-3.78202	0.71138	749.3025	762.0630	764.8464
H	3.01091	-2.41813	1.84182	811.8579	815.2085	817.1398
H	1.50926	-3.29160	1.50535	834.3364	855.8372	865.2598
C	0.28576	-3.44372	-1.19141	885.7272	893.0047	950.0680
H	0.85409	-4.25527	-1.66499	953.6470	972.1295	975.1389
H	-0.03319	-3.78498	-0.20083	975.3648	1028.2311	1031.6617
H	-0.61947	-3.26807	-1.78266	1037.5567	1038.3525	1039.8291
C	0.45053	-1.02089	-3.33527	1045.4522	1047.4913	1049.8101
H	-0.39240	-1.71756	-3.39227	1086.3913	1089.7268	1090.9138
H	0.05262	-0.01146	-3.48452	1110.7401	1113.3851	1117.6776
H	1.14058	-1.25272	-4.15692	1141.1017	1143.7897	1177.6123
Ir	0.34022	-0.43056	-0.13334	1184.4442	1188.1440	1199.9406
O	-1.32386	1.11279	-1.95359	1223.0362	1263.3377	1281.1669
N	-1.06080	1.28241	1.80778	1300.4179	1342.5452	1373.2059
N	-2.15592	1.32234	2.04572	1380.8323	1381.3140	1383.3412
C	-2.35427	-1.19205	0.58991	1390.5848	1394.9271	1395.8013
O	-1.14201	-1.37816	1.06236	1401.1231	1421.2547	1428.7705
C	-3.82585	-0.08865	-1.02381	1434.6521	1439.8464	1443.6621
C	-3.48654	-1.77989	1.18959	1452.0766	1454.9947	1459.0990
C	-4.74369	-1.52416	0.67117	1464.2635	1467.2564	1469.0965
C	-4.92899	-0.68146	-0.43609	1471.3286	1477.7754	1483.4988
H	-3.34657	-2.42949	2.05080	1484.6756	1487.5665	1492.1195
H	-5.61104	-1.98786	1.13872	1498.4591	1508.8592	1510.9103
H	-5.92921	-0.49804	-0.82021	1513.2851	1529.1524	1574.7596
H	-3.91925	0.58044	-1.87740	1619.8260	1657.7311	1745.3496
C	0.73837	2.40868	0.73796	1831.1552	1878.0071	2293.6220
C	-0.04251	4.05893	-0.75604	3025.1417	3028.7302	3033.1091
H	0.46239	4.92289	-0.30697	3035.2316	3036.2922	3037.0606
H	0.64619	3.59847	-1.47517	3046.0966	3054.2480	3096.1900
C	-1.36433	4.40419	-1.38564	3105.7327	3110.5171	3117.3218
H	-2.05282	4.82789	-0.64691	3118.0349	3121.0539	3129.5131
H	-1.21826	5.14329	-2.17985	3136.2580	3140.8132	3140.9207
H	-1.81325	3.50316	-1.81727	3145.2159	3150.1073	3166.2605
C	1.08926	0.58483	2.62528	3170.2045	3172.0506	3175.9171
O	1.89555	2.69187	0.55639	3184.1006	3194.6765	3201.3226
O	-0.31014	3.09356	0.28139			
C	0.36930	-0.35060	3.55305			
H	-0.26049	-1.05589	2.99665			
H	1.11517	-0.87276	4.15563			
H	-0.27866	0.22082	4.23129			
O	2.25753	0.86916	2.74519			
C	0.42980	0.30815	2.30634			
C	2.65568	0.71500	2.91114			
H	2.32955	0.91778	3.93866			
H	2.92774	-0.34753	2.85725			

C	3.79449	1.59958	2.48075
H	3.48375	2.65056	2.46660
H	4.63320	1.49808	3.17760
H	4.13091	1.31161	1.47927
O	0.33368	-0.44917	3.26261
O	1.55723	0.95591	2.02270
C	-2.36009	0.68610	3.26416
H	-3.44394	0.72569	3.39627
H	-1.92099	0.01076	4.00591
H	-1.91041	1.67249	3.43323
O	-2.88701	-0.42384	1.23902
H	5.67274	-0.47492	-2.32853
C	0.63389	0.75102	-2.26539
C	2.92715	1.58077	-1.45499
C	4.85170	2.36254	-0.35019
H	4.58554	3.41370	-0.51439
H	5.46963	2.04686	-1.20246
C	5.53081	2.13074	0.97347
H	6.47248	2.68645	1.02514
H	4.88756	2.45610	1.79667
H	5.74242	1.06336	1.11047
O	3.65827	1.57347	-0.34098
O	3.14601	2.29349	-2.40703
C	0.92000	0.94807	-3.71343
H	-0.00533	0.88337	-4.29044
H	1.41585	1.91119	-3.86642
H	1.63737	0.18240	-4.03787
O	-0.52197	0.63428	-1.87363

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.461795 Electronic Energy = -1482.12490082
Internal Energy (E)= -1481.63084882 Enthalpy (H)= -1481.62990482
Gibbs Free Energy (G)=-1481.72260382 Gibbs Free Energy of Solvation=-1481.75894005

St.Pt.	General Structure	Ball & Stick model
TS-5C		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.28336	-1.43745	-2.04827
C	1.12731	-1.32402	-1.71784
C	1.38556	-2.19204	-0.59169
C	0.13679	-2.74741	-0.16480
C	-0.90000	-2.28510	-1.08110
C	-0.74041	1.39835	-0.61960
C	-2.17977	1.41291	-0.29219

Frequencies

-314.1503	31.7660	43.4392
51.6962	67.4707	95.2563
100.8651	102.2048	111.0611
116.5169	119.9981	125.6149
139.3124	153.6050	167.2130
170.8463	180.5408	184.1819
192.4851	195.6807	203.0331
211.5339	213.4734	226.2604
227.1090	237.2776	242.6254
247.0071	259.0710	269.9316
279.1562	292.8043	297.7153

C	1.11945	0.68164	1.30986	302.4471	308.8954	316.0171
C	2.12254	-0.53676	-2.49843	319.9025	327.3206	336.0217
H	2.36370	-1.02419	-3.45213	359.0121	395.8584	403.6772
H	1.72922	0.46480	-2.71627	408.2702	414.3012	428.3652
H	3.05303	-0.41720	-1.93335	440.5797	461.0400	468.0349
C	2.69606	-2.49391	0.04443	503.3889	526.1423	537.1690
H	2.96243	-3.54042	-0.15431	537.9706	544.2608	549.4795
H	3.49435	-1.85165	-0.33131	560.4557	581.8208	588.0965
H	2.65401	-2.34122	1.12894	594.8846	599.9747	613.7653
C	-0.05391	-3.65058	1.00194	627.8765	650.4529	667.8132
H	0.05117	-4.70655	0.71712	758.7477	761.8881	768.4300
H	0.68620	-3.43270	1.78053	798.2510	807.5791	810.0012
H	-1.04722	-3.51790	1.44421	813.3071	840.0646	857.4688
C	-2.34075	-2.64325	-0.98203	872.1610	891.3881	949.0709
H	-2.52383	-3.65084	-1.37658	953.6206	958.3189	968.7553
H	-2.67176	-2.62017	0.06232	974.9043	996.0467	1030.3429
H	-2.96910	-1.93861	-1.53581	1036.6529	1042.3514	1045.2022
C	-0.94446	-0.74281	-3.18710	1046.4541	1048.0924	1056.8512
H	-2.02101	-0.63136	-3.02301	1060.5140	1091.2309	1093.6613
H	-0.52784	0.25985	-3.32940	1108.2185	1109.6956	1111.2929
H	-0.79976	-1.30773	-4.11709	1144.8581	1145.2859	1170.5298
Ir	-0.02643	-0.56098	-0.01456	1182.9377	1184.6872	1189.8355
O	-0.19890	2.05042	-1.48834	1236.3459	1264.1169	1278.8586
N	0.14059	1.72609	1.09463	1299.0387	1336.6260	1366.8388
N	-0.42977	2.61055	1.54917	1377.1401	1377.9851	1383.1358
C	-2.58986	0.50166	0.70874	1383.8611	1395.8752	1401.4155
O	-1.70792	-0.30158	1.27000	1407.7546	1423.5633	1434.4640
C	-3.09169	2.26484	-0.91809	1440.7182	1442.9928	1447.4040
C	-3.94686	0.49193	1.08079	1450.7622	1451.5005	1452.3368
C	-4.83948	1.33943	0.44569	1460.7058	1463.2495	1468.3532
C	-4.42861	2.22703	-0.55942	1469.7127	1474.9453	1478.6345
H	-4.26984	-0.19911	1.85635	1484.5176	1485.5079	1494.2756
H	-5.88938	1.30980	0.73275	1497.7116	1500.3153	1507.4914
H	-5.15177	2.87805	-1.04358	1509.8694	1516.4445	1540.2500
H	-2.72138	2.94597	-1.68264	1617.1940	1659.1698	1760.7078
C	2.41271	1.04637	0.64871	1798.8971	1862.9537	2049.9443
C	3.45263	2.60449	-0.77272	3028.4576	3029.4017	3036.6016
H	4.29720	2.78229	-0.09551	3038.6397	3039.3965	3040.2945
H	3.73308	1.76950	-1.42866	3048.4191	3056.8352	3098.7362
C	3.05779	3.82970	-1.55126	3101.6416	3110.1454	3119.6645
H	2.77973	4.64741	-0.87890	3120.3606	3121.7685	3127.8868
H	3.89084	4.16523	-2.17702	3136.3162	3141.7513	3144.4743
H	2.19901	3.60919	-2.19250	3145.8342	3146.2124	3155.8486
C	1.15343	0.03735	2.67194	3167.5555	3168.0191	3175.8216
O	3.41672	0.37767	0.68808	3182.3704	3194.3852	3204.2118
O	2.31134	2.21535	0.00567			
C	0.16082	0.48605	3.70236			
H	-0.85377	0.30081	3.32537			
H	0.33148	-0.08572	4.61642			
H	0.25052	1.55800	3.91129			
O	1.94303	-0.86644	2.86553			
C	0.42980	0.30815	2.30634			
C	2.65568	0.71500	2.91114			
H	2.32955	0.91778	3.93866			
H	2.92774	-0.34753	2.85725			
C	3.79449	1.59958	2.48075			
H	3.48375	2.65056	2.46660			
H	4.63320	1.49808	3.17760			
H	4.13091	1.31161	1.47927			
O	0.33368	-0.44917	3.26261			
O	1.55723	0.95591	2.02270			

C	-2.36009	0.68610	3.26416
H	-3.44394	0.72569	3.39627
H	-1.92099	0.01076	4.00591
H	-1.91041	1.67249	3.43323
O	-2.88701	-0.42384	1.23902
H	5.67274	-0.47492	-2.32853
C	0.63389	0.75102	-2.26539
C	2.92715	1.58077	-1.45499
C	4.85170	2.36254	-0.35019
H	4.58554	3.41370	-0.51439
H	5.46963	2.04686	-1.20246
C	5.53081	2.13074	0.97347
H	6.47248	2.68645	1.02514
H	4.88756	2.45610	1.79667
H	5.74242	1.06336	1.11047
O	3.65827	1.57347	-0.34098
O	3.14601	2.29349	-2.40703
C	0.92000	0.94807	-3.71343
H	-0.00533	0.88337	-4.29044
H	1.41585	1.91119	-3.86642
H	1.63737	0.18240	-4.03787
O	-0.52197	0.63428	-1.87363

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.459833 Electronic Energy = -1482.06427040
Internal Energy (E)= -1481.5725944 Enthalpy (H)= -1481.5716504
Gibbs Free Energy (G)=-1481.6636834 Gibbs Free Energy of Solvation=-1481.70025931

St.Pt.	General Structure	Ball & Stick model
VI-1C		

Cartesian co-ordinate

Atoms	X	Y	Z
C	0.78513	1.09174	-1.74320
C	-0.65672	1.21649	-1.74079
C	-1.00126	2.33825	-0.91000
C	0.24515	2.96257	-0.47906
C	1.33335	2.22034	-1.00078
C	0.49791	-2.27516	-0.33305
C	1.92525	-2.04920	-0.11842
C	-1.08405	-0.75879	1.02747
C	-1.58812	0.33168	-2.49171
H	-1.52320	0.54616	-3.56608
H	-1.34653	-0.72770	-2.33773
H	-2.62507	0.49477	-2.17874
C	-2.37150	2.84489	-0.62198

Frequencies

40.6926	51.8624	62.9009
80.1627	86.4024	95.6488
98.1419	105.3115	109.0234
110.7614	122.1253	127.2913
133.9257	155.6280	160.2123
171.9259	177.9432	187.8288
191.5034	195.1241	204.5812
207.3222	212.1903	225.9699
235.5253	242.9554	250.3681
261.9189	263.7920	275.6603
296.5078	302.5336	314.7827
317.9058	325.5994	326.6934
330.9942	344.5103	354.4026
384.5709	397.1192	400.4047
416.2272	441.0348	444.5788
452.3034	455.1409	516.8627
529.8255	535.6447	537.4729

H	-2.69796	3.56650	-1.38233	544.6576	547.9148	555.9620
H	-3.09617	2.02485	-0.58147	584.2058	597.6852	602.2785
H	-2.40749	3.34335	0.35289	605.8103	640.2894	671.4349
C	0.31158	4.13264	0.43765	677.8934	715.5705	761.9897
H	0.03240	5.05499	-0.08750	769.0711	789.8624	800.8009
H	-0.38018	4.00686	1.27873	810.1717	811.8371	829.5499
H	1.31512	4.26482	0.85182	854.9297	869.4579	877.6298
C	2.78573	2.45576	-0.78231	897.3442	940.0776	953.6942
H	3.25380	2.87292	-1.68350	956.0884	970.9430	978.7433
H	2.96201	3.15146	0.04357	998.0179	1011.4350	1033.1841
H	3.30315	1.51845	-0.54239	1039.6563	1044.2271	1045.5279
C	1.57894	0.12648	-2.55172	1050.7768	1058.4714	1060.4487
H	2.53346	-0.11015	-2.06740	1070.2798	1091.6948	1093.2588
H	1.04282	-0.81854	-2.69321	1111.9009	1119.1925	1126.2725
H	1.79514	0.55162	-3.54113	1145.2532	1149.1278	1171.1244
Ir	0.06842	0.86285	0.26158	1183.9393	1187.5479	1217.6008
O	-0.02710	-2.70531	-1.33179	1273.3030	1276.0929	1284.6642
N	-0.36431	-2.09937	0.92097	1319.0696	1337.6699	1374.1627
N	-0.41637	-3.02312	1.69460	1379.1012	1381.7443	1386.8969
C	2.37748	-1.00734	0.73294	1399.9224	1402.1446	1402.5728
O	1.56463	-0.17674	1.34468	1408.7774	1413.0087	1425.6888
C	2.83410	-2.84191	-0.83085	1433.4302	1436.6745	1441.1569
C	3.77274	-0.86389	0.88746	1441.4803	1443.4602	1447.5599
C	4.65619	-1.68196	0.20340	1453.6358	1458.0771	1467.0932
C	4.19777	-2.67287	-0.67279	1472.7332	1476.2601	1477.7615
H	4.12390	-0.07670	1.55174	1480.7594	1487.2064	1489.6587
H	5.72684	-1.53864	0.34031	1498.4360	1500.3156	1511.4247
H	4.90034	-3.30174	-1.21267	1516.9897	1520.2182	1553.1358
H	2.43301	-3.60185	-1.49916	1609.8766	1660.5287	1696.4025
C	-2.47138	-0.80323	0.49762	1723.6173	1804.7331	1829.1884
C	-3.94283	-1.90998	-0.97702	3019.2892	3030.4752	3034.3009
H	-4.65063	-2.21898	-0.19726	3036.1074	3038.5095	3039.3729
H	-4.27490	-0.92803	-1.33965	3046.3690	3055.8912	3096.0269
C	-3.82127	-2.92594	-2.08149	3099.6630	3104.4637	3114.1918
H	-3.44741	-3.87695	-1.68999	3117.3331	3119.2189	3120.5010
H	-4.79400	-3.09747	-2.55318	3139.5776	3140.9828	3142.7016
H	-3.11751	-2.58182	-2.84714	3147.5946	3148.4135	3149.3926
C	-1.06427	-0.16017	2.39871	3154.0277	3171.0636	3171.1615
O	-3.34326	-0.01704	0.82051	3186.0060	3192.7813	3209.1141
O	-2.64175	-1.78262	-0.39122			
C	-1.51601	-0.85778	3.61332			
H	-1.07695	-1.86639	3.60773			
H	-1.27052	-0.29215	4.51443			
H	-2.60171	-1.00327	3.53853			
O	-0.62984	1.00494	2.39399			
C	0.42980	0.30815	2.30634			
C	2.65568	0.71500	2.91114			
H	2.32955	0.91778	3.93866			
H	2.92774	-0.34753	2.85725			
C	3.79449	1.59958	2.48075			
H	3.48375	2.65056	2.46660			
H	4.63320	1.49808	3.17760			
H	4.13091	1.31161	1.47927			
O	0.33368	-0.44917	3.26261			
O	1.55723	0.95591	2.02270			
C	-2.36009	0.68610	3.26416			
H	-3.44394	0.72569	3.39627			
H	-1.92099	0.01076	4.00591			
H	-1.91041	1.67249	3.43323			
O	-2.88701	-0.42384	1.23902			
H	5.67274	-0.47492	-2.32853			

C	0.63389	0.75102	-2.26539
C	2.92715	1.58077	-1.45499
C	4.85170	2.36254	-0.35019
H	4.58554	3.41370	-0.51439
H	5.46963	2.04686	-1.20246
C	5.53081	2.13074	0.97347
H	6.47248	2.68645	1.02514
H	4.88756	2.45610	1.79667
H	5.74242	1.06336	1.11047
O	3.65827	1.57347	-0.34098
O	3.14601	2.29349	-2.40703
C	0.92000	0.94807	-3.71343
H	-0.00533	0.88337	-4.29044
H	1.41585	1.91119	-3.86642
H	1.63737	0.18240	-4.03787
O	-0.52197	0.63428	-1.87363

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.461821 Electronic Energy = -1482.07454869
Internal Energy (E)= -1481.58081869 Enthalpy (H)= -1481.57987569
Gibbs Free Energy (G)=-1481.67197969 Gibbs Free Energy of Solvation=-1481.71629325

St.Pt.	General Structure	Ball & Stick model
VI'-1C		

Cartesian co-ordinate

Atoms	X	Y	Z
C	0.20936	1.89601	1.25379
C	1.30462	1.94124	0.30871
C	0.73895	2.10800	-1.01084
C	-0.68363	2.14305	-0.86682
C	-1.01801	2.05647	0.52359
C	-2.23088	-0.82950	1.58910
C	-2.99943	-0.99665	0.37931
C	-2.42547	-1.20300	-0.91218
C	1.52741	-1.19075	-0.36369
Ir	0.15070	0.09880	-0.06938
C	1.30121	-2.64460	-0.31827
H	0.36100	-2.91322	-0.81292

Frequencies

30.1545	31.8831	46.5421
63.6618	64.9866	65.7289
89.8495	103.5438	114.5334
123.2468	134.7262	137.8544
148.1627	152.2200	157.3407
172.8681	179.7631	181.9114
199.5329	200.6381	213.2666
227.7540	239.0337	243.7050
249.7889	255.3479	271.3448
276.6063	289.2983	299.2683
305.7663	312.3848	315.8702
333.9259	346.9288	354.5547
366.2167	380.7145	393.6475
417.6317	421.9213	427.0324
439.5032	444.9332	451.3285
482.3277	527.5157	533.9556

H	2.13658	-3.24988	-0.68891	536.0100	547.9774	566.5755
H	1.14498	-2.87463	0.76176	578.6198	586.2808	598.4349
C	2.95128	-0.81204	-0.52961	606.3559	628.3253	650.2722
O	3.67117	-1.21301	0.53126	692.6984	727.1494	740.8612
C	5.08955	-0.98176	0.46739	765.6215	792.5237	811.7606
H	5.27205	-0.00461	0.00562	816.4379	820.3440	821.9991
H	5.41142	-0.94853	1.51239	853.6997	867.2668	877.0973
C	5.77127	-2.08841	-0.29902	901.4309	928.0616	955.1293
H	6.85710	-1.94744	-0.28869	961.0239	964.5190	983.6234
H	5.54706	-3.06265	0.14770	984.0171	1037.7294	1041.1331
H	5.43741	-2.09215	-1.34134	1045.3763	1049.5998	1052.9639
O	3.42306	-0.23740	-1.48927	1054.2387	1056.3110	1094.6951
O	-2.59629	-0.47968	2.68124	1097.3525	1114.1187	1118.6375
O	-1.15753	-1.13129	-1.19876	1125.4415	1137.4756	1148.1126
C	-3.32723	-1.47138	-1.97456	1182.1833	1187.8164	1192.9889
C	-4.40282	-0.96649	0.53846	1196.7152	1212.6941	1253.7132
C	-4.69020	-1.46627	-1.78143	1299.6147	1325.6127	1338.9083
C	-5.24950	-1.19787	-0.51923	1348.6916	1383.1873	1385.2808
H	-2.89054	-1.64442	-2.95534	1389.3165	1396.4179	1399.1190
H	-5.34561	-1.65992	-2.62893	1406.0412	1407.2877	1412.5886
H	-6.32693	-1.18956	-0.38158	1416.7224	1440.2981	1442.1798
H	-4.78669	-0.77769	1.53913	1449.4524	1456.1401	1458.8949
N	-0.74347	-1.21920	1.46107	1459.4577	1463.9201	1464.3460
N	-0.29031	-2.08135	2.12471	1469.3658	1469.5038	1473.9507
C	0.34102	1.79299	2.73475	1480.5748	1482.4973	1485.0913
H	1.23466	1.22164	3.00833	1501.8555	1504.8376	1508.3052
H	0.42093	2.78702	3.19473	1519.7958	1524.3375	1525.3734
H	-0.52172	1.28057	3.17587	1531.0363	1597.6402	1672.7647
C	2.74451	2.07339	0.67055	1814.5178	1825.3419	1870.8524
H	2.97172	3.11424	0.93589	2856.0010	3031.9671	3036.3741
H	3.00226	1.44693	1.53230	3037.4151	3037.7022	3041.0652
H	3.39269	1.79243	-0.16526	3051.4983	3065.4216	3067.4823
C	1.50112	2.30480	-2.27468	3109.9496	3114.4590	3117.5677
H	1.81138	3.35391	-2.37598	3120.0379	3121.5033	3126.0071
H	2.39414	1.67483	-2.30335	3137.2086	3139.4867	3140.6485
H	0.89194	2.05394	-3.14874	3143.8816	3154.7866	3157.0565
C	-1.66562	2.22263	-1.98350	3162.1958	3173.9528	3187.6354
H	-1.83858	3.26363	-2.28622	3190.9280	3197.1782	3210.1633
H	-1.31161	1.67043	-2.86098			
H	-2.63155	1.79207	-1.69731			
C	-2.37348	2.28324	1.10198			
H	-2.60122	3.35748	1.10937			
H	-3.16074	1.78442	0.52491			
H	-2.44721	1.92005	2.13068			
H	-2.60171	-1.00327	3.53853			
O	-0.62984	1.00494	2.39399			
C	0.42980	0.30815	2.30634			
C	2.65568	0.71500	2.91114			
H	2.32955	0.91778	3.93866			
H	2.92774	-0.34753	2.85725			
C	3.79449	1.59958	2.48075			
H	3.48375	2.65056	2.46660			
H	4.63320	1.49808	3.17760			
H	4.13091	1.31161	1.47927			
O	0.33368	-0.44917	3.26261			
O	1.55723	0.95591	2.02270			
C	-2.36009	0.68610	3.26416			
H	-3.44394	0.72569	3.39627			
H	-1.92099	0.01076	4.00591			
H	-1.91041	1.67249	3.43323			
O	-2.88701	-0.42384	1.23902			

H	5.67274	-0.47492	-2.32853
C	0.63389	0.75102	-2.26539
C	2.92715	1.58077	-1.45499
C	4.85170	2.36254	-0.35019
H	4.58554	3.41370	-0.51439
H	5.46963	2.04686	-1.20246
C	5.53081	2.13074	0.97347
H	6.47248	2.68645	1.02514
H	4.88756	2.45610	1.79667
H	5.74242	1.06336	1.11047
O	3.65827	1.57347	-0.34098
O	3.14601	2.29349	-2.40703
C	0.92000	0.94807	-3.71343
H	-0.00533	0.88337	-4.29044
H	1.41585	1.91119	-3.86642
H	1.63737	0.18240	-4.03787
O	-0.52197	0.63428	-1.87363

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.450883 Electronic Energy = -1368.79356929
Internal Energy (E)= -1368.31195229 Enthalpy (H)= -1368.31100829
Gibbs Free Energy (G)=-1368.40226729 Gibbs Free Energy of Solvation=-1369.53383758

St.Pt.	General Structure	Ball & Stick model
TS-6C		

Cartesian co-ordinate

Atoms	X	Y	Z
C	0.49268	2.46700	-0.66555
C	-0.85969	2.39095	-0.13306
C	-0.74893	2.07919	1.27679
C	0.63960	1.85277	1.55446
C	1.40028	2.15980	0.37231
C	2.70249	-0.18805	-1.54784
C	3.15181	-0.92020	-0.45037
C	2.30317	-1.56911	0.52686
C	-1.63201	-0.85249	-0.19944
Ir	-0.16867	0.32752	0.04160
C	-1.41887	-2.34269	-0.21892
C	-3.05036	-0.46418	-0.22659
O	-3.81461	-1.48435	-0.69838
C	-5.22774	-1.26841	-0.72176
H	-5.43012	-0.23885	-1.03696
H	-5.60564	-1.95532	-1.48561
C	-5.83519	-1.55305	0.63217
H	-6.92467	-1.44572	0.59638

Frequencies

-326.2260	16.5648	32.4604
35.0514	50.7666	57.9876
66.1274	78.4781	79.8936
85.7895	95.1714	101.5024
109.1509	116.6216	120.3309
134.5115	139.6645	147.0527
150.0146	157.3184	158.4519
167.8460	176.2756	183.0605
186.4381	201.5837	209.1656
215.1931	228.8472	235.0818
244.3883	251.9885	253.5617
270.3489	274.5147	282.4529
298.5379	306.3770	327.4196
334.3523	347.8849	355.8141
361.9252	387.3250	395.0111
401.7976	420.6426	430.1757
461.4066	492.5731	513.9116
526.3909	530.3970	537.0688
543.7141	553.4856	573.3901
583.0718	587.9798	604.5135
607.4780	624.7757	638.5838
738.7051	752.2563	754.1336

H	-5.60155	-2.57441	0.95240	758.6135	777.2160	802.5236
H	-5.44665	-0.85155	1.37765	816.2225	819.4297	854.5074
O	-3.54109	0.59926	0.11255	881.2537	886.3870	946.2972
O	3.01065	0.55983	-2.39769	949.8277	950.7746	960.7844
O	1.05704	-1.38179	0.68026	983.4933	997.5842	1012.7005
C	2.97725	-2.46784	1.41475	1027.5252	1031.4031	1038.2661
C	4.57593	-1.05160	-0.39418	1039.0895	1042.4065	1044.5996
C	4.33816	-2.59748	1.41881	1050.3559	1083.6102	1090.3027
C	5.16396	-1.87265	0.52193	1107.2635	1115.2216	1139.1690
H	2.35006	-2.99952	2.12533	1143.6036	1157.1091	1179.0014
H	4.80228	-3.26757	2.14020	1181.0865	1191.2606	1192.9620
H	6.24324	-1.98624	0.55196	1226.5989	1245.6490	1257.2007
H	5.16875	-0.50760	-1.12664	1319.7023	1363.5669	1364.5512
N	0.92156	-0.75581	-1.88847	1371.1177	1379.1019	1384.3116
N	0.49268	-1.24435	-2.80745	1386.5509	1396.7344	1407.2545
C	0.79325	2.91201	-2.05414	1410.7739	1426.6985	1433.4933
H	0.17434	2.37475	-2.78269	1437.0993	1438.0060	1439.9272
H	0.57149	3.98274	-2.16775	1444.1881	1453.5422	1455.0469
H	1.83914	2.75451	-2.32631	1458.6166	1462.3673	1464.5030
C	-2.02465	2.98991	-0.84860	1467.9499	1471.1692	1473.4080
H	-1.83717	4.05815	-1.02791	1474.5708	1475.2881	1485.7744
H	-2.18362	2.51438	-1.82380	1487.5264	1491.6800	1509.1772
H	-2.94771	2.88594	-0.27934	1513.3851	1555.9854	1571.1107
C	-1.81455	2.14290	2.31296	1591.2586	1687.0305	1782.1407
H	-1.88238	3.16550	2.70984	1816.0850	2035.9879	2188.4308
H	-2.78266	1.85600	1.90133	3022.8512	3027.3034	3029.4226
H	-1.58836	1.47768	3.15320	3035.4074	3038.9561	3041.8900
C	1.22271	1.46497	2.86914	3046.5545	3068.5777	3098.4739
H	1.46370	2.34636	3.48041	3103.1170	3103.6893	3109.1950
H	0.53012	0.83898	3.44132	3113.7919	3124.4656	3131.9856
H	2.14841	0.89152	2.74063	3132.7724	3138.2721	3145.7819
C	2.88640	2.29066	0.35683	3149.8775	3159.7308	3165.5145
H	3.17226	3.22443	0.86012	3180.5332	3191.8974	3194.5296
H	3.38504	1.47669	0.89555	3204.4221	3213.7605	3217.3687
H	3.29628	2.32995	-0.65599			
C	-1.76846	-3.06353	1.05843			
H	-1.78668	-4.14339	0.88666			
H	-0.99357	-2.82499	1.79773			
H	-2.72961	-2.72460	1.46130			
O	-0.95203	-2.93160	-1.17437			
C	0.42980	0.30815	2.30634			
C	2.65568	0.71500	2.91114			
H	2.32955	0.91778	3.93866			
H	2.92774	-0.34753	2.85725			
C	3.79449	1.59958	2.48075			
H	3.48375	2.65056	2.46660			
H	4.63320	1.49808	3.17760			
H	4.13091	1.31161	1.47927			
O	0.33368	-0.44917	3.26261			
O	1.55723	0.95591	2.02270			
C	-2.36009	0.68610	3.26416			
H	-3.44394	0.72569	3.39627			
H	-1.92099	0.01076	4.00591			
H	-1.91041	1.67249	3.43323			
O	-2.88701	-0.42384	1.23902			
H	5.67274	-0.47492	-2.32853			
C	0.63389	0.75102	-2.26539			
C	2.92715	1.58077	-1.45499			
C	4.85170	2.36254	-0.35019			
H	4.58554	3.41370	-0.51439			
H	5.46963	2.04686	-1.20246			

C	5.53081	2.13074	0.97347
H	6.47248	2.68645	1.02514
H	4.88756	2.45610	1.79667
H	5.74242	1.06336	1.11047
O	3.65827	1.57347	-0.34098
O	3.14601	2.29349	-2.40703
C	0.92000	0.94807	-3.71343
H	-0.00533	0.88337	-4.29044
H	1.41585	1.91119	-3.86642
H	1.63737	0.18240	-4.03787
O	-0.52197	0.63428	-1.87363

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.456206 Electronic Energy = -1482.04762081
Internal Energy (E)= -1481.55701581 Enthalpy (H)= -1481.55607181
Gibbs Free Energy (G)=-1481.65701981 Gibbs Free Energy of Solvation=-1481.69140748

St.Pt.	General Structure	Ball & Stick model
VII-1C		

Cartesian co-ordinate

Atoms	X	Y	Z
C	2.11147	-1.51572	1.24468
C	0.87466	-2.27513	1.18278
C	0.72089	-2.73942	-0.16941
C	1.78980	-2.16658	-0.95482
C	2.65070	-1.42914	-0.06108
C	0.60542	1.04663	1.24993
C	1.08843	2.26539	0.61824
C	1.30652	2.19574	-0.77477
C	-1.27561	-0.12900	-0.66034
Ir	0.51619	-0.50733	-0.17033
C	-1.61131	0.89951	-1.70704
C	-2.46536	-0.87481	-0.16076
O	-3.58531	-0.16744	-0.40214
C	-4.80035	-0.68761	0.15162
H	-5.03149	-1.64120	-0.33951
H	-4.63826	-0.89787	1.21628
C	-5.86665	0.35089	-0.07393
H	-6.82628	0.00494	0.32266
H	-5.60563	1.28875	0.42981
H	-5.98865	0.55834	-1.14190
O	-2.47472	-1.92846	0.44015
O	0.30479	0.90695	2.41256
O	1.05572	1.08952	-1.42733
C	1.74877	3.36020	-1.43946
C	1.25910	3.46638	1.32769
C	1.92798	4.52645	-0.72229

Frequencies

33.6961	36.4373	43.7479
56.3979	59.6844	74.5898
74.8409	84.0949	91.5606
104.5893	107.2967	112.7232
127.8548	140.4980	145.9344
151.5653	152.7770	155.4740
158.6234	162.8573	171.1977
179.2435	184.1035	189.8506
198.3320	202.7028	209.5562
216.7640	223.2911	233.8102
251.8978	258.9744	267.4436
278.4050	290.7097	295.8001
310.9632	314.1142	321.9475
336.5368	345.4501	351.6564
364.9736	373.0554	409.2442
415.6526	422.7244	426.0267
470.5271	532.6083	536.3379
539.6641	548.2768	550.7916
554.9219	570.2508	583.9226
590.0607	599.0718	605.7790
626.6313	633.0182	664.3530
754.5532	765.5769	785.7936
799.6374	805.7974	813.4583
817.1877	852.7485	858.3629
879.3742	887.1049	946.6499
953.8821	961.5914	975.3069
980.8016	1005.7266	1017.5147
1032.2626	1034.0890	1036.8650
1041.4437	1043.2772	1050.2119
1056.9409	1093.6642	1095.4420

C	1.68250	4.59719	0.66193
H	1.91657	3.31462	-2.51252
H	2.25957	5.42060	-1.24772
H	1.82449	5.53453	1.19302
H	1.04387	3.47076	2.39454
N	-2.86454	1.31343	2.09858
N	-2.29490	2.25985	2.05592
C	-0.27553	-3.72344	-0.67121
H	0.16007	-4.73114	-0.64893
H	-1.18366	-3.71639	-0.06650
H	-0.56497	-3.50662	-1.70506
C	0.04768	-2.63876	2.36553
H	-0.96580	-2.91595	2.06490
H	0.49687	-3.47458	2.91885
H	-0.03378	-1.78380	3.04553
C	2.70028	-0.97477	2.49742
H	1.93001	-0.53857	3.14075
H	3.19147	-1.78355	3.05409
H	3.44746	-0.20009	2.29624
C	3.84764	-0.65569	-0.49383
H	3.61127	-0.04932	-1.37606
H	4.18978	0.02577	0.29147
H	4.68041	-1.32084	-0.75515
C	2.04534	-2.37266	-2.40743
H	2.42421	-1.45473	-2.87043
H	2.79097	-3.16306	-2.56946
H	1.13215	-2.65337	-2.94073
O	-1.71708	0.49565	-2.84852
C	-1.88315	2.32144	-1.31778
H	-1.71017	2.97404	-2.17839
H	-2.94103	2.38792	-1.03089
H	-1.28296	2.65032	-0.46246
C	0.42980	0.30815	2.30634
C	2.65568	0.71500	2.91114
H	2.32955	0.91778	3.93866
H	2.92774	-0.34753	2.85725
C	3.79449	1.59958	2.48075
H	3.48375	2.65056	2.46660
H	4.63320	1.49808	3.17760
H	4.13091	1.31161	1.47927
O	0.33368	-0.44917	3.26261
O	1.55723	0.95591	2.02270
C	-2.36009	0.68610	3.26416
H	-3.44394	0.72569	3.39627
H	-1.92099	0.01076	4.00591
H	-1.91041	1.67249	3.43323
O	-2.88701	-0.42384	1.23902
H	5.67274	-0.47492	-2.32853
C	0.63389	0.75102	-2.26539
C	2.92715	1.58077	-1.45499
C	4.85170	2.36254	-0.35019
H	4.58554	3.41370	-0.51439
H	5.46963	2.04686	-1.20246
C	5.53081	2.13074	0.97347
H	6.47248	2.68645	1.02514
H	4.88756	2.45610	1.79667
H	5.74242	1.06336	1.11047
O	3.65827	1.57347	-0.34098
O	3.14601	2.29349	-2.40703
C	0.92000	0.94807	-3.71343
H	-0.00533	0.88337	-4.29044

1111.0849	1119.1987	1138.7835
1142.7258	1145.2209	1179.2434
1185.6226	1187.5202	1208.5448
1251.5332	1262.0855	1267.7755
1286.0568	1345.6861	1373.4884
1378.0577	1378.8729	1381.5095
1395.9749	1398.7889	1400.3962
1406.8548	1421.0617	1433.3830
1438.6456	1440.5122	1440.8204
1446.1334	1449.6962	1455.0851
1460.1232	1467.3367	1467.7500
1473.9646	1476.6279	1477.3274
1482.9301	1483.5837	1490.8136
1496.5953	1502.9676	1516.3048
1518.3907	1520.7216	1553.7220
1616.2099	1660.7684	1806.7045
1813.9066	1819.0060	2462.2681
3030.6833	3037.9515	3039.5331
3039.8090	3040.6346	3042.8236
3048.7840	3052.9823	3102.6145
3111.8057	3115.6855	3118.5329
3124.3820	3128.3584	3130.7585
3139.4617	3142.9371	3145.8181
3148.0889	3163.5300	3166.0785
3174.2728	3174.5347	3179.3359
3190.6769	3203.7423	3208.1208

H	1.41585	1.91119	-3.86642
H	1.63737	0.18240	-4.03787
O	-0.52197	0.63428	-1.87363

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.458621 Electronic Energy = -1482.15556477
Internal Energy (E)= -1481.66258977 Enthalpy (H)= -1481.66164577
Gibbs Free Energy (G)=-1481.76104277 Gibbs Free Energy of Solvation=-1481.7942226

St.Pt.	General Structure	Ball & Stick model
TS-7C		

Cartesian co-ordinate

Atoms	X	Y	Z
C	2.40756	-0.20694	1.53715
C	1.76074	-1.51099	1.39627
C	2.14475	-2.05213	0.13026
C	2.97247	-1.05508	-0.53653
C	3.17539	0.04543	0.37599
C	-0.75614	0.75863	0.86716
C	-0.64179	2.15557	0.49272
C	0.14702	2.48248	-0.64303
C	-0.86746	-0.50594	-0.72391
Ir	0.98592	-0.23836	-0.22832
C	-1.53911	0.11507	-1.93927
C	-1.67229	-1.64910	-0.19096
O	-2.96799	-1.52205	-0.53035
C	-3.84877	-2.55257	-0.06366
H	-3.48960	-3.52076	-0.43387
H	-3.79851	-2.58284	1.03267
C	-5.22905	-2.22026	-0.56446
H	-5.94317	-2.98560	-0.24481
H	-5.56373	-1.25421	-0.16960
H	-5.24371	-2.16689	-1.65761
O	-1.25687	-2.57216	0.47413
O	-1.27657	0.29489	1.85407
O	0.79737	1.56785	-1.30484
C	0.16592	3.83399	-1.05996
C	-1.35492	3.14336	1.19491
C	-0.55126	4.78394	-0.36185
C	-1.31672	4.45444	0.77278

Frequencies

-271.6288	25.5466	40.8741
51.7439	60.5341	66.0438
72.4567	74.1025	88.7570
99.6740	117.2992	119.8424
124.6169	136.9494	142.7100
149.2009	159.7818	161.6108
167.9124	172.8375	179.0185
186.0841	197.6012	199.7822
205.1383	218.0457	223.2933
231.0950	244.8111	246.8051
249.3986	259.0060	279.3811
282.2311	295.6893	298.1382
308.0640	314.8615	322.2164
334.4213	354.2613	356.7586
373.9973	388.3238	406.3591
420.3059	431.4674	444.3770
461.1527	473.1854	536.4603
543.2364	547.1197	550.9050
556.6698	575.7890	592.3086
595.5066	599.3815	605.3793
608.0858	619.1700	647.4206
752.2777	776.7618	780.7858
799.8286	808.3835	817.4831
825.2461	832.5501	870.8717
878.2010	889.7455	957.6178
958.4858	967.6903	985.7991
994.9225	1010.8162	1033.7695
1037.7457	1043.3343	1045.9507
1048.5498	1051.4668	1058.3280
1060.1054	1090.0119	1096.5813
1110.3155	1124.6275	1131.8352

H	0.75266	4.09041	-1.93857	1140.9672	1149.6457	1174.3496
H	-0.52287	5.81848	-0.70008	1184.6177	1186.3744	1207.8955
H	-1.86966	5.22549	1.30200	1236.9784	1264.7772	1274.3179
H	-1.94365	2.83648	2.05730	1295.2633	1348.7668	1376.5764
N	-4.40092	-0.09019	1.99269	1378.8202	1380.7248	1387.4490
N	-4.08688	0.82144	1.45248	1395.5132	1399.6983	1400.1489
C	1.77375	-3.38902	-0.40500	1409.9290	1424.1277	1434.3421
H	2.44640	-4.16464	-0.01623	1438.5782	1441.6954	1451.9171
H	0.74541	-3.63676	-0.12399	1455.1657	1455.9032	1463.1219
H	1.83450	-3.40641	-1.49770	1463.8326	1465.2760	1471.1690
C	0.97451	-2.18276	2.46641	1475.0744	1481.1729	1482.1666
H	0.53382	-3.11485	2.10726	1485.1464	1491.1805	1493.0703
H	1.62006	-2.39784	3.32807	1504.0767	1505.7476	1508.7899
H	0.14484	-1.55097	2.80134	1522.2535	1527.1714	1556.3601
C	2.25325	0.69227	2.71430	1602.8561	1665.9194	1796.0379
H	1.32546	0.47834	3.25397	1818.3647	1835.9617	2462.8727
H	3.08684	0.56390	3.41695	3030.7923	3036.6121	3037.8217
H	2.22502	1.74506	2.41205	3041.5769	3047.5591	3048.5055
C	3.92214	1.29305	0.05740	3056.8053	3060.0827	3108.7844
H	3.73513	1.60877	-0.97497	3113.9423	3114.9159	3118.3636
H	3.61648	2.11795	0.70953	3125.2703	3137.7140	3140.4408
H	5.00366	1.15049	0.17626	3142.3172	3142.7699	3147.5011
C	3.60728	-1.19558	-1.87547	3148.4667	3150.0123	3170.0642
H	3.72544	-0.21994	-2.35822	3172.2994	3180.1347	3184.3814
H	4.60125	-1.65668	-1.79570	3185.2199	3198.3748	3205.9917
H	2.99874	-1.81571	-2.54084			
O	-1.31116	-0.43561	-2.99731			
C	-2.53650	1.23583	-1.83665			
H	-2.03163	2.20683	-1.90542			
H	-3.22787	1.14815	-2.67921			
H	-3.08553	1.21339	-0.88902			
C	0.42980	0.30815	2.30634			
C	2.65568	0.71500	2.91114			
H	2.32955	0.91778	3.93866			
H	2.92774	-0.34753	2.85725			
C	3.79449	1.59958	2.48075			
H	3.48375	2.65056	2.46660			
H	4.63320	1.49808	3.17760			
H	4.13091	1.31161	1.47927			
O	0.33368	-0.44917	3.26261			
O	1.55723	0.95591	2.02270			
C	-2.36009	0.68610	3.26416			
H	-3.44394	0.72569	3.39627			
H	-1.92099	0.01076	4.00591			
H	-1.91041	1.67249	3.43323			
O	-2.88701	-0.42384	1.23902			
H	5.67274	-0.47492	-2.32853			
C	0.63389	0.75102	-2.26539			
C	2.92715	1.58077	-1.45499			
C	4.85170	2.36254	-0.35019			
H	4.58554	3.41370	-0.51439			
H	5.46963	2.04686	-1.20246			
C	5.53081	2.13074	0.97347			
H	6.47248	2.68645	1.02514			
H	4.88756	2.45610	1.79667			
H	5.74242	1.06336	1.11047			
O	3.65827	1.57347	-0.34098			
O	3.14601	2.29349	-2.40703			
C	0.92000	0.94807	-3.71343			
H	-0.00533	0.88337	-4.29044			
H	1.41585	1.91119	-3.86642			

H	1.63737	0.18240	-4.03787
O	-0.52197	0.63428	-1.87363

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.459402 Electronic Energy = -1482.13708549
Internal Energy (E)= -1481.64440449 Enthalpy (H)= -1481.64346049
Gibbs Free Energy (G)=-1481.74017149 Gibbs Free Energy of Solvation=-1481.77630004

St.Pt.	General Structure	Ball & Stick model
VIII-1C		

Cartesian co-ordinate

Atoms	X	Y	Z
C	2.52636	0.33482	1.18229
C	1.87879	-0.87784	1.63588
C	2.12735	-1.90042	0.65237
C	2.99696	-1.32160	-0.36235
C	3.27664	0.03141	-0.02646
C	-1.51976	0.87343	0.79400
C	-1.20445	2.25086	0.37546
C	-0.15487	2.56545	-0.52845
C	-1.05648	-0.25071	-0.08224
Ir	1.07178	-0.21839	-0.25281
C	-1.16124	-0.17267	-1.57646
C	-1.61932	-1.56159	0.40069
O	-2.66503	-1.91789	-0.37422
C	-3.38394	-3.09286	0.02640
H	-2.68722	-3.93795	0.08194
H	-3.78173	-2.92810	1.03606
C	-4.47517	-3.30814	-0.98862
H	-5.06840	-4.19097	-0.73092
H	-5.14784	-2.44361	-1.02365
H	-4.05423	-3.45493	-1.98882
O	-1.25567	-2.22086	1.34307
O	-2.14134	0.63350	1.82506
O	0.68962	1.69170	-1.03217
C	-0.00395	3.91930	-0.90619
C	-2.01191	3.27493	0.89616
C	-0.82720	4.90294	-0.39354
C	-1.84174	4.59282	0.52115
H	0.79670	4.15511	-1.60414

Frequencies

-3.2624	30.9011	41.1962
49.8100	54.9799	77.4854
83.7871	90.9783	101.8549
107.8573	113.4427	130.1848
131.9783	138.5674	146.2573
158.3697	162.2239	163.9124
171.6015	183.5779	187.7323
202.1928	206.5915	212.0589
216.9844	225.7381	226.8177
229.6944	234.6424	240.5773
243.8695	255.6709	266.0056
277.7679	296.1136	309.7137
314.9145	321.5602	325.5705
335.4494	349.7292	365.7430
399.6732	408.4417	416.9391
433.2802	442.6348	468.1471
496.7604	533.0851	536.1650
542.3820	545.4528	547.5893
559.3550	586.8757	595.3164
599.1127	608.7745	623.8931
645.0310	679.9037	705.9054
752.0244	764.6313	776.6093
807.0633	816.9615	819.1283
845.3744	862.0359	871.9256
895.6918	942.4393	963.1345
965.6450	977.8945	981.3919
983.3002	1028.8193	1031.8263
1036.3906	1042.7346	1048.2853
1050.5520	1053.7978	1058.1000
1089.9332	1096.9599	1099.7734
1110.0977	1119.0887	1141.4555
1142.9273	1154.8950	1180.5615

H	-0.67590	5.93585	-0.70363	1185.4931	1190.3253	1239.3445
H	-2.48525	5.37207	0.92069	1264.1332	1282.5283	1284.4294
H	-2.79110	2.98011	1.59681	1295.9515	1346.3516	1377.8341
N	-5.07125	-0.20818	0.93171	1379.0590	1384.4334	1386.1464
N	-4.60799	0.55495	0.28019	1387.2406	1399.4215	1402.9102
C	1.71658	-3.32962	0.72923	1412.2856	1420.2843	1428.2829
H	2.45196	-3.92101	1.29105	1438.3208	1441.9803	1444.1298
H	0.74222	-3.43121	1.21735	1444.6394	1450.6653	1456.0541
H	1.63481	-3.76707	-0.27201	1460.4182	1461.6989	1466.3847
C	1.11505	-1.00915	2.90523	1471.0639	1474.3553	1480.5866
H	0.45667	-1.87936	2.88739	1481.3996	1490.0794	1490.4779
H	1.81030	-1.09143	3.75107	1498.4123	1505.0714	1511.2074
H	0.47602	-0.13481	3.07434	1522.1332	1524.5015	1548.5974
C	2.51423	1.64972	1.87901	1607.8262	1665.3486	1686.4398
H	1.58032	1.79191	2.43314	1744.8847	1862.8870	2463.9480
H	3.34937	1.72799	2.58742	3030.8723	3035.8973	3038.0066
H	2.59514	2.47168	1.15963	3039.1166	3042.5288	3046.3504
C	4.05615	1.03549	-0.80031	3047.3704	3053.6514	3103.9653
H	4.44307	0.61579	-1.73351	3106.1321	3115.5871	3116.4866
H	3.42288	1.89353	-1.06008	3118.0345	3122.4876	3134.5151
H	4.90917	1.40595	-0.21785	3137.2167	3139.0591	3141.5485
C	3.44044	-2.04687	-1.58376	3144.0410	3147.7755	3167.7626
H	3.85699	-1.36402	-2.32970	3170.8773	3177.3247	3182.6662
H	4.20456	-2.79506	-1.33733	3189.3963	3193.3876	3205.8679
H	2.59725	-2.57085	-2.04872			
O	-0.17246	-0.67365	-2.14392			
C	-2.28123	0.44282	-2.32751			
H	-2.32916	1.50933	-2.07024			
H	-2.13575	0.32656	-3.40355			
H	-3.22788	-0.00444	-2.00392			
C	0.42980	0.30815	2.30634			
C	2.65568	0.71500	2.91114			
H	2.32955	0.91778	3.93866			
H	2.92774	-0.34753	2.85725			
C	3.79449	1.59958	2.48075			
H	3.48375	2.65056	2.46660			
H	4.63320	1.49808	3.17760			
H	4.13091	1.31161	1.47927			
O	0.33368	-0.44917	3.26261			
O	1.55723	0.95591	2.02270			
C	-2.36009	0.68610	3.26416			
H	-3.44394	0.72569	3.39627			
H	-1.92099	0.01076	4.00591			
H	-1.91041	1.67249	3.43323			
O	-2.88701	-0.42384	1.23902			
H	5.67274	-0.47492	-2.32853			
C	0.63389	0.75102	-2.26539			
C	2.92715	1.58077	-1.45499			
C	4.85170	2.36254	-0.35019			
H	4.58554	3.41370	-0.51439			
H	5.46963	2.04686	-1.20246			
C	5.53081	2.13074	0.97347			
H	6.47248	2.68645	1.02514			
H	4.88756	2.45610	1.79667			
H	5.74242	1.06336	1.11047			
O	3.65827	1.57347	-0.34098			
O	3.14601	2.29349	-2.40703			
C	0.92000	0.94807	-3.71343			
H	-0.00533	0.88337	-4.29044			
H	1.41585	1.91119	-3.86642			
H	1.63737	0.18240	-4.03787			

O	-0.52197	0.63428	-1.87363

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.460596 Electronic Energy = -1482.18200732
Internal Energy (E)= -1481.68872032 Enthalpy (H)= -1481.68777632
Gibbs Free Energy (G)=-1481.78278232 Gibbs Free Energy of Solvation=-1481.82176301

St.Pt.	General Structure	Ball & Stick model
X-1		

Cartesian co-ordinate

Atoms	X	Y	Z
C	2.18086	0.65404	0.11708
C	1.73245	-0.64804	-0.07243
C	0.29976	-0.92573	-0.28908
C	-0.01102	1.51137	-0.05260
O	1.31156	1.71008	0.11127
C	2.66905	-1.68634	-0.06096
C	3.52630	0.94798	0.31835
C	4.00915	-1.41669	0.14141
C	4.43481	-0.09652	0.33025
H	2.29396	-2.69485	-0.21679
H	4.73480	-2.22540	0.15255
H	5.48931	0.11555	0.48808
H	3.82821	1.98171	0.46060
O	-0.09891	-2.05275	-0.53578
C	-0.55514	0.27030	-0.21547
C	-0.73005	2.81342	-0.02450
H	-0.91310	3.16220	-1.04649
H	-1.70870	2.72645	0.44898
H	-0.11616	3.55240	0.49615
C	-2.02783	0.16804	-0.38309
C	-3.92118	-1.17410	0.00774
H	-4.03251	-2.26097	0.05923
H	-4.23524	-0.82940	-0.98326
C	-4.69599	-0.47931	1.10071
H	-5.75940	-0.73125	1.03185

Frequencies

37.9986	48.2314	75.8867
103.5721	115.0127	147.3091
150.9988	189.1005	220.8960
246.5561	279.7456	283.2309
303.0066	356.9778	372.5615
394.6257	432.9286	454.4443
473.3339	531.9558	546.5059
570.0029	587.2556	641.4769
672.6953	689.6102	755.4528
771.0897	779.5322	815.0531
832.6464	865.6759	875.8972
895.1731	920.3047	969.3136
995.4173	1013.2063	1033.6783
1046.5480	1049.8593	1110.1776
1121.0776	1130.1934	1150.0932
1169.8403	1199.1676	1237.0822
1263.2154	1287.8048	1316.4388
1342.8258	1383.3937	1389.2153
1393.7019	1410.6278	1423.5423
1453.0925	1463.5896	1469.0155
1474.4836	1490.3486	1505.6250
1510.4655	1632.5950	1670.2560
1683.7480	1804.8843	1829.0885
3048.5348	3065.0908	3072.0439
3129.7466	3140.4830	3148.1541
3153.9869	3184.5310	3188.2735
3199.8711	3209.3918	3214.6747

H	-4.33388	-0.78827	2.08667
H	-4.59534	0.60639	1.01083
O	-2.71596	1.01341	-0.91882
O	-2.51158	-0.95136	0.15674

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.226940 Electronic Energy = -803.032983981
Internal Energy (E)= -802.791102981 Enthalpy (H)= -802.790158981
Gibbs Free Energy (G)=-802.848610981 Gibbs Free Energy of Solvation=-802.868080771

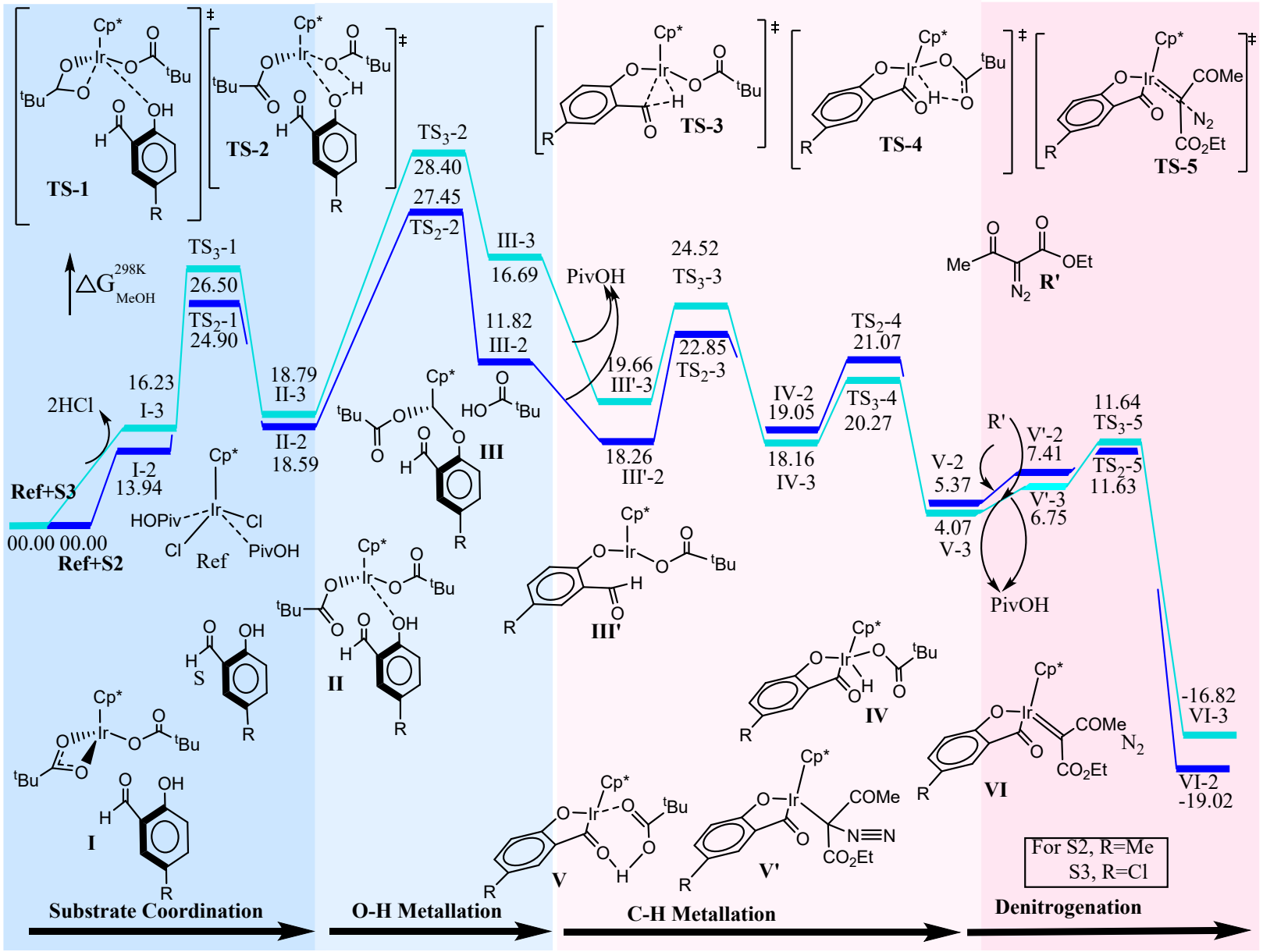


Fig-23: PES with Gibbs free energy (kcal/mol) and the structures of the stationary points of first part of path using M06 functional & 6-31G(d,p) basis set. (Blue colour for S2 and Cyan colour for S3)

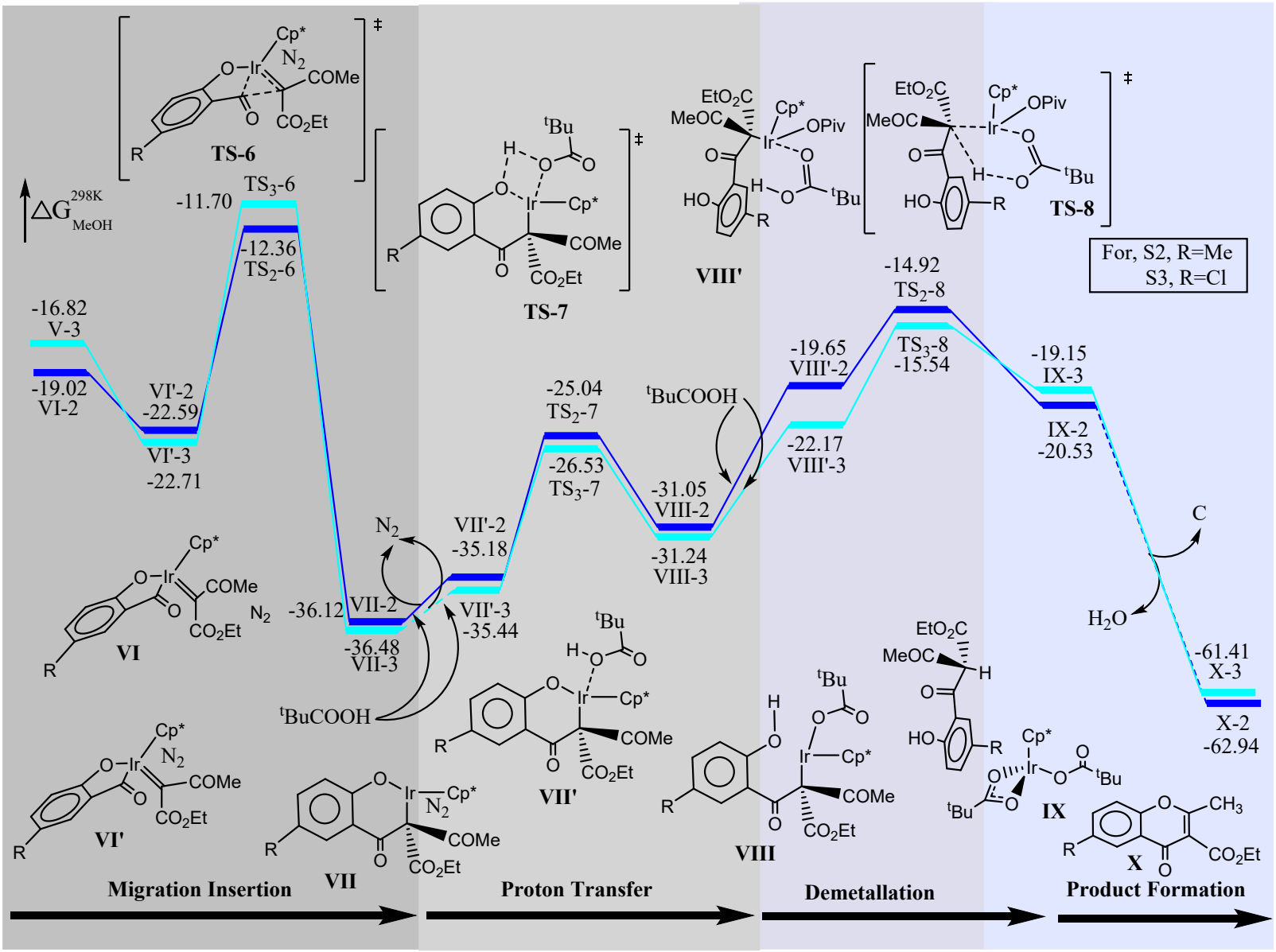


Fig-24: PES with Gibbs free energy (kcal/mol) and the structures of the stationary points of second part of path using M06 functional & 6-31G(d,p) basis set. (Blue colour for S2 and Cyan colour for S3)

St.Pt.	General Structure	Ball & Stick model
S2		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.74412	0.91750	0.00197
O	-1.97586	1.45792	0.00557
C	0.40559	1.70978	-0.00176
C	1.66443	1.13045	-0.00644
C	-0.60670	-0.48282	-0.00123
C	1.83244	-0.25734	-0.00620
C	0.68040	-1.03110	-0.00617
H	0.76764	-2.11933	-0.01031
H	2.54421	1.77331	-0.01143
C	-1.74270	-1.41903	-0.00240
H	-1.40587	-2.48746	-0.00793
O	-2.91893	-1.14166	0.00230
H	0.30321	2.79506	-0.00384
H	-1.89637	2.41890	0.00513
C	3.20078	-0.86978	0.00894
H	3.68644	-0.74817	0.98540
H	3.16032	-1.94259	-0.20467
H	3.85807	-0.40577	-0.73555

Frequencies

88.7026	90.7695	136.5505
178.7657	234.6471	294.2184
336.2679	404.2494	413.9829
442.1407	450.4665	483.3244
561.8327	678.6823	723.4892
773.3123	801.5432	813.2558
895.6303	948.7472	952.4873
1009.1335	1031.8652	1048.1981
1139.5954	1172.9430	1196.0046
1275.1611	1316.7237	1340.2348
1388.8169	1405.0965	1407.0189
1452.9394	1460.7630	1488.7854
1554.6250	1649.4619	1690.2023
1853.7158	2835.3976	3032.3839
3105.9166	3134.4365	3148.9724
3153.7792	3169.2156	3873.4890

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.141333 Electronic Energy = -459.812785569
Internal Energy (E)= -459.662145569 Enthalpy (H)= -459.661201569
Gibbs Free Energy (G)=-459.705891569 Gibbs Free Energy of Solvation=-459.726345099

St.Pt.	General Structure	Ball & Stick model
I-2		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.79049	-1.87133	1.44279
C	-3.00008	-1.12842	1.23026
C	-3.35709	-1.22950	-0.17927
C	-2.34274	-2.01628	-0.82545
C	-1.35465	-2.39772	0.16786
C	1.70147	-0.93977	-2.01470

Frequencies

32.8274	44.0822	46.8878
50.6867	59.5808	63.9435
70.8457	75.5617	77.4571
92.8067	108.6759	114.1719
121.5695	125.4847	127.5215
130.1970	149.9544	152.4790
160.5354	168.0781	172.1131
177.2777	180.2056	184.4690
192.6370	198.1712	204.4451
206.0411	210.2709	219.8118

C	-0.77566	3.32394	-1.75765	228.7057	237.3763	247.8371
C	-1.16724	1.99500	-1.14780	257.8937	278.1204	293.3390
O	-1.84345	1.91729	-0.08126	296.1885	305.0993	305.8648
O	-0.79806	0.90919	-1.70088	308.6895	313.9611	318.5751
C	-4.55430	-0.61243	-0.81350	325.7953	330.9405	334.4860
H	-4.73202	0.39393	-0.41826	344.7292	347.3635	353.3080
H	-4.42180	-0.51874	-1.89578	364.1810	379.0027	383.8972
H	-5.45535	-1.21248	-0.63314	387.4450	398.4144	408.3914
C	-2.23526	-2.31378	-2.27763	415.6726	416.5507	419.1613
H	-1.20098	-2.17683	-2.61530	423.4671	446.3722	447.9826
H	-2.53513	-3.34923	-2.48334	454.1137	464.9718	468.3689
H	-2.87278	-1.64820	-2.86765	471.6208	489.4044	534.3146
C	-0.15745	-3.26032	-0.03130	539.1896	547.3887	551.4913
H	0.11583	-3.35287	-1.08582	569.1252	571.1478	585.7038
H	0.71484	-2.83406	0.48113	593.6762	605.9216	620.9264
H	-0.33528	-4.26260	0.38159	643.7365	681.7600	731.7788
C	-1.09903	-2.09325	2.73950	777.3750	792.7453	794.8934
H	-0.01642	-2.17939	2.59142	801.8430	808.9608	813.5938
H	-1.27244	-1.26605	3.43145	818.4576	819.5007	832.2962
H	-1.45007	-3.03006	3.19270	921.8393	927.2809	936.4823
C	-3.71882	-0.35081	2.27469	947.5542	950.5959	951.8770
H	-4.42564	0.35509	1.82811	953.2742	959.8560	962.6654
H	-4.27778	-1.01686	2.94430	962.8281	965.9280	966.2267
H	-2.99670	0.22586	2.86410	994.3920	1014.3671	1037.6292
C	0.35640	0.93046	2.00414	1040.6545	1042.0437	1043.9978
O	0.36457	0.50219	0.77395	1047.4057	1049.1697	1049.9988
O	-0.61306	0.92590	2.75699	1051.6681	1054.9009	1064.6852
C	1.73232	1.42114	2.48103	1089.0666	1097.9043	1101.3427
O	1.07481	-1.86633	-2.49158	1123.4103	1136.5339	1170.0417
C	2.66463	0.20666	2.53477	1188.0454	1192.7879	1197.3489
H	2.76892	-0.26543	1.55005	1241.8755	1244.4531	1248.7148
H	3.66395	0.50803	2.88056	1258.0536	1266.0438	1268.8387
H	2.28020	-0.54255	3.24091	1276.2319	1314.6088	1333.3237
C	1.61175	2.03663	3.86904	1368.6542	1370.7931	1378.7516
H	2.59739	2.37262	4.21864	1379.7210	1385.7429	1386.6625
H	0.93368	2.89731	3.86238	1387.9675	1392.2904	1397.4997
H	1.21286	1.31349	4.58783	1403.5365	1405.4730	1407.6336
C	2.27843	2.45852	1.50258	1410.7559	1411.1726	1417.3994
H	1.60463	3.32383	1.42894	1429.0445	1440.0826	1443.6723
H	3.25773	2.82545	1.84163	1445.0357	1447.3390	1451.3645
H	2.39450	2.02899	0.50153	1453.6311	1458.3795	1459.4413
C	0.71216	3.25840	-2.10551	1460.9883	1464.3171	1464.8907
H	0.90596	2.49523	-2.86754	1465.9693	1467.2990	1469.1333
H	1.05348	4.22934	-2.48650	1473.8039	1476.4973	1479.4853
H	1.30179	3.00867	-1.21227	1481.9127	1483.7743	1486.5956
C	-1.03751	4.45781	-0.77444	1486.9689	1495.0965	1495.8158
H	-0.76380	5.41659	-1.23300	1500.2862	1500.9468	1514.7774
H	-2.09213	4.49762	-0.48325	1518.3745	1519.5779	1531.9339
H	-0.44703	4.33031	0.14091	1543.1137	1553.3783	1607.5698
C	-1.60226	3.52160	-3.03162	1651.3096	1688.8585	1759.4599
H	-2.67381	3.57546	-2.80206	1818.5676	2948.0205	3017.2050
H	-1.31337	4.46117	-3.51993	3019.3661	3021.8943	3026.7403
H	-1.43920	2.70039	-3.73850	3029.0145	3032.3174	3033.2607
Ir	-1.44326	-0.26168	0.04737	3035.7140	3036.3593	3036.8465
H	1.29480	0.09548	-2.04677	3038.1600	3038.4472	3092.7454
C	3.01327	-1.02596	-1.35397	3094.2294	3101.8719	3102.9131
C	3.65248	0.18498	-1.06554	3109.8681	3112.7410	3115.9442
C	3.65255	-2.22772	-0.99974	3117.5678	3120.5075	3122.9206
C	4.89480	0.25752	-0.44889	3124.2302	3124.7183	3127.1966
H	3.13604	1.10508	-1.34731	3132.1606	3133.8258	3139.7683
C	4.89795	-2.17232	-0.37060	3139.8882	3140.4656	3141.9366

C	5.50395	-0.95279	-0.10567	3145.4879	3145.8160	3146.9844
H	5.39514	-3.10154	-0.09048	3158.2515	3160.2013	3165.6918
H	6.47729	-0.93957	0.38435	3174.8353	3175.7875	3878.6548
O	3.04692	-3.40427	-1.26316			
H	3.61122	-4.12054	-0.95054			
C	5.54309	1.56920	-0.12368			
H	5.05900	2.39634	-0.65357			
H	5.47672	1.78890	0.95052			
H	6.60649	1.57246	-0.39013			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.642036 Electronic Energy = -1646.78541337
Internal Energy (E)= -1646.10327437 Enthalpy (H)= -1646.10233037
Gibbs Free Energy (G)=-1646.21173537 Gibbs Free Energy of Solvation=-1646.27282437

St.Pt.	General Structure	Ball & Stick model
TS_2-1		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-2.00866	-2.15024	0.99330
C	-2.96412	-1.05782	1.05612
C	-3.35005	-0.71860	-0.31012
C	-2.61216	-1.57454	-1.19180
C	-1.77341	-2.45583	-0.39721
C	1.48983	-0.19004	-1.78093
C	-1.04701	3.65484	-0.99516
C	-1.14627	2.15606	-0.74651
O	-1.25628	1.72714	0.45214
O	-1.08491	1.35101	-1.71134
C	-4.27522	0.38013	-0.70107
H	-4.17476	1.22889	-0.01460
H	-4.03737	0.74807	-1.70430
H	-5.32188	0.05178	-0.68862
C	-2.62221	-1.55176	-2.67783
H	-1.59768	-1.56725	-3.06222
H	-3.15404	-2.43073	-3.06496
H	-3.11041	-0.65367	-3.06492
C	-0.88729	-3.51905	-0.93999
H	-0.36039	-3.16694	-1.83164
H	-0.12307	-3.79919	-0.20816
H	-1.46561	-4.41756	-1.19437
C	-1.39506	-2.83055	2.16319
H	-0.43035	-3.27292	1.89385
H	-1.21477	-2.11315	2.96839
H	-2.05038	-3.63364	2.52496

Frequencies

-80.5794	31.1055	37.5201
46.7935	51.4437	56.4645
71.3185	73.2878	80.0201
88.5242	94.8622	99.1166
108.2751	113.7150	118.2644
124.6821	129.4564	137.7128
139.2622	145.7673	161.1876
167.5360	172.6564	182.6904
188.2761	192.4699	201.4401
204.9951	215.8837	221.4059
227.1958	235.5080	244.0365
250.6355	258.8619	276.1881
289.4308	295.9329	300.5170
306.7025	312.9173	314.1958
316.6977	320.1481	324.9112
340.3325	348.7062	350.4286
372.7895	376.3888	378.0736
380.6785	390.5767	397.7072
414.1373	415.2593	424.6208
444.5040	448.5136	451.2475
458.8080	462.9445	471.4981
492.7938	502.4728	535.7855
538.0073	547.5603	548.4835
566.6268	567.6853	580.3870
589.2438	602.6928	620.7711
630.9480	683.0279	726.8049
782.2038	788.5446	799.6128
801.2665	804.8925	812.1290
813.0342	814.3058	826.5037
905.6900	916.4357	926.8228

C	-3.45122	-0.41719	2.30419	944.9732	945.8068	946.2340
H	-3.90729	0.55556	2.09688	948.1354	954.1314	954.1895
H	-4.19957	-1.05131	2.79743	955.3949	963.9055	964.6495
H	-2.60796	-0.25401	2.98455	972.0886	1012.3225	1034.1741
C	0.63400	0.10778	2.25342	1037.2899	1037.9233	1039.4011
O	0.60788	-0.21814	0.99619	1045.0353	1047.5281	1048.3436
O	-0.29964	0.01690	3.04553	1052.9042	1056.0765	1056.4006
C	1.99460	0.68069	2.68285	1060.7663	1090.5299	1100.7357
O	0.57756	-0.96383	-2.00603	1114.6252	1141.7762	1171.6204
C	3.10740	-0.31556	2.35857	1184.3147	1186.8049	1198.2281
H	3.10482	-0.58199	1.29665	1240.0637	1241.9877	1249.9050
H	4.08744	0.11788	2.60535	1255.7347	1268.8960	1270.1012
H	2.99310	-1.23669	2.94520	1283.5865	1319.9027	1335.7185
C	1.98812	0.98706	4.17394	1359.2047	1369.8310	1372.0630
H	2.95988	1.39857	4.47921	1375.3681	1378.0820	1385.0766
H	1.20613	1.71166	4.42420	1385.9446	1387.0443	1389.7963
H	1.79338	0.08215	4.76046	1392.6750	1404.8504	1409.3466
C	2.20418	1.97251	1.88756	1410.5756	1411.5989	1412.3720
H	1.39112	2.68581	2.08173	1423.4097	1432.4474	1438.0375
H	3.15389	2.44899	2.17050	1445.1179	1450.3032	1452.1170
H	2.21745	1.76338	0.81139	1454.1056	1456.2389	1458.9267
C	0.41660	3.94219	-1.34710	1459.9464	1462.2409	1464.1965
H	0.71901	3.38222	-2.24063	1464.7949	1468.1670	1471.6413
H	0.55527	5.01311	-1.54510	1474.7592	1476.3956	1478.9283
H	1.08003	3.66219	-0.51707	1480.0211	1484.7178	1486.0839
C	-1.45119	4.45226	0.23842	1487.9560	1492.7453	1494.8455
H	-1.35903	5.52718	0.03457	1498.6984	1508.3126	1509.7294
H	-2.49041	4.24521	0.52098	1511.2020	1520.8136	1530.6592
H	-0.82073	4.20438	1.09869	1542.0546	1556.5141	1632.1084
C	-1.94175	4.01850	-2.17883	1654.5717	1687.4189	1763.0285
H	-2.99607	3.80827	-1.95413	1805.6592	2930.4824	3012.8384
H	-1.85289	5.08925	-2.40388	3014.5326	3023.8441	3025.2559
H	-1.66414	3.44546	-3.06909	3031.1363	3032.9823	3034.4650
Ir	-1.25225	-0.41200	0.01388	3036.3018	3038.9772	3040.1996
H	1.28795	0.90617	-1.75785	3041.5653	3047.5738	3092.2718
C	2.88640	-0.52604	-1.49257	3098.9150	3101.2539	3104.2013
C	3.74454	0.54318	-1.21932	3105.7795	3116.0317	3118.5321
C	3.39198	-1.83805	-1.40794	3118.6747	3121.3291	3123.3010
C	5.07210	0.37319	-0.84375	3126.5637	3129.8131	3133.6538
H	3.33203	1.55263	-1.28770	3134.5874	3137.5907	3138.5247
C	4.72584	-2.02441	-1.04767	3140.0579	3143.5104	3143.6653
C	5.54481	-0.93775	-0.76729	3147.5819	3154.8952	3156.8454
H	5.12415	-3.03725	-0.98164	3162.5433	3164.8886	3167.1410
H	6.57987	-1.11570	-0.47770	3169.6027	3178.5481	3881.5833
O	2.58043	-2.88018	-1.67914			
H	3.07796	-3.69761	-1.56233			
C	5.93073	1.54968	-0.48965			
H	5.84786	2.34880	-1.23522			
H	5.63061	1.97893	0.47571			
H	6.98652	1.26981	-0.41270			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.640755 Electronic Energy = -1646.77064733
Internal Energy (E)= -1646.09007233 Enthalpy (H)= -1646.08912833
Gibbs Free Energy (G)=-1646.19830333 Gibbs Free Energy of Solvation=-1646.26504489

St.Pt.	General Structure	Ball & Stick model
II-2		

Cartesian co-ordinate

Atoms	X	Y	Z
C	2.93737	-0.16624	-1.64517
C	3.35858	-0.16309	-0.25309
C	2.95835	-1.43605	0.32521
C	2.23836	-2.17541	-0.66351
C	2.22739	-1.38465	-1.89192
C	-1.80118	-0.38323	-0.37020
C	-0.51411	-0.27809	3.68493
C	0.04911	-0.79750	2.35145
O	0.37134	0.16404	1.53776
O	0.14896	-2.00052	2.12300
C	3.23906	-1.85784	1.72324
H	3.16975	-1.00345	2.40647
H	2.52329	-2.60820	2.06587
H	4.25580	-2.26544	1.79664
C	1.58546	-3.49871	-0.47062
H	0.79943	-3.65850	-1.21623
H	2.31312	-4.31543	-0.56224
H	1.11363	-3.54087	0.51648
C	1.57304	-1.79723	-3.16357
H	0.57187	-2.20260	-2.97704
H	1.46360	-0.94651	-3.84304
H	2.16265	-2.56869	-3.67565
C	3.16670	0.94287	-2.60872
H	2.42876	0.92223	-3.41726
H	3.08122	1.90796	-2.09943
H	4.16586	0.86128	-3.05621
C	4.19030	0.87766	0.40684
H	4.06350	0.84532	1.49390
H	5.25474	0.72276	0.18385
H	3.88355	1.87376	0.07699
C	0.71983	2.65655	-0.55648
O	0.21099	1.48448	-0.77217
O	1.90050	2.90580	-0.33100
C	-0.34121	3.77077	-0.54173
O	-0.82371	-1.00470	-0.78703
C	-1.36058	3.58315	-1.66220
H	-1.86189	2.61216	-1.58387
H	-2.12121	4.37455	-1.61556
H	-0.88219	3.63564	-2.64853
C	0.33068	5.13199	-0.66648
H	-0.42078	5.93148	-0.61641

Frequencies

22.0323	32.1274	39.4528
40.8556	60.1674	61.7328
68.3222	72.8057	82.9475
89.8233	93.3414	105.0037
107.9439	112.5423	118.1126
125.4836	128.9086	135.1163
143.2004	154.5909	155.7812
157.7503	164.2699	165.8336
181.1728	184.2137	196.5695
200.8893	208.2757	213.8923
220.1935	232.3942	245.0949
250.3332	266.0903	276.9570
283.3853	295.4009	301.3812
309.8292	312.8336	318.3613
321.6088	324.5719	330.2925
331.9048	335.1343	337.5864
343.6646	349.1861	364.0153
371.5298	392.1489	393.7815
398.4379	398.4829	425.4636
434.0087	439.4702	441.8486
447.4034	463.7733	467.3278
474.2544	498.6580	537.0105
539.9762	546.7779	568.4684
571.8327	575.4341	583.5711
589.2536	602.1135	633.0384
643.5388	684.3031	732.6294
785.8427	791.8630	797.5294
805.0551	806.7456	812.7436
817.0584	817.3008	818.3726
914.5045	916.8281	929.8480
946.5654	947.2621	949.8579
950.4183	952.6929	958.9531
961.4000	961.6793	971.8764
981.1507	1015.6971	1033.1472
1035.8771	1038.3929	1038.7641
1041.4863	1043.7423	1046.6352
1047.5000	1048.7828	1050.2428
1056.5075	1094.4949	1099.8646
1111.5353	1144.0796	1178.3719
1186.7800	1188.7405	1213.0406
1239.7613	1245.2511	1246.4392
1254.4070	1266.0805	1269.3199
1280.6136	1330.9154	1337.9647
1365.4765	1369.1817	1372.7024
1373.5003	1375.1144	1378.6013

H	1.06237	5.28301	0.13293	1388.7509	1390.4874	1394.2886
H	0.86419	5.22183	-1.62038	1394.8785	1397.3941	1400.8954
C	-1.04686	3.66579	0.81403	1406.3080	1413.9743	1420.2514
H	-0.32505	3.73425	1.63854	1420.9612	1430.9405	1434.0736
H	-1.78128	4.47460	0.92908	1439.1443	1442.3536	1442.7029
H	-1.57159	2.70574	0.90638	1449.7080	1452.6626	1454.1763
C	-1.80142	0.49963	3.40180	1458.3741	1461.1124	1462.6680
H	-2.54561	-0.14103	2.90631	1463.2481	1464.3007	1469.3042
H	-2.24444	0.85632	4.34148	1470.6774	1472.3771	1474.8836
H	-1.60647	1.37014	2.76352	1477.0625	1478.7169	1482.7978
C	0.51701	0.65015	4.32745	1483.5235	1484.3645	1489.9134
H	0.13497	1.04355	5.27929	1491.1351	1495.3252	1499.1092
H	1.44940	0.10953	4.54114	1506.7652	1511.4191	1522.3807
H	0.75436	1.49101	3.66745	1537.8209	1556.5210	1648.2187
C	-0.81410	-1.44691	4.61338	1690.6822	1741.5606	1761.3228
H	0.09135	-2.02920	4.81741	1768.7836	3010.4085	3018.1604
H	-1.21366	-1.07740	5.56741	3022.4323	3023.6486	3025.9438
H	-1.54548	-2.12978	4.16771	3031.9158	3032.7615	3035.5794
Ir	1.23465	-0.29161	-0.32023	3035.9746	3037.1405	3038.3095
H	-1.64368	0.47723	0.30469	3040.0527	3042.1947	3090.2460
C	-3.18164	-0.68887	-0.69599	3100.5827	3103.4481	3110.4748
C	-4.16135	0.14311	-0.13037	3113.4809	3113.9025	3119.1430
C	-3.58554	-1.74568	-1.53671	3120.2800	3121.1420	3121.3479
C	-5.51687	-0.03227	-0.36126	3122.6484	3122.9232	3125.3098
H	-3.82610	0.95771	0.51450	3125.3988	3134.3003	3136.0851
C	-4.94823	-1.93085	-1.77634	3139.5434	3143.6064	3144.5673
C	-5.88741	-1.09049	-1.19954	3144.6295	3147.6931	3150.5825
H	-5.26915	-2.74517	-2.42591	3160.5969	3165.6019	3170.8069
H	-6.94415	-1.25844	-1.40615	3173.6521	3177.0301	3875.9676
O	-2.65484	-2.54543	-2.08767			
H	-3.09511	-3.22033	-2.61740			
C	-6.55053	0.85833	0.25923			
H	-6.08738	1.70031	0.78297			
H	-7.23316	1.26832	-0.49438			
H	-7.16446	0.31377	0.98712			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.640416 Electronic Energy = -1646.78348091
Internal Energy (E)= -1646.10211691 Enthalpy (H)= -1646.10117291
Gibbs Free Energy (G)=-1646.21390991 Gibbs Free Energy of Solvation=-1646.27469087

St.Pt.	General Structure	Ball & Stick model
II'-2		

Cartesian co-ordinate

Atoms	X	Y	Z

Frequencies

20.0744	29.3744	48.9783
52.6922	62.6322	71.6485
78.6146	85.5435	102.7368
107.7594	114.3509	125.5434

C	1.07541	-2.50972	-0.88658	137.5374	141.3507	152.0275
C	2.16408	-1.55519	-1.06062	157.3046	166.6753	177.1511
C	2.65470	-1.19695	0.25299	179.8444	183.3429	189.2985
C	1.81580	-1.84120	1.23111	198.8367	202.6518	218.5455
C	0.85835	-2.67787	0.51405	224.1933	229.4175	238.6966
O	0.67989	1.43437	0.53690	280.7524	294.5548	302.8653
C	1.38755	2.27426	-0.19927	306.3899	312.5015	316.7158
O	2.13813	1.91024	-1.08898	327.2327	330.0313	340.5639
C	1.18928	3.73682	0.19267	342.6930	352.5477	367.7980
C	-2.54664	0.08291	0.75155	375.1420	388.3604	429.0263
H	-0.85922	0.99306	1.22641	441.3319	450.0821	456.9283
C	2.71527	-1.06440	-2.34918	462.0792	472.6599	477.9132
H	2.84379	0.02250	-2.30995	495.7418	534.7981	538.4697
H	3.68711	-1.53105	-2.55258	544.9586	548.9842	577.2898
H	2.04715	-1.29775	-3.18289	586.7001	592.4911	601.9791
C	3.78521	-0.27716	0.53094	637.5193	676.7225	710.5163
H	3.87506	0.48240	-0.25007	773.3995	786.2497	796.3614
H	3.65778	0.23583	1.48960	803.9118	806.6905	809.7328
H	4.71911	-0.85174	0.57871	819.7726	850.0496	899.6841
C	-0.18929	-3.50969	1.16078	919.1666	947.8313	952.8967
H	-1.00494	-3.74131	0.46951	955.9375	958.7364	961.7579
H	0.23680	-4.45885	1.50890	973.5327	985.7794	1018.4141
H	-0.61852	-3.00112	2.03075	1024.2622	1029.2953	1031.2102
C	0.30737	-3.13888	-1.99337	1032.6551	1036.1203	1038.1256
H	-0.65960	-3.51691	-1.64851	1038.8072	1043.8580	1052.7310
H	0.12130	-2.42189	-2.79980	1090.3894	1096.5326	1108.8513
H	0.86560	-3.98168	-2.41842	1144.1061	1188.3902	1190.4433
C	1.95768	-1.75961	2.70873	1194.9509	1214.4344	1243.4309
H	2.63386	-2.54230	3.07464	1253.9675	1260.2129	1264.2898
H	2.36443	-0.79261	3.01857	1283.7844	1322.4877	1354.7479
H	0.99326	-1.89016	3.20961	1380.1871	1382.1684	1382.5412
Ir	0.60056	-0.58205	0.00499	1390.7500	1392.2223	1395.4717
C	-0.30335	4.07428	0.17385	1398.4755	1400.7515	1407.6703
H	-0.86346	3.51021	0.92986	1414.9096	1417.5497	1425.4537
H	-0.44581	5.14078	0.38566	1430.2393	1435.5419	1440.1313
H	-0.74399	3.87244	-0.81186	1443.7317	1447.4253	1449.6929
C	1.75298	3.92933	1.60407	1453.9275	1454.0651	1458.4959
H	2.82018	3.67555	1.63827	1458.7608	1464.0258	1465.1863
H	1.65089	4.97862	1.90626	1467.8758	1472.0434	1479.0946
H	1.22681	3.30813	2.33735	1482.1434	1488.8749	1490.1399
C	1.93391	4.63060	-0.79117	1491.3450	1500.1058	1500.8804
H	3.00011	4.38526	-0.81748	1513.7199	1538.3110	1540.5318
H	1.54428	4.51486	-1.80855	1633.6164	1676.9223	1724.7848
H	1.82430	5.68099	-0.49631	1790.6153	3016.5070	3021.9587
O	-1.25880	0.08503	1.24264	3033.3123	3045.4698	3045.9283
C	-3.57816	-0.19333	1.63255	3047.0139	3047.5066	3048.2445
C	-4.89554	-0.15379	1.18898	3048.6332	3048.6642	3106.6949
C	-2.83035	0.36759	-0.59697	3119.4643	3124.6658	3126.9860
C	-5.22308	0.17116	-0.13367	3127.3685	3129.8269	3130.2849
C	-4.17484	0.42880	-1.00605	3131.8743	3134.1397	3136.8076
H	-4.39148	0.66502	-2.04837	3137.4037	3146.6617	3148.6777
H	-5.69775	-0.36435	1.89463	3150.2523	3153.0388	3153.4208
C	-1.83722	0.50188	-1.63822	3160.3408	3168.6466	3169.8228
H	-2.22486	0.84894	-2.61243	3183.2310	3209.6223	3399.4346
O	-0.63489	0.21949	-1.59393			
H	-3.33593	-0.41281	2.66891			
C	-6.65251	0.23771	-0.57334			
H	-6.73684	0.40222	-1.65116			
H	-7.18616	-0.68766	-0.33040			
H	-7.18090	1.05499	-0.06903			
H	-1.64368	0.47723	0.30469			

C	-3.18164	-0.68887	-0.69599
C	-4.16135	0.14311	-0.13037
C	-3.58554	-1.74568	-1.53671
C	-5.51687	-0.03227	-0.36126
H	-3.82610	0.95771	0.51450
C	-4.94823	-1.93085	-1.77634
C	-5.88741	-1.09049	-1.19954
H	-5.26915	-2.74517	-2.42591
H	-6.94415	-1.25844	-1.40615
O	-2.65484	-2.54543	-2.08767
H	-3.09511	-3.22033	-2.61740
C	-6.55053	0.85833	0.25923
H	-6.08738	1.70031	0.78297
H	-7.23316	1.26832	-0.49438
H	-7.16446	0.31377	0.98712

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.503387 Electronic Energy = -1300.34761965
Internal Energy (E)= -1299.81216465 Enthalpy (H)= -1299.81122065
Gibbs Free Energy (G)=-1299.90620465 Gibbs Free Energy of Solvation=-1300.00827188

St.Pt.	General Structure	Ball & Stick model
TS_2-2		

Cartesian co-ordinate

Atoms	X	Y	Z
C	2.09476	-2.21342	-0.44385
C	2.79322	-0.95652	-0.48180
C	2.63679	-0.31688	0.81735
C	1.81945	-1.16252	1.63278
C	1.45441	-2.33420	0.84908
O	0.01464	1.45217	-0.73069
C	0.81120	2.55954	-0.79654
O	1.86921	2.49453	-1.36742
C	0.26584	3.77352	-0.06223
C	-2.41889	-0.03937	0.55323
H	-0.65725	1.35174	0.09375
C	3.57748	-0.39586	-1.61058
H	3.35924	0.66938	-1.74089
H	4.65131	-0.51016	-1.41489
H	3.34976	-0.90531	-2.55054
C	3.28368	0.95877	1.21494
H	3.32268	1.66397	0.37880
H	2.76479	1.43720	2.05152
H	4.31498	0.76075	1.53408
C	0.65028	-3.48553	1.33558
H	0.14165	-3.99644	0.51262
H	1.29498	-4.21788	1.83739

Frequencies

-362.0498	21.4204	35.3869
40.6666	52.6371	67.1309
80.2105	96.2371	97.3259
111.1473	122.7926	136.6811
138.4154	143.4812	145.4917
150.5693	159.3508	166.8609
170.1808	179.1166	181.9617
186.4033	200.8321	204.2169
218.7593	234.3215	238.4722
256.0662	293.9181	304.0441
310.3046	318.6636	323.5773
333.2830	336.0501	341.2307
354.7297	356.6942	377.7848
384.5587	395.7571	417.0617
440.7783	442.3606	452.8198
455.5628	468.4793	496.4780
503.3173	526.2445	536.4479
537.7877	547.5708	551.3181
574.8783	586.5201	593.4361
602.3305	671.3168	710.2198
743.7231	779.3790	787.5559
807.8553	810.5527	810.8972
842.4425	844.3937	886.7042
932.1789	942.5759	953.1740
958.1045	959.8956	961.7482
968.7862	981.6419	1014.4481

H	-0.11107	-3.16294	2.05267	1017.0646	1024.9141	1025.9419
C	1.97121	-3.18103	-1.56222	1029.3631	1034.6111	1035.2089
H	0.98721	-3.65928	-1.56678	1038.9246	1043.0226	1051.3503
H	2.10544	-2.69057	-2.53047	1091.4576	1093.8050	1106.7360
H	2.73119	-3.96589	-1.46778	1149.3742	1163.3818	1188.5202
C	1.35192	-0.88809	3.01518	1190.7855	1196.4029	1227.1158
H	1.92617	-1.48160	3.73711	1237.4820	1258.7432	1264.8053
H	1.46653	0.16767	3.27690	1273.0838	1305.9001	1348.6984
H	0.29392	-1.14643	3.12724	1379.6053	1379.9915	1385.7939
Ir	0.69034	-0.60795	-0.12215	1393.7695	1394.3708	1396.1457
C	-1.22987	3.96520	-0.32502	1398.4856	1402.4121	1407.2323
H	-1.84681	3.15670	0.08785	1421.5851	1430.3307	1431.1474
H	-1.55963	4.89455	0.15308	1431.8815	1434.9915	1435.4685
H	-1.44343	4.04726	-1.39668	1440.8070	1445.1771	1449.6439
C	0.50894	3.51741	1.43460	1453.3344	1453.5912	1456.4710
H	1.58269	3.43933	1.64806	1458.6930	1460.2161	1465.2079
H	0.11319	4.35857	2.01536	1467.0084	1476.4050	1480.5286
H	0.01021	2.60482	1.79222	1484.5757	1485.3580	1491.0980
C	1.04046	5.00868	-0.50631	1492.4184	1500.5462	1505.1574
H	2.11524	4.88453	-0.34277	1514.4514	1521.1503	1533.9341
H	0.88590	5.21150	-1.57154	1595.7999	1678.6793	1691.1015
H	0.70007	5.88163	0.06191	1874.6613	2292.7195	3028.6554
O	-1.17010	0.27428	0.85934	3033.8991	3037.0970	3042.8261
C	-3.43448	0.29957	1.46363	3048.2967	3048.9570	3049.5228
C	-4.76179	0.07301	1.16274	3049.9681	3051.2023	3052.8168
C	-2.80685	-0.64731	-0.67462	3115.7008	3118.9106	3122.0491
C	-5.17312	-0.51005	-0.05461	3131.6250	3133.6477	3135.1196
C	-4.18410	-0.85696	-0.94617	3135.8692	3136.1475	3136.5591
H	-4.45652	-1.31840	-1.89624	3137.9357	3141.0361	3145.2468
H	-5.52368	0.35709	1.88837	3150.2630	3153.0932	3156.5636
C	-1.89881	-1.11872	-1.66286	3162.6512	3163.7149	3166.3630
H	-2.36631	-1.51758	-2.57836	3169.6104	3174.7412	3210.5571
O	-0.64903	-1.18935	-1.64283			
H	-3.13843	0.75978	2.40284			
C	-6.62587	-0.73702	-0.33754			
H	-6.77798	-1.17731	-1.32736			
H	-7.07448	-1.41206	0.40063			
H	-7.19081	0.20154	-0.29864			
H	-1.64368	0.47723	0.30469			
C	-3.18164	-0.68887	-0.69599			
C	-4.16135	0.14311	-0.13037			
C	-3.58554	-1.74568	-1.53671			
C	-5.51687	-0.03227	-0.36126			
H	-3.82610	0.95771	0.51450			
C	-4.94823	-1.93085	-1.77634			
C	-5.88741	-1.09049	-1.19954			
H	-5.26915	-2.74517	-2.42591			
H	-6.94415	-1.25844	-1.40615			
O	-2.65484	-2.54543	-2.08767			
H	-3.09511	-3.22033	-2.61740			
C	-6.55053	0.85833	0.25923			
H	-6.08738	1.70031	0.78297			
H	-7.23316	1.26832	-0.49438			
H	-7.16446	0.31377	0.98712			

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm

Zero-point correction= 0.500279	Electronic Energy = -1300.34507399
Internal Energy (E)= -1299.81340599	Enthalpy (H)= -1299.81246199
Gibbs Free Energy (G)=-1299.90555599	Gibbs Free Energy of Solvation=-1300.00601288

St.Pt.	General Structure	Ball & Stick model
III-2		

Cartesian co-ordinate

Atoms	X	Y	Z
C	2.99610	-0.95551	-0.65053
C	2.90939	0.46371	-0.54675
C	2.51983	0.80131	0.82091
C	2.36917	-0.41338	1.55644
C	2.62683	-1.51852	0.64130
O	-0.64497	1.33156	-1.19869
C	-0.59052	2.63581	-0.78699
O	0.42400	3.25514	-0.97246
C	-1.79987	3.15813	-0.02536
C	-1.92292	-0.97692	0.65615
H	-1.53615	0.97579	-1.04762
C	3.15896	1.46222	-1.61535
H	2.35361	2.20370	-1.64524
H	4.10033	1.99086	-1.41761
H	3.23730	0.99282	-2.59915
C	2.37532	2.18153	1.34695
H	1.99789	2.86282	0.57881
H	1.69546	2.21928	2.20416
H	3.35277	2.55401	1.68002
C	2.62936	-2.96051	0.99245
H	2.31751	-3.57786	0.14465
H	3.64172	-3.27314	1.27954
H	1.96251	-3.17247	1.83300
C	3.33900	-1.74204	-1.86400
H	2.77994	-2.68236	-1.89935
H	3.10494	-1.18726	-2.77716
H	4.40843	-1.98406	-1.87669
C	1.95011	-0.55243	2.97447
H	2.81659	-0.75595	3.61495
H	1.46525	0.35869	3.33655
H	1.23549	-1.37312	3.09382
Ir	0.96468	-0.44048	-0.08055
C	-3.10755	2.47837	-0.43650
H	-3.15874	1.41638	-0.14661
H	-3.94110	2.96387	0.08273
H	-3.29856	2.56949	-1.51285
C	-1.49026	2.86582	1.45341
H	-0.59738	3.41889	1.77028
H	-2.33227	3.19483	2.07394
H	-1.32182	1.79450	1.63680
C	-1.90609	4.66409	-0.24735

Frequencies

28.7520	35.0146	51.0168
66.5888	71.9024	75.9666
90.7762	95.7351	101.4807
106.3216	109.6986	117.5751
136.7290	151.8083	158.2183
161.9706	166.6370	173.5018
176.3756	185.6614	192.2451
203.4382	208.4540	223.0905
224.5632	227.6590	232.6044
265.1380	286.2284	294.9332
306.7000	318.4625	325.9135
328.3058	336.7801	341.4133
346.5925	360.9797	377.6926
383.6695	402.0374	412.1100
433.0141	445.5681	456.8121
460.8979	478.1401	501.3771
512.9497	532.8457	537.0918
546.2883	553.0144	575.2198
582.5593	583.8141	588.6452
602.0324	625.6015	688.8966
749.8784	763.8857	771.9885
792.8185	806.3590	810.6673
835.3090	849.6731	879.1423
890.2191	944.9115	952.1311
953.4254	956.6883	963.4347
965.1254	996.0614	1009.0669
1018.9310	1026.1181	1030.8219
1031.7709	1033.1647	1036.2555
1041.3103	1043.7804	1052.0602
1089.6795	1093.9575	1105.2209
1138.4852	1157.4512	1188.0537
1189.6740	1201.1760	1227.4456
1255.9122	1260.8524	1264.5671
1270.1239	1340.3850	1356.8682
1377.7797	1380.9501	1387.0292
1390.8569	1392.5368	1396.2896
1399.9662	1402.5276	1406.4068
1420.3064	1430.0598	1431.6869
1434.0298	1435.3125	1435.6372
1441.3690	1447.6014	1451.3827
1454.6129	1456.8813	1458.0225
1459.0950	1464.4176	1465.4895
1467.9705	1472.9151	1478.1279
1482.7313	1487.3510	1490.0863
1492.0778	1496.9600	1504.2316

H	-0.96802	5.16603	0.00484	1510.8319	1523.9655	1545.6437
H	-2.14544	4.89797	-1.29095	1585.5673	1665.2137	1700.4664
H	-2.70220	5.07320	0.38467	1892.8109	3018.5984	3026.8101
O	-0.75507	-0.53374	1.02496	3037.9010	3041.8596	3046.2860
C	-2.98805	-0.87680	1.58441	3046.8508	3048.7798	3050.0376
C	-4.25741	-1.28377	1.25329	3050.2808	3051.4057	3103.4757
C	-2.22216	-1.54515	-0.62415	3117.0072	3119.4060	3121.9634
C	-4.57747	-1.83581	-0.01363	3129.4289	3129.6920	3133.7874
C	-3.55243	-1.96437	-0.91500	3134.3920	3135.5036	3136.2650
H	-3.74736	-2.40195	-1.89495	3136.6708	3143.1433	3145.7203
H	-5.05306	-1.18230	1.99123	3153.0624	3155.1012	3158.0334
C	-1.23906	-1.79404	-1.61209	3161.8101	3163.6095	3168.1279
H	-1.57538	-2.34109	-2.50689	3168.8011	3208.1610	3768.2502
O	-0.02241	-1.47831	-1.60611			
H	-2.76123	-0.45782	2.56170			
C	-5.97968	-2.26199	-0.31783			
H	-6.06048	-2.69363	-1.31970			
H	-6.33164	-3.01280	0.39931			
H	-6.67522	-1.41624	-0.26110			
H	-1.64368	0.47723	0.30469			
C	-3.18164	-0.68887	-0.69599			
C	-4.16135	0.14311	-0.13037			
C	-3.58554	-1.74568	-1.53671			
C	-5.51687	-0.03227	-0.36126			
H	-3.82610	0.95771	0.51450			
C	-4.94823	-1.93085	-1.77634			
C	-5.88741	-1.09049	-1.19954			
H	-5.26915	-2.74517	-2.42591			
H	-6.94415	-1.25844	-1.40615			
O	-2.65484	-2.54543	-2.08767			
H	-3.09511	-3.22033	-2.61740			
C	-6.55053	0.85833	0.25923			
H	-6.08738	1.70031	0.78297			
H	-7.23316	1.26832	-0.49438			
H	-7.16446	0.31377	0.98712			

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.503789 Electronic Energy = -1300.35898633
Internal Energy (E)= -1299.82321433 Enthalpy (H)= -1299.82227033
Gibbs Free Energy (G)=-1299.91608533 Gibbs Free Energy of Solvation=-1300.01818946

St.Pt.	General Structure	Ball & Stick model
III'-2		

Cartesian co-ordinate

Atoms	X	Y	Z

Frequencies

20.8743	36.1718	44.3079
47.6848	63.9882	67.0506
79.9820	90.4817	92.2496
113.1737	125.3191	149.8214

C	0.94547	-2.45196	-0.99208
C	2.05626	-2.05241	-0.18930
C	1.59269	-1.94406	1.18726
C	0.19643	-2.36571	1.21717
C	-0.20697	-2.66424	-0.12095
C	-2.45610	0.50672	-0.50993
Ir	0.47397	-0.57801	0.03275
C	-3.82401	0.64282	-0.82186
C	-4.71718	1.18300	0.07687
C	-1.95905	0.88682	0.76557
C	-4.20761	1.60165	1.32812
C	-2.88248	1.46690	1.67007
H	-2.50883	1.78189	2.64147
H	-4.89827	2.04102	2.04948
H	-0.43908	0.40334	-1.36662
O	1.77945	1.02348	0.04602
C	1.45764	2.15106	-0.53232
C	2.37162	3.31420	-0.13054
O	0.50104	2.31687	-1.27657
H	-4.15193	0.31877	-1.80945
C	-1.54004	0.02008	-1.51152
O	-1.78851	-0.56435	-2.54891
O	-0.72477	0.70120	1.14704
C	2.28163	4.42125	-1.17390
H	1.24516	4.74222	-1.31318
H	2.88281	5.28470	-0.85985
H	2.65554	4.08001	-2.14696
C	1.82634	3.81958	1.21009
H	1.87639	3.03512	1.97451
H	2.41062	4.68319	1.55492
H	0.77865	4.12873	1.10815
C	3.82109	2.86553	0.03504
H	4.21729	2.44781	-0.89998
H	4.44824	3.72411	0.31014
H	3.91896	2.10357	0.81561
C	3.42668	-1.68772	-0.63880
H	3.67014	-0.66499	-0.32402
H	4.17131	-2.37004	-0.21064
H	3.51432	-1.72869	-1.72805
C	0.90847	-2.60748	-2.47069
H	1.81263	-2.20505	-2.93623
H	0.82317	-3.66654	-2.74573
H	0.04583	-2.07432	-2.89203
C	-1.53163	-3.17730	-0.56468
H	-1.76137	-2.85108	-1.58377
H	-1.54202	-4.27468	-0.54494
H	-2.33879	-2.81985	0.08320
C	-0.67490	-2.37729	2.42182
H	-1.72341	-2.21912	2.14898
H	-0.59639	-3.33307	2.95435
H	-0.39746	-1.57278	3.11006
C	2.44522	-1.56857	2.34608
H	1.84101	-1.25275	3.20163
H	3.07029	-2.41382	2.66310
H	3.10508	-0.73525	2.08106
C	-6.17403	1.34094	-0.23960
H	-6.48461	2.39302	-0.20383
H	-6.40545	0.96223	-1.24058
H	-6.80646	0.79859	0.47520
H	-6.67522	-1.41624	-0.26110
H	-1.64368	0.47723	0.30469

154.8496	164.0287	164.5216
168.8445	173.1781	179.6150
184.9250	193.7839	200.3294
209.9459	216.2697	218.8683
231.9153	237.2907	242.0462
267.7984	275.1406	284.5779
300.6006	304.5714	306.5550
316.8299	319.9498	324.7481
335.2879	352.2321	374.2323
391.0362	417.5441	423.9420
428.0465	440.0530	458.9242
468.2371	489.4322	536.0787
537.7189	540.1136	546.1405
572.2011	581.5471	591.9960
598.1530	605.8361	620.0171
640.8497	652.1550	736.2677
748.5215	789.7600	804.3741
812.7607	818.4612	834.8409
854.7165	898.9977	916.6834
945.3512	947.9682	948.6062
953.8351	960.0831	961.1766
971.6386	1018.1598	1034.9495
1039.4973	1040.3402	1043.5933
1045.0682	1046.6080	1047.6081
1048.0619	1070.7354	1090.0084
1095.7679	1105.4089	1140.5566
1155.2739	1182.5137	1188.3190
1226.6426	1236.3836	1244.4448
1265.7616	1273.0211	1339.6517
1356.5476	1372.2535	1376.0558
1380.3681	1385.9043	1394.2141
1397.6893	1400.9673	1403.3976
1404.2504	1410.5079	1437.2345
1437.7636	1440.7821	1446.3584
1448.7346	1449.3656	1452.8424
1455.0735	1456.9448	1459.1743
1459.7167	1460.6334	1461.4882
1465.7028	1466.0242	1471.2348
1474.4522	1477.4749	1479.1846
1487.3490	1490.1864	1497.0417
1502.3137	1521.0106	1535.7105
1543.5895	1598.0972	1690.6112
1781.9205	1802.1037	2313.9836
3023.4477	3025.8069	3028.6461
3034.0012	3034.3448	3036.1109
3036.7592	3042.8174	3044.5407
3097.8482	3104.0850	3113.3693
3113.6802	3114.9323	3115.3702
3121.2059	3125.8039	3129.2267
3129.8175	3133.5272	3133.9335
3145.1210	3147.6164	3147.9698
3150.1098	3150.9078	3152.2181
3153.7427	3178.6554	3200.1775

C	-3.18164	-0.68887	-0.69599
C	-4.16135	0.14311	-0.13037
C	-3.58554	-1.74568	-1.53671
C	-5.51687	-0.03227	-0.36126
H	-3.82610	0.95771	0.51450
C	-4.94823	-1.93085	-1.77634
C	-5.88741	-1.09049	-1.19954
H	-5.26915	-2.74517	-2.42591
H	-6.94415	-1.25844	-1.40615
O	-2.65484	-2.54543	-2.08767
H	-3.09511	-3.22033	-2.61740
C	-6.55053	0.85833	0.25923
H	-6.08738	1.70031	0.78297
H	-7.23316	1.26832	-0.49438
H	-7.16446	0.31377	0.98712

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.489734 Electronic Energy = -1299.93516804
Internal Energy (E)= -1299.41379904 Enthalpy (H)= -1299.41285504
Gibbs Free Energy (G)=-1299.50667604 Gibbs Free Energy of Solvation=-1300.03259846

St.Pt.	General Structure	Ball & Stick model
TS_2-3		

Cartesian co-ordinate

Atoms	X	Y	Z
C	1.40542	-2.33034	-0.92083
C	2.40954	-1.55852	-0.26022
C	2.07481	-1.48963	1.15753
C	0.87179	-2.23790	1.35700
C	0.42557	-2.72439	0.07727
C	-2.43510	-0.03479	-0.38781
Ir	0.48988	-0.50870	-0.03325
C	-3.78367	-0.06471	-0.78677
C	-4.76278	0.50775	-0.00179
C	-2.04204	0.56052	0.82777
C	-4.35878	1.12100	1.20643
C	-3.04629	1.15721	1.62280
H	-2.75486	1.63079	2.55703
H	-5.12335	1.58254	1.83302
H	-0.25198	0.29690	-1.31922
O	1.45845	1.32684	0.02137
C	0.92529	2.34139	-0.60186
C	1.53290	3.68358	-0.18139
O	-0.00919	2.27795	-1.39168
H	-4.03116	-0.54132	-1.73464

Frequencies

-294.0967	-157.4336	-23.5044
24.3028	34.3561	37.7231
52.0164	64.7373	72.9212
83.9380	86.1907	110.2838
122.1226	132.6960	148.1008
153.7445	159.5093	165.1175
168.0953	175.3686	178.1913
186.4847	199.7208	209.4055
226.8833	233.1996	240.6859
251.9471	262.6682	275.3826
283.0458	291.0584	306.9004
316.2256	322.3645	327.4276
329.4522	344.4112	363.9224
378.4826	392.2229	406.9199
424.9169	428.3031	442.0907
468.5854	484.7403	496.2889
537.1604	538.9788	541.6607
545.9409	570.7651	586.4351
592.0648	603.5996	639.6059
644.1499	656.0810	710.0559
747.2654	776.4834	792.2833
806.3319	812.4465	821.4745
827.2856	856.8537	874.1113
898.3447	921.9208	946.4469

C	-1.38887	-0.60637	-1.20943
O	-1.51608	-1.27663	-2.21074
O	-0.79464	0.54127	1.21509
C	1.25699	4.73572	-1.24817
H	0.18491	4.81866	-1.44903
H	1.63300	5.71239	-0.91616
H	1.75276	4.48196	-2.19305
C	0.81430	4.05810	1.12065
H	0.96898	3.28974	1.88754
H	1.19233	5.01706	1.49948
H	-0.26541	4.15475	0.95097
C	3.03416	3.56856	0.06741
H	3.56288	3.23820	-0.83643
H	3.44106	4.54700	0.35497
H	3.25276	2.85526	0.86914
C	3.59972	-0.90227	-0.86410
H	3.64520	0.15160	-0.56309
H	4.52340	-1.39490	-0.53472
H	3.56337	-0.93536	-1.95656
C	1.35371	-2.70176	-2.36003
H	2.13542	-2.19253	-2.93097
H	1.49330	-3.78347	-2.48103
H	0.38508	-2.42772	-2.79081
C	-0.74163	-3.61540	-0.16840
H	-1.15393	-3.45391	-1.16909
H	-0.44582	-4.66919	-0.08336
H	-1.54442	-3.43130	0.55409
C	0.12561	-2.38256	2.63422
H	-0.95530	-2.34767	2.45975
H	0.36150	-3.33853	3.11811
H	0.36935	-1.57372	3.32901
C	2.88996	-0.78024	2.18137
H	2.37059	-0.72824	3.14263
H	3.84850	-1.29015	2.34299
H	3.10156	0.24738	1.86353
C	-6.20942	0.49709	-0.39684
H	-6.60944	1.51413	-0.49788
H	-6.35548	-0.01148	-1.35548
H	-6.83059	-0.01641	0.34851
H	-6.67522	-1.41624	-0.26110
H	-1.64368	0.47723	0.30469
C	-3.18164	-0.68887	-0.69599
C	-4.16135	0.14311	-0.13037
C	-3.58554	-1.74568	-1.53671
C	-5.51687	-0.03227	-0.36126
H	-3.82610	0.95771	0.51450
C	-4.94823	-1.93085	-1.77634
C	-5.88741	-1.09049	-1.19954
H	-5.26915	-2.74517	-2.42591
H	-6.94415	-1.25844	-1.40615
O	-2.65484	-2.54543	-2.08767
H	-3.09511	-3.22033	-2.61740
C	-6.55053	0.85833	0.25923
H	-6.08738	1.70031	0.78297
H	-7.23316	1.26832	-0.49438
H	-7.16446	0.31377	0.98712

949.8508	951.0237	951.8244
954.1959	955.0078	962.0621
1018.6285	1019.4390	1036.6081
1037.9559	1041.6903	1042.9361
1045.4963	1048.9553	1049.2705
1083.7842	1090.2266	1104.4257
1140.0005	1152.4769	1182.7533
1184.6800	1231.0569	1236.5242
1247.0283	1266.9531	1267.9520
1349.2905	1355.6571	1370.2225
1373.8534	1377.8300	1385.8162
1388.0422	1394.6357	1395.4155
1399.5291	1412.5238	1414.5292
1421.7909	1430.7450	1435.3070
1441.8250	1442.4888	1447.0329
1448.7227	1450.8792	1455.1644
1457.9718	1459.8883	1461.3699
1461.5073	1464.4455	1466.9242
1469.2491	1476.8177	1478.3286
1482.8370	1483.9854	1502.6157
1505.2559	1517.1431	1540.7435
1545.6251	1611.2043	1685.9846
1738.5370	1784.2964	1853.1230
3024.1354	3026.5837	3028.7787
3034.4759	3035.9270	3037.5681
3038.3663	3043.1388	3044.2971
3098.7483	3106.7248	3112.4120
3115.4323	3116.9278	3117.0769
3119.1089	3126.0212	3127.6274
3131.1084	3131.1755	3132.4582
3142.8337	3144.7485	3148.1751
3150.1392	3152.8155	3156.6724
3160.5396	3185.0414	3204.2085

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.484330 Electronic Energy = -1299.92992170
Internal Energy (E)= -1299.4152707 Enthalpy (H)= -1299.4143267
Gibbs Free Energy (G)=-1299.5055027 Gibbs Free Energy of Solvation=-1299.54698466

St.Pt.	General Structure	Ball & Stick model
IV-2		

Cartesian co-ordinate

Atoms	X	Y	Z
C	0.48616	-2.42881	-0.99962
C	1.79338	-1.94247	-0.60703
C	1.89949	-2.01764	0.84302
C	0.65288	-2.39904	1.34589
C	-0.26610	-2.58658	0.21416
C	-2.45745	0.59484	-0.41766
Ir	0.22849	-0.47609	-0.07155
C	-3.68287	1.02610	-0.94469
C	-4.69222	1.46352	-0.10541
C	-2.21848	0.58594	0.96513
C	-4.44354	1.44848	1.28241
C	-3.24525	1.02309	1.82292
H	-3.07199	1.02141	2.89621
H	-5.23266	1.78903	1.95432
H	0.86626	0.08919	-1.41969
O	1.14248	1.32227	0.42704
C	1.93258	1.89765	-0.43215
C	2.63571	3.13681	0.13612
O	2.15428	1.49702	-1.57375
H	-3.81652	1.00983	-2.02575
C	-1.36808	0.08952	-1.25688
O	-1.42102	-0.05977	-2.45566
O	-1.05716	0.16435	1.42006
C	-1.66368	-3.08617	0.35044
H	-2.22835	-2.95241	-0.57754
H	-1.67650	-4.15351	0.60725
H	-2.19669	-2.54269	1.13905
C	0.05713	-2.74098	-2.39040
H	0.63908	-3.58340	-2.78381
H	-1.00201	-3.00967	-2.42762
H	0.18286	-1.87675	-3.05152
C	2.94018	-1.68661	-1.52212
H	3.60926	-2.55712	-1.54282
H	2.59517	-1.48971	-2.54123
H	3.51838	-0.81223	-1.20515
C	3.10547	-1.58359	1.59752
H	3.98795	-2.16627	1.30530
H	3.32673	-0.52739	1.39047
H	2.96983	-1.68718	2.67748

Frequencies

21.2937	32.3270	42.8059
52.0702	55.8794	58.8492
75.8436	87.3001	107.8969
128.7963	141.7687	151.4943
153.4986	159.9386	167.7156
174.0369	176.1886	189.6062
199.2984	203.3613	204.2115
210.0928	228.8006	231.7042
240.0091	244.4557	249.4648
263.7687	283.7635	286.2598
298.4475	300.2695	307.7079
326.6997	333.0884	341.5149
355.5344	360.1810	367.2513
382.4206	393.2485	427.1399
430.3871	439.6826	447.4083
477.5140	496.7275	533.1986
535.8731	541.3435	554.2847
570.9459	594.0899	615.9479
621.2859	633.7856	646.3130
650.6313	672.0044	745.3643
758.2441	791.0474	810.6475
812.9480	814.3231	827.0599
830.7871	871.3385	907.5498
914.4166	946.7919	949.3935
952.6642	953.8713	957.0205
959.2673	959.9278	973.8831
1015.4206	1027.4851	1039.0159
1041.0564	1042.3290	1048.5976
1049.5352	1050.7182	1056.6072
1087.6972	1090.3792	1107.4411
1134.6101	1146.5920	1176.7224
1189.1535	1225.7541	1241.8206
1249.0729	1267.7240	1269.0371
1336.6147	1360.1194	1366.4375
1375.7186	1376.6937	1390.5829
1391.4998	1393.2056	1396.7510
1397.7269	1404.3158	1413.9921
1429.2545	1434.9922	1440.2814
1446.8468	1448.0842	1450.3653
1452.1310	1453.6590	1454.8332
1458.8312	1462.0642	1462.2409
1462.8044	1464.8477	1468.4468
1472.5087	1477.5783	1480.4583

C	0.21081	-2.45458	2.76128	1482.4321	1483.7895	1494.1479
H	1.04851	-2.36001	3.45759	1508.0149	1515.7238	1536.0043
H	-0.49127	-1.62933	2.95268	1585.7302	1620.6152	1678.6810
H	-0.31238	-3.39475	2.97339	1734.2117	1812.1487	2093.1198
C	3.65048	2.64021	1.17058	3015.7552	3017.7990	3028.2759
H	4.21755	3.48665	1.57906	3030.5118	3031.4228	3033.5069
H	3.14783	2.12900	1.99968	3037.8796	3038.9617	3045.7738
H	4.36956	1.94593	0.71258	3098.7720	3099.2211	3099.7374
C	3.35796	3.87848	-0.98043	3101.3360	3111.9271	3112.7188
H	2.65317	4.22535	-1.74426	3124.1798	3125.1415	3127.6601
H	3.88064	4.75188	-0.56921	3131.8393	3132.4270	3139.1964
H	4.08835	3.23142	-1.47659	3145.2899	3145.8349	3146.1915
C	1.62030	4.05685	0.81215	3147.4913	3151.4681	3154.1066
H	2.13435	4.93043	1.23447	3155.1775	3184.1250	3200.8701
H	0.87648	4.42116	0.09279			
H	1.08854	3.53882	1.61579			
C	-6.00916	1.95042	-0.63394			
H	-6.15968	3.01811	-0.42796			
H	-6.07726	1.81290	-1.71810			
H	-6.85220	1.41659	-0.17717			
H	-6.67522	-1.41624	-0.26110			
H	-1.64368	0.47723	0.30469			
C	-3.18164	-0.68887	-0.69599			
C	-4.16135	0.14311	-0.13037			
C	-3.58554	-1.74568	-1.53671			
C	-5.51687	-0.03227	-0.36126			
H	-3.82610	0.95771	0.51450			
C	-4.94823	-1.93085	-1.77634			
C	-5.88741	-1.09049	-1.19954			
H	-5.26915	-2.74517	-2.42591			
H	-6.94415	-1.25844	-1.40615			
O	-2.65484	-2.54543	-2.08767			
H	-3.09511	-3.22033	-2.61740			
C	-6.55053	0.85833	0.25923			
H	-6.08738	1.70031	0.78297			
H	-7.23316	1.26832	-0.49438			
H	-7.16446	0.31377	0.98712			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.488106 Electronic Energy = -1299.93739201
Internal Energy (E)= -1299.41788701 Enthalpy (H)= -1299.41694301
Gibbs Free Energy (G)=-1299.51024201 Gibbs Free Energy of Solvation=-1299.55304533

St.Pt.	General Structure	Ball & Stick model
TS_2-4		

Cartesian co-ordinate

Atoms	X	Y	Z

Frequencies

-286.2848	22.8946	33.6469
45.2210	54.1231	71.0819

C	-0.82203	-2.25367	1.17835
C	-2.03739	-1.66676	0.66225
C	-2.10257	-1.92135	-0.77380
C	-0.90055	-2.51805	-1.15959
C	-0.05094	-2.65968	0.03192
C	2.45257	0.42494	0.38689
Ir	-0.28364	-0.50207	0.01124
C	3.67301	0.85298	0.92715
C	4.74275	1.14780	0.10016
C	2.27931	0.27438	-0.99838
C	4.55928	0.99265	-1.28939
C	3.36700	0.56752	-1.84292
H	3.24418	0.45709	-2.91758
H	5.39572	1.22165	-1.95142
H	-0.92204	0.37479	1.26754
O	-0.98206	1.38452	-0.62556
C	-1.55701	2.09337	0.28155
C	-2.18015	3.39810	-0.20492
O	-1.66371	1.73754	1.47022
H	3.75443	0.95138	2.00918
C	1.28998	0.08345	1.21228
O	1.27460	0.07445	2.42328
O	1.12087	-0.13799	-1.46572
C	1.28107	-3.32909	0.03386
H	1.83842	-3.10034	0.94806
H	1.18033	-4.41968	-0.04265
H	1.88790	-2.98414	-0.81111
C	-0.47935	-2.42191	2.61645
H	-1.14342	-3.16264	3.07894
H	0.55297	-2.75920	2.74198
H	-0.56376	-1.47453	3.15931
C	-3.17662	-1.15773	1.47702
H	-3.92718	-1.94648	1.62060
H	-2.84061	-0.81645	2.46040
H	-3.66790	-0.30773	0.99007
C	-3.21523	-1.44448	-1.63961
H	-4.17751	-1.86095	-1.31638
H	-3.29818	-0.34962	-1.59198
H	-3.06128	-1.71768	-2.68721
C	-0.41731	-2.80664	-2.53390
H	-1.20867	-2.69107	-3.27969
H	0.39529	-2.11047	-2.78820
H	-0.01940	-3.82597	-2.60654
C	-3.43752	3.00524	-0.98952
H	-3.96276	3.90682	-1.32950
H	-3.18033	2.40368	-1.86923
H	-4.13040	2.43006	-0.35951
C	-2.56233	4.27621	0.97979
H	-1.68267	4.53901	1.57801
H	-3.02276	5.20460	0.61842
H	-3.27111	3.76698	1.64052
C	-1.20796	4.13666	-1.12258
H	-1.67610	5.05848	-1.49116
H	-0.29282	4.41513	-0.58619
H	-0.92289	3.51908	-1.97938
C	6.05737	1.62633	0.64221
H	6.29651	2.63895	0.29228
H	6.04946	1.65046	1.73691
H	6.88677	0.97849	0.33053

96.8001	107.0709	114.3423
120.0723	135.7310	145.1398
157.5666	160.9874	169.3231
173.9368	189.1233	190.3318
198.0535	205.5368	212.6701
216.3820	220.8383	234.5289
241.3982	249.3995	255.5347
262.1645	271.3004	291.4492
300.7974	305.4355	309.8148
327.1066	332.3746	334.7854
341.9990	353.3892	359.7255
374.6267	396.2503	422.0473
432.0107	436.1140	451.1000
475.7047	496.8319	517.0569
536.3678	540.2870	544.7216
553.7712	596.2792	620.1672
621.9811	633.1494	640.8683
648.0917	662.3009	679.8945
758.5226	762.9859	793.3192
809.5275	817.2648	835.4512
841.1120	864.9017	906.9014
915.1537	950.0328	953.5060
957.2442	958.4058	961.3119
962.7027	963.7674	967.5116
1015.5497	1032.0073	1041.0287
1042.3176	1043.7240	1045.0417
1050.0455	1052.6980	1058.6100
1088.6184	1089.6914	1108.0723
1134.5914	1149.8906	1177.8945
1186.8279	1230.5963	1241.4920
1255.2166	1268.1258	1270.7666
1340.3684	1370.9108	1374.1190
1380.0940	1384.6172	1392.9981
1394.2705	1399.4600	1402.3184
1403.0940	1404.2304	1427.9071
1429.1168	1434.3248	1439.0863
1448.8316	1449.8006	1450.7087
1452.7566	1456.3335	1459.0632
1459.6466	1461.3494	1463.5204
1465.1688	1466.3192	1468.0602
1476.9079	1478.7996	1480.5882
1482.3467	1482.5969	1500.3130
1505.7172	1510.0885	1538.0587
1585.1993	1590.2858	1622.8217
1680.4184	1770.7450	1819.0895
3018.0136	3028.2407	3030.0201
3030.4735	3033.9687	3034.7377
3034.7907	3039.9510	3044.7753
3097.0692	3099.2416	3103.6236
3106.2705	3113.9219	3115.2103
3118.2740	3125.4762	3127.9718
3131.2948	3131.8552	3136.7811
3144.7805	3145.5331	3147.6598
3150.2458	3150.9566	3151.9209
3154.9454	3178.1238	3196.0261

H	-6.67522	-1.41624	-0.26110
H	-1.64368	0.47723	0.30469
C	-3.18164	-0.68887	-0.69599
C	-4.16135	0.14311	-0.13037
C	-3.58554	-1.74568	-1.53671
C	-5.51687	-0.03227	-0.36126
H	-3.82610	0.95771	0.51450
C	-4.94823	-1.93085	-1.77634
C	-5.88741	-1.09049	-1.19954
H	-5.26915	-2.74517	-2.42591
H	-6.94415	-1.25844	-1.40615
O	-2.65484	-2.54543	-2.08767
H	-3.09511	-3.22033	-2.61740
C	-6.55053	0.85833	0.25923
H	-6.08738	1.70031	0.78297
H	-7.23316	1.26832	-0.49438
H	-7.16446	0.31377	0.98712

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.487024 Electronic Energy = -1299.93645448
Internal Energy (E)= -1299.41890548 Enthalpy (H)= -1299.41796148
Gibbs Free Energy (G)=-1299.50836548 Gibbs Free Energy of Solvation=-1299.54981933

St.Pt.	General Structure	Ball & Stick model
V-2		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.41680	-2.07332	1.44534
C	-1.70479	-1.64607	0.98678
C	-1.88728	-2.14407	-0.38436
C	-0.70193	-2.75624	-0.79495
C	0.27426	-2.63763	0.29977
C	2.38970	0.79055	0.27887
Ir	-0.11990	-0.59894	-0.10213
C	3.49377	1.45162	0.83856
C	4.64191	1.65628	0.09637
C	2.39916	0.34586	-1.06312
C	4.64820	1.19939	-1.24060
C	3.56795	0.56965	-1.82387
H	3.59121	0.23987	-2.85994
H	5.54817	1.36150	-1.83638
H	-0.75992	1.55950	1.65632
O	-1.18002	1.25120	-0.72028
C	-1.78588	1.99465	0.06169
C	-2.89901	2.90237	-0.42974

Frequencies

25.9116	39.5514	64.2013
69.2993	79.7181	88.1598
107.7791	112.1727	125.1286
135.5280	142.6626	149.2133
154.8861	166.3952	167.0315
171.8833	178.3326	202.8175
205.3514	208.3898	219.9779
226.1348	235.0720	246.5402
247.3348	250.9407	277.6542
288.7071	290.6307	310.4867
315.1442	323.7936	325.5580
332.9416	336.2659	343.0851
358.9915	363.7408	372.5847
397.2479	401.3672	413.1860
422.1601	430.8617	468.2082
488.4976	495.2262	534.1903
539.1268	541.3405	548.4742
554.6308	594.5528	604.1891
611.6433	628.6041	641.8325
669.3130	690.7893	760.8204
770.2793	776.3774	787.6238
806.4411	808.3029	832.4099

O	-1.58665	2.05042	1.35033
H	3.42343	1.79422	1.87106
C	1.11624	0.58245	0.94688
O	0.79392	1.12181	2.01958
O	1.33528	-0.22802	-1.56393
C	1.63958	-3.23454	0.28025
H	2.27798	-2.77743	1.04400
H	1.61330	-4.31825	0.45633
H	2.12127	-3.05685	-0.68805
C	0.10994	-1.91806	2.82880
H	-0.33224	-2.66594	3.49901
H	1.19764	-2.03867	2.85678
H	-0.10927	-0.91888	3.22148
C	-2.78029	-1.04222	1.82443
H	-3.46503	-1.80933	2.21189
H	-2.35966	-0.50317	2.68043
H	-3.38102	-0.32355	1.25303
C	-3.11171	-1.87783	-1.18849
H	-3.99492	-2.34737	-0.73550
H	-3.31151	-0.79845	-1.24971
H	-3.01723	-2.25148	-2.21228
C	-0.35047	-3.28771	-2.13938
H	-1.18496	-3.20413	-2.84179
H	0.49607	-2.72790	-2.55805
H	-0.05850	-4.34437	-2.08374
C	-4.21058	2.34681	0.14197
H	-5.04688	2.97718	-0.18399
H	-4.40226	1.32761	-0.22265
H	-4.19613	2.33001	1.23723
C	-2.67037	4.32403	0.08746
H	-1.72500	4.73491	-0.28671
H	-3.48132	4.97318	-0.26455
H	-2.64940	4.35696	1.18076
C	-2.95407	2.89580	-1.95211
H	-3.77328	3.54231	-2.28905
H	-2.02006	3.26707	-2.38744
H	-3.12415	1.88769	-2.34527
C	5.84825	2.34256	0.66607
H	6.11855	3.23699	0.08950
H	5.67251	2.65783	1.70018
H	6.72994	1.68804	0.66613
H	-6.67522	-1.41624	-0.26110
H	-1.64368	0.47723	0.30469
C	-3.18164	-0.68887	-0.69599
C	-4.16135	0.14311	-0.13037
C	-3.58554	-1.74568	-1.53671
C	-5.51687	-0.03227	-0.36126
H	-3.82610	0.95771	0.51450
C	-4.94823	-1.93085	-1.77634
C	-5.88741	-1.09049	-1.19954
H	-5.26915	-2.74517	-2.42591
H	-6.94415	-1.25844	-1.40615
O	-2.65484	-2.54543	-2.08767
H	-3.09511	-3.22033	-2.61740
C	-6.55053	0.85833	0.25923
H	-6.08738	1.70031	0.78297
H	-7.23316	1.26832	-0.49438
H	-7.16446	0.31377	0.98712

873.5144	898.0157	900.2471
946.6262	950.0495	953.2728
957.2989	957.7673	960.8132
964.6949	967.1371	1018.6744
1036.0284	1042.1606	1044.5977
1047.8312	1048.8758	1049.7079
1052.2525	1056.3910	1084.8544
1091.7179	1103.5576	1137.5939
1156.2270	1180.6644	1183.0039
1223.3635	1234.8532	1249.5203
1263.7316	1272.3005	1341.0302
1347.7313	1369.2264	1376.0969
1379.9235	1389.0045	1393.7308
1396.9400	1401.6980	1403.6626
1405.7713	1417.2902	1427.0066
1434.3563	1444.1450	1447.7290
1452.3222	1454.5397	1456.0530
1457.9288	1459.1757	1461.1498
1462.5365	1464.1666	1465.9180
1471.2949	1472.5970	1476.0111
1480.4883	1484.3805	1485.9507
1486.9583	1495.4858	1503.4832
1512.5154	1520.7677	1539.8870
1591.3275	1606.7005	1656.2141
1683.5875	1742.8442	3022.6575
3023.1066	3025.6825	3030.2201
3031.7819	3032.2416	3039.4730
3039.8801	3046.6243	3053.5223
3090.3121	3091.2512	3101.5354
3106.0966	3112.6787	3114.4029
3124.0009	3124.2541	3127.0205
3132.7200	3134.1730	3138.0093
3140.3660	3141.1818	3142.4059
3143.5604	3148.7437	3148.9673
3152.1251	3172.1200	3193.2503

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.492606 Electronic Energy = -1299.97034305
Internal Energy (E)= -1299.44713005 Enthalpy (H)= -1299.44618505
Gibbs Free Energy (G)=-1299.53608705 Gibbs Free Energy of Solvation=-1299.57483814

St.Pt.	General Structure	Ball & Stick model
V'-2		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.37434	2.62858	0.46876
C	0.87861	2.24986	1.06981
C	1.82768	2.04277	-0.01165
C	1.16971	2.19786	-1.25529
C	-0.22140	2.49750	-0.95773
C	-2.62906	-0.49024	0.39953
Ir	0.05918	0.52556	-0.04202
C	-2.37509	-0.68040	-0.97544
C	-3.43446	-1.14286	-1.78534
C	-3.88965	-0.75413	0.95338
C	-4.67221	-1.37690	-1.21874
C	-4.93355	-1.18943	0.15557
H	-4.02402	-0.60529	2.02515
H	-5.48589	-1.72649	-1.85640
H	-3.25146	-1.30692	-2.84476
C	1.16274	-1.36762	0.13897
C	2.61578	-1.22429	-0.25245
C	0.45685	-2.50001	-0.65095
O	0.85774	-2.77316	-1.75106
N	1.03353	-1.52721	1.51739
N	0.85811	-1.61370	2.62530
C	3.27710	1.78159	0.19818
H	3.75079	1.38333	-0.70392
H	3.78706	2.71365	0.47392
H	3.44083	1.06903	1.01647
C	1.16366	2.22387	2.53311
H	2.10952	1.71007	2.74159
H	1.23397	3.23347	2.95969
H	0.37110	1.67625	3.05993
C	-1.58738	3.08505	1.20232
H	-1.64123	2.63040	2.19644
H	-1.56985	4.17562	1.32739
H	-2.50778	2.82287	0.66898
C	-1.28364	2.71598	-1.97793
H	-2.28160	2.60080	-1.54225
H	-1.21025	3.71970	-2.41550
H	-1.19856	1.97984	-2.78408

Frequencies

23.1859	28.9335	34.8334
50.9235	68.5001	80.2592
86.7880	100.6912	104.9129
114.3659	122.0237	132.7133
133.9148	138.6172	142.6237
151.5691	161.6004	166.6094
174.1549	182.8222	187.9704
192.6409	197.4148	200.8907
214.4230	215.6132	222.3383
231.5623	236.0736	248.5784
264.5014	271.3069	289.1528
295.5295	305.9399	315.4215
320.7998	332.7284	335.4860
339.5901	356.5432	360.4731
362.3259	371.2441	380.4800
409.0497	430.6609	433.6131
452.8337	479.5466	491.3871
493.3410	502.5926	532.5733
536.2309	537.6698	545.0141
546.9431	585.2015	590.2382
597.8240	605.0970	622.9936
637.3312	670.7804	678.4723
752.5728	756.4445	764.0650
774.4632	811.6708	813.5534
822.8318	833.4210	867.7127
878.5815	903.2455	953.6914
953.8730	957.6755	958.8159
966.8288	971.0491	1018.2264
1032.3209	1033.5799	1038.0182
1044.9407	1049.6841	1049.7708
1052.0629	1059.6630	1090.3299
1093.8029	1095.3645	1110.9490
1123.5842	1134.5613	1145.3759
1176.3893	1180.5175	1187.6185
1194.1575	1228.2322	1262.9320
1270.0064	1319.5309	1343.0117
1377.1921	1381.2375	1384.7102
1385.4085	1389.4668	1396.0443
1396.7745	1402.2439	1405.3994
1416.4485	1439.3860	1439.5278
1446.4177	1450.0268	1450.9622

C	1.75554	2.02068	-2.61445	1452.9394	1454.8522	1459.8685
H	2.15819	2.96106	-3.01536	1463.1930	1464.1144	1465.5600
H	2.55694	1.27327	-2.60592	1468.9434	1470.7390	1472.1193
H	0.99773	1.65751	-3.31718	1480.5047	1483.0062	1487.2100
C	-1.45724	-0.07642	1.17832	1492.8827	1493.3273	1500.4122
O	-1.17072	-0.47351	-1.45106	1508.1538	1512.3264	1536.2001
O	-1.42040	-0.03375	2.40222	1546.9506	1608.6289	1679.0631
O	2.98028	-0.90249	-1.35158	1734.5227	1853.0524	1894.6027
C	4.84496	-1.51289	0.48566	2255.9220	3023.9459	3025.6480
H	5.31934	-1.34507	1.45715	3029.3218	3036.6064	3036.9842
H	5.06981	-0.66750	-0.17313	3039.3756	3043.2004	3053.0303
O	3.43150	-1.51913	0.77392	3073.9131	3094.5665	3102.8452
C	5.26508	-2.82154	-0.13506	3107.5817	3112.7484	3116.7999
H	4.78348	-2.95664	-1.10838	3123.3360	3124.8507	3128.8292
H	6.34939	-2.83555	-0.28550	3131.2393	3136.5183	3139.9389
H	4.99792	-3.66313	0.51197	3141.5001	3146.7896	3148.3014
C	-0.63522	-3.25411	0.04714	3151.0309	3157.0949	3158.2410
H	-1.19496	-3.81388	-0.70529	3170.3482	3180.0224	3197.3953
H	-0.18579	-3.96570	0.75262			
H	-1.32110	-2.60799	0.60387			
C	-6.30206	-1.45375	0.71113			
H	-6.31408	-1.34781	1.80116			
H	-7.04882	-0.75838	0.30539			
H	-6.65018	-2.46691	0.47231			
C	-3.18164	-0.68887	-0.69599			
C	-4.16135	0.14311	-0.13037			
C	-3.58554	-1.74568	-1.53671			
C	-5.51687	-0.03227	-0.36126			
H	-3.82610	0.95771	0.51450			
C	-4.94823	-1.93085	-1.77634			
C	-5.88741	-1.09049	-1.19954			
H	-5.26915	-2.74517	-2.42591			
H	-6.94415	-1.25844	-1.40615			
O	-2.65484	-2.54543	-2.08767			
H	-3.09511	-3.22033	-2.61740			
C	-6.55053	0.85833	0.25923			
H	-6.08738	1.70031	0.78297			
H	-7.23316	1.26832	-0.49438			
H	-7.16446	0.31377	0.98712			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.488065 Electronic Energy = -1521.39530407
Internal Energy (E)= -1520.87269207 Enthalpy (H)= -1520.87174707
Gibbs Free Energy (G)=-1520.97103207 Gibbs Free Energy of Solvation=-1522.22368415

St.Pt.	General Structure	Ball & Stick model
TS_2-5		

Cartesian co-ordinate

Frequencies

-398.7991	18.7427	29.6523
37.6777	55.1765	80.4389

Atoms	X	Y	Z
C	-0.54074	2.61503	0.44148
C	0.65889	2.26199	1.16021
C	1.70861	2.07318	0.18038
C	1.16799	2.27183	-1.12661
C	-0.23638	2.55723	-0.95908
C	-2.59394	-0.57486	0.37921
Ir	0.07197	0.50610	-0.06166
C	-2.36054	-0.69406	-1.00636
C	-3.42851	-1.12494	-1.82247
C	-3.84427	-0.87437	0.93984
C	-4.65522	-1.39493	-1.24902
C	-4.89691	-1.27598	0.13703
H	-3.96483	-0.77781	2.01905
H	-5.47673	-1.71808	-1.89048
H	-3.26113	-1.23426	-2.89130
C	1.17232	-1.22834	0.03319
C	2.64947	-1.12099	-0.27021
C	0.57733	-2.43293	-0.71906
O	0.98984	-2.67579	-1.82703
N	1.13576	-1.64674	1.61784
N	0.82037	-1.56126	2.68823
C	3.14350	1.85232	0.51488
H	3.70828	1.51002	-0.35703
H	3.59547	2.78840	0.86764
H	3.26456	1.11028	1.31427
C	0.80674	2.24024	2.64347
H	1.81147	1.91682	2.93673
H	0.64073	3.23640	3.07400
H	0.08572	1.54511	3.09328
C	-1.84034	2.99078	1.06682
H	-1.98632	2.46620	2.01728
H	-1.87736	4.06962	1.26808
H	-2.68947	2.74114	0.42177
C	-1.19829	2.76587	-2.07621
H	-2.23359	2.75112	-1.72094
H	-1.02191	3.73034	-2.56908
H	-1.09732	1.97314	-2.82614
C	1.89819	2.20554	-2.42374
H	2.40014	3.15571	-2.65362
H	2.64779	1.40796	-2.41781
H	1.20827	1.98892	-3.24584
C	-1.41604	-0.18407	1.15540
O	-1.16800	-0.44508	-1.48878
O	-1.36071	-0.20001	2.37883
O	3.06017	-0.71221	-1.32608
C	4.85025	-1.54195	0.47708
H	5.31040	-1.46290	1.46652
H	5.10420	-0.65131	-0.10808
O	3.43234	-1.53971	0.73758
C	5.25109	-2.80655	-0.24030
H	4.76616	-2.86036	-1.21990
H	6.33509	-2.82771	-0.39234
H	4.96911	-3.68978	0.34185
C	-0.46509	-3.27385	-0.03913
H	-1.00741	-3.82661	-0.80985
H	0.03193	-3.99726	0.62056
H	-1.17195	-2.69573	0.56324

83.3278	88.7999	99.3782
113.4440	118.6139	131.3231
134.1087	141.3897	145.2391
148.8037	151.1019	153.2944
159.4593	177.0891	177.8540
179.7661	189.7045	195.4706
199.8725	202.5916	210.8424
220.9348	222.0505	226.7936
243.2733	254.6937	255.9997
259.3353	278.6770	284.2337
294.7951	302.2289	328.0682
330.0899	340.0232	348.1666
357.1596	362.4299	369.2292
403.4853	414.7666	415.7838
428.7281	438.9544	452.7501
483.2691	492.6636	508.0266
535.7163	539.1561	545.2813
546.5462	570.6367	589.4068
591.2307	601.6170	610.9918
640.5859	666.3912	676.8341
709.0065	755.1565	760.0006
763.9776	809.7865	812.3796
814.4225	834.9164	868.3171
885.2207	896.6842	904.1042
945.9868	953.5321	955.8133
961.5728	964.1830	1018.0045
1018.4589	1032.2796	1036.3414
1039.1587	1043.5266	1048.5289
1049.7809	1054.4772	1083.0495
1087.7463	1091.5573	1110.4945
1124.2184	1136.3134	1147.5498
1178.2676	1185.3033	1191.0317
1208.2127	1228.2781	1269.9330
1276.1107	1332.5988	1344.7376
1377.3449	1379.0636	1383.9179
1387.9805	1389.9131	1393.6015
1396.6055	1400.8542	1402.5352
1419.6082	1436.7231	1439.6898
1444.5232	1448.0867	1450.1600
1451.0435	1453.4916	1455.1769
1458.0368	1462.6222	1463.6241
1470.5070	1471.0686	1475.3779
1476.6681	1479.4139	1482.2908
1490.2832	1491.6078	1493.9378
1502.0462	1519.4117	1535.4139
1537.8038	1610.7241	1678.7987
1728.3989	1837.8768	1877.3698
2259.4247	3025.5569	3026.0058
3033.0123	3033.5896	3035.9095
3039.0049	3046.3167	3051.6567
3072.9990	3094.8806	3104.9117
3106.2562	3113.0155	3118.5700
3120.5333	3126.7430	3128.9618
3130.1293	3135.6402	3136.7753
3144.0824	3145.6814	3150.0931
3155.1812	3157.6621	3169.6589
3170.7821	3177.0064	3199.3909

C	-6.25604	-1.57531	0.69754
H	-6.26175	-1.49055	1.78940
H	-7.01745	-0.88568	0.30990
H	-6.58811	-2.58979	0.44191
C	-3.18164	-0.68887	-0.69599
C	-4.16135	0.14311	-0.13037
C	-3.58554	-1.74568	-1.53671
C	-5.51687	-0.03227	-0.36126
H	-3.82610	0.95771	0.51450
C	-4.94823	-1.93085	-1.77634
C	-5.88741	-1.09049	-1.19954
H	-5.26915	-2.74517	-2.42591
H	-6.94415	-1.25844	-1.40615
O	-2.65484	-2.54543	-2.08767
H	-3.09511	-3.22033	-2.61740
C	-6.55053	0.85833	0.25923
H	-6.08738	1.70031	0.78297
H	-7.23316	1.26832	-0.49438
H	-7.16446	0.31377	0.98712

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.485815 Electronic Energy = -1521.39030742
Internal Energy (E)= -1520.86986142 Enthalpy (H)= -1520.86891742
Gibbs Free Energy (G)=-1520.96833042 Gibbs Free Energy of Solvation=-1521.00650477

St.Pt.	General Structure	Ball & Stick model
VI-2		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.82669	2.36847	0.79742
C	0.40808	1.97724	1.43669
C	1.47029	2.10343	0.46218
C	0.88696	2.55138	-0.77126
C	-0.52444	2.70012	-0.55580
C	-2.55270	-0.80922	0.26665
Ir	0.05002	0.44094	-0.14371
C	-2.47536	-0.49598	-1.10010
C	-3.62924	-0.66323	-1.89065
C	-3.73474	-1.30001	0.83913
C	-4.78583	-1.13946	-1.30417
C	-4.86950	-1.46836	0.06541
H	-3.73895	-1.53481	1.90314
H	-5.67475	-1.26904	-1.92293
H	-3.58152	-0.42454	-2.95031
C	1.23553	-0.99774	-0.50441

Frequencies

19.3135	36.1646	38.5375
49.3872	51.1225	56.9392
71.0017	75.7407	82.3814
95.2624	99.9230	102.7187
121.6400	125.0358	131.7800
136.8615	143.0307	149.5574
153.7448	157.3902	164.0298
166.9960	177.6573	181.0976
192.2479	198.4098	205.4996
214.9386	221.3827	225.0190
237.4803	247.6573	257.8252
259.4998	274.9544	291.8917
297.8118	304.3834	322.5066
332.5411	340.0434	352.7117
360.6394	369.6659	375.1183
392.7580	397.2211	411.8886
434.0407	435.9949	449.3468
479.0199	488.6671	491.8323
531.8156	539.9260	542.8327
551.2806	572.4265	587.6303

C	2.70554	-0.73798	-0.63720
C	0.97238	-2.41260	-0.94352
O	1.82015	-2.94237	-1.64626
N	1.47555	-2.15893	2.43041
N	1.89690	-1.41826	3.13391
C	2.92405	2.00603	0.77328
H	3.52196	1.89192	-0.13521
H	3.25718	2.91182	1.29619
H	3.13453	1.14933	1.42483
C	0.57765	1.70209	2.89081
H	1.62340	1.49426	3.13782
H	0.25919	2.57169	3.47989
H	-0.01837	0.83670	3.20207
C	-2.15338	2.45781	1.47336
H	-2.20402	1.76994	2.32424
H	-2.33369	3.47284	1.85074
H	-2.97491	2.19736	0.79663
C	-1.50718	3.05506	-1.61570
H	-2.53204	3.04601	-1.23263
H	-1.30436	4.05337	-2.02165
H	-1.45715	2.33094	-2.43876
C	1.61473	2.83722	-2.03831
H	2.09172	3.82621	-2.00285
H	2.38961	2.08549	-2.21996
H	0.93140	2.82749	-2.89338
C	-1.32302	-0.58308	1.02897
O	-1.33636	-0.07818	-1.60864
O	-1.17840	-0.83832	2.20464
O	3.20307	-0.05428	-1.50538
C	4.83284	-1.32622	0.20159
H	5.20152	-1.51182	1.21507
H	5.14808	-0.32479	-0.11373
O	3.39938	-1.35005	0.32956
C	5.28826	-2.38476	-0.77243
H	4.92372	-2.16086	-1.77921
H	6.38211	-2.43076	-0.79973
H	4.90332	-3.36671	-0.47937
C	-0.27342	-3.13261	-0.53950
H	-1.14019	-2.70011	-1.05101
H	-0.17578	-4.18279	-0.82317
H	-0.44895	-3.04635	0.53894
C	-6.15874	-1.97315	0.64284
H	-6.05676	-2.19305	1.71056
H	-6.96779	-1.23988	0.53120
H	-6.49213	-2.89256	0.14515
C	-3.18164	-0.68887	-0.69599
C	-4.16135	0.14311	-0.13037
C	-3.58554	-1.74568	-1.53671
C	-5.51687	-0.03227	-0.36126
H	-3.82610	0.95771	0.51450
C	-4.94823	-1.93085	-1.77634
C	-5.88741	-1.09049	-1.19954
H	-5.26915	-2.74517	-2.42591
H	-6.94415	-1.25844	-1.40615
O	-2.65484	-2.54543	-2.08767
H	-3.09511	-3.22033	-2.61740
C	-6.55053	0.85833	0.25923
H	-6.08738	1.70031	0.78297
H	-7.23316	1.26832	-0.49438
H	-7.16446	0.31377	0.98712

597.4803	602.8977	636.2330
651.4476	669.3695	672.8464
734.1887	750.6416	756.5981
757.6105	809.8409	814.0046
818.1442	830.3355	862.7782
886.0635	904.6074	950.1844
950.4619	952.7751	959.3061
966.3610	1004.8782	1010.5921
1014.9878	1024.1727	1037.6962
1041.2867	1045.1114	1045.7390
1049.8887	1050.8355	1085.7021
1092.9257	1110.2428	1117.2393
1128.3998	1134.4911	1148.3911
1177.9608	1186.4305	1189.0141
1232.8637	1242.6055	1268.4030
1288.0811	1313.0612	1335.4963
1366.2708	1372.4298	1380.6668
1381.3395	1388.0208	1390.9521
1393.1674	1399.2258	1402.3181
1415.3582	1419.6723	1435.8927
1439.2480	1444.1165	1447.2268
1448.2356	1455.6644	1460.1230
1461.9780	1463.4222	1471.4652
1474.2879	1474.7992	1478.8307
1481.3348	1482.4217	1488.5706
1494.9329	1508.8041	1516.6893
1523.3111	1528.2088	1532.5864
1541.2063	1618.8680	1675.4109
1777.7221	1795.4474	1821.4563
2460.5419	3029.8635	3031.6476
3032.5401	3036.2526	3038.3706
3040.3084	3055.5422	3060.1579
3069.0174	3100.2867	3110.5741
3112.9787	3113.9839	3116.7112
3123.7104	3128.9373	3132.6316
3134.0858	3142.7831	3145.4728
3145.9732	3150.2842	3156.8762
3157.4987	3166.2361	3171.4302
3174.3448	3180.0037	3199.4407

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.486291 Electronic Energy = -1521.44111907
Internal Energy (E)= -1520.91884007 Enthalpy (H)= -1520.91789607
Gibbs Free Energy (G)=-1521.02177207 Gibbs Free Energy of Solvation=-1521.05534055

St.Pt.	General Structure	Ball & Stick model
VI'-2		

Cartesian co-ordinate

Atoms	X	Y	Z
C	1.20257	-2.54295	-0.29216
C	2.12196	-1.68935	-1.02379
C	2.84297	-0.90285	-0.05896
C	2.31471	-1.22355	1.25149
C	1.31648	-2.24227	1.09000
C	-2.18581	-0.77160	-0.29265
Ir	0.69326	-0.28048	-0.02545
C	-1.99515	-0.20296	0.97920
C	-3.11751	-0.09358	1.82808
C	-3.44772	-1.21179	-0.71935
C	-4.34861	-0.54317	1.39254
C	-4.54625	-1.11430	0.11662
H	-3.53917	-1.62875	-1.72213
H	-5.20766	-0.45449	2.05912
H	-2.98744	0.35149	2.81198
C	0.65889	1.49859	-0.68500
C	1.77503	2.08111	-1.48433
C	-0.41149	2.44480	-0.26188
C	-2.70020	2.94872	-0.30222
H	-2.83297	2.73013	0.76650
H	-2.43703	4.00916	-0.39333
C	-3.91057	2.57640	-1.11437
H	-4.78003	3.15131	-0.77967
H	-3.74526	2.78748	-2.17598
H	-4.13613	1.50965	-1.00658
O	-1.60152	2.15355	-0.78172
O	-0.19683	3.38327	0.47756
C	4.01276	-0.02315	-0.33007
H	4.08197	0.79020	0.40226
H	4.94226	-0.60394	-0.27342
H	3.95276	0.43020	-1.32441
C	2.35740	-1.76398	-2.49184
H	2.94982	-0.91602	-2.84167
H	2.87316	-2.69709	-2.75514
H	1.40271	-1.73009	-3.02774

Frequencies

33.9384	42.0257	52.9466
55.5591	66.8233	70.3071
84.3384	88.2315	94.3234
103.6148	109.8362	117.9250
118.8646	125.2613	134.2879
143.7589	150.9629	155.6322
159.5211	164.5676	172.9606
179.3725	182.9351	188.2618
197.5554	203.1521	214.8953
222.2744	227.5215	232.4556
244.0821	249.7876	257.8778
263.3284	276.0259	289.0119
290.4176	296.4220	315.2428
320.8336	333.4298	336.5605
346.5479	356.3718	360.3926
363.7638	371.6431	399.4504
407.2729	418.4788	433.7293
478.6065	499.8417	526.5059
532.5197	543.8619	545.1448
557.0501	577.9403	586.9297
596.3846	606.9948	631.9190
648.4819	657.2074	668.3560
740.9753	755.2659	758.4439
801.0637	806.7538	815.7078
823.8589	838.9901	860.6429
887.8984	911.0419	939.8279
953.4351	964.1810	966.0647
972.9586	1016.7959	1021.2842
1022.3547	1034.8039	1037.7033
1039.7805	1046.5936	1049.9148
1054.4406	1070.1607	1093.8525
1097.8989	1110.5998	1115.3824
1136.4262	1142.3952	1149.6979
1173.4159	1184.6000	1188.0621
1229.7745	1243.2511	1267.2066
1268.0861	1312.0159	1342.7424
1376.6458	1381.3463	1383.4329
1387.5730	1394.4563	1398.4827
1403.0041	1405.4945	1408.4265

C	0.35685	-3.60248	-0.90603	1416.8915	1435.4871	1440.1059
H	0.04530	-3.32748	-1.91762	1445.2057	1446.6344	1449.7618
H	0.92385	-4.54065	-0.96816	1450.6731	1457.6131	1459.1717
H	-0.54814	-3.79602	-0.31990	1459.9139	1462.0140	1462.7070
C	0.49343	-2.79162	2.20285	1462.9921	1472.2432	1474.5909
H	-0.32248	-3.41693	1.82842	1481.0642	1482.9631	1484.7168
H	1.10261	-3.39784	2.88520	1487.8892	1499.1178	1504.2690
H	0.04538	-1.97579	2.78356	1511.0089	1518.1248	1536.6257
C	2.77700	-0.70915	2.57029	1548.9861	1615.4081	1678.2573
H	3.36788	-1.46887	3.09982	1775.3708	1815.4955	1828.0133
H	3.39842	0.18505	2.46452	2464.4824	3026.1717	3026.8903
H	1.92347	-0.44706	3.20740	3037.2250	3039.3075	3039.7689
C	-1.00770	-0.81001	-1.15354	3044.3638	3046.2193	3050.1616
O	-0.81156	0.23133	1.34167	3062.3686	3096.5773	3098.4668
O	-0.96523	-1.16276	-2.30524	3103.3192	3114.2202	3117.3721
N	1.96863	2.43209	2.39146	3117.6035	3126.2015	3128.9574
N	1.23473	2.49913	3.21484	3142.9586	3145.7328	3147.4555
C	2.30351	3.43584	-1.09718	3147.9225	3151.5213	3155.2200
H	2.60752	3.44296	-0.04422	3157.6305	3170.1563	3174.3284
H	3.15141	3.67804	-1.74242	3174.8686	3178.8995	3192.0365
H	1.52667	4.20231	-1.18474			
O	2.26460	1.45174	-2.40940			
C	-5.90624	-1.59342	-0.29735			
H	-6.66542	-0.81070	-0.17420			
H	-5.91547	-1.90163	-1.34803			
H	-6.23605	-2.45277	0.30102			
C	-3.18164	-0.68887	-0.69599			
C	-4.16135	0.14311	-0.13037			
C	-3.58554	-1.74568	-1.53671			
C	-5.51687	-0.03227	-0.36126			
H	-3.82610	0.95771	0.51450			
C	-4.94823	-1.93085	-1.77634			
C	-5.88741	-1.09049	-1.19954			
H	-5.26915	-2.74517	-2.42591			
H	-6.94415	-1.25844	-1.40615			
O	-2.65484	-2.54543	-2.08767			
H	-3.09511	-3.22033	-2.61740			
C	-6.55053	0.85833	0.25923			
H	-6.08738	1.70031	0.78297			
H	-7.23316	1.26832	-0.49438			
H	-7.16446	0.31377	0.98712			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.486866 Electronic Energy = -1521.44808054
Internal Energy (E)= -1520.92554054 Enthalpy (H)= -1520.92459654
Gibbs Free Energy (G)=-1521.02592654 Gibbs Free Energy of Solvation=-1521.06104041

St.Pt.	General Structure	Ball & Stick model
TS_2-6		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.29777	-2.45411	0.41342
C	-2.12115	-1.50727	1.16268
C	-2.90934	-0.77704	0.22583
C	-2.54205	-1.24166	-1.10804
C	-1.59625	-2.31898	-0.96626
C	2.08964	-0.59086	0.47499
Ir	-0.79817	-0.33641	-0.17377
C	1.95107	-0.54966	-0.93404
C	3.07940	-0.90395	-1.70623
C	3.28732	-1.00610	1.07974
C	4.24516	-1.30806	-1.08702
C	4.37924	-1.37590	0.31668
H	3.33675	-1.02233	2.16807
H	5.09977	-1.59059	-1.70374
H	2.99437	-0.85903	-2.78947
C	-0.16052	1.38129	0.49483
C	-0.79964	2.06276	1.65381
C	0.70467	2.24812	-0.37090
C	2.88480	2.88556	-0.97233
H	2.66258	2.52298	-1.98484
H	2.67167	3.96167	-0.95566
C	4.29222	2.56125	-0.54774
H	5.01165	3.05462	-1.20924
H	4.47789	2.89874	0.47728
H	4.46487	1.47908	-0.59093
O	2.00450	2.21984	-0.05451
O	0.24408	2.96539	-1.23158
C	-3.94267	0.23667	0.56679
H	-4.23337	0.82063	-0.31160
H	-4.84615	-0.24788	0.95925
H	-3.55976	0.92466	1.33030
C	-2.20096	-1.44575	2.64754
H	-2.95752	-0.72793	2.97093
H	-2.45989	-2.43590	3.04507
H	-1.25064	-1.12562	3.08776
C	-0.33531	-3.40477	1.03620
H	0.04441	-3.01279	1.98543
H	-0.82083	-4.36778	1.24293
H	0.52603	-3.59423	0.38675
C	-0.92563	-3.02466	-2.09242
H	-0.00397	-3.51392	-1.76081
H	-1.57955	-3.79078	-2.52745
H	-0.65189	-2.32107	-2.88636
C	-3.13201	-0.77638	-2.39232
H	-4.02289	-1.36485	-2.65119
H	-3.42769	0.27601	-2.34054
H	-2.41437	-0.87302	-3.21341
C	0.97115	-0.15444	1.29622
O	0.83341	-0.17715	-1.50268
O	0.85653	-0.21218	2.49022
N	-2.72202	3.32242	-0.73974
N	-3.00861	2.91948	-1.72779
C	-0.47946	3.51739	1.87926
H	-0.79007	4.11249	1.01246

Frequencies

-259.2547	29.5639	35.2321
45.3142	55.2507	69.7943
81.1726	84.1605	89.4766
94.8835	109.6390	113.2516
120.7556	123.1292	132.0593
133.6388	138.6469	144.6666
160.3912	165.9206	177.0548
180.2678	184.2831	194.1045
196.3483	204.8201	207.8484
211.2126	222.3948	223.3518
233.1632	236.4697	242.1033
251.3887	267.9775	280.6628
284.9590	304.0503	314.3164
318.3396	321.6598	332.0222
334.2492	342.6884	358.8648
363.9056	385.1766	398.7537
407.1270	422.1577	443.8157
462.3082	472.8265	487.3202
527.2152	538.6145	543.3152
554.3002	560.5089	577.4830
591.7703	601.9163	609.8501
628.4020	641.1751	681.3437
724.4969	736.7605	753.7617
793.7150	811.7839	814.3082
820.7728	839.5459	844.1653
892.3013	903.8133	927.9895
945.2675	961.0875	970.9151
971.1673	1014.3241	1019.2680
1031.4236	1033.9402	1037.9172
1044.7113	1047.5135	1048.7435
1050.1393	1054.3668	1092.7604
1097.0023	1109.6883	1113.1418
1135.0377	1137.2335	1143.1133
1174.4594	1184.6867	1190.3298
1227.4628	1244.0497	1264.5738
1289.1598	1313.6126	1341.1601
1374.4808	1379.2462	1381.5142
1387.6661	1395.0504	1399.0597
1399.7414	1404.0670	1405.1612
1420.1956	1434.5051	1441.6392
1442.1529	1443.3911	1445.0629
1447.6071	1451.5034	1456.1451
1458.0640	1462.0344	1469.9785
1471.7863	1472.4957	1473.3188
1477.2115	1480.3318	1484.3680
1488.9336	1498.2400	1507.3492
1517.3589	1524.2415	1535.7829
1555.4411	1601.9526	1678.9479
1775.8311	1829.4191	1842.3278
2468.9242	3026.7690	3036.0205
3036.4633	3038.9241	3040.2278
3044.4301	3046.8202	3047.7781
3051.4562	3096.2713	3097.7100
3116.0333	3117.9134	3120.2680
3121.1751	3131.4605	3140.6127
3142.4049	3142.6660	3142.8727
3144.1749	3144.8829	3149.2190
3156.5555	3159.8373	3173.0718

H	-0.99795	3.86709	2.77408	3180.4919	3180.7825	3196.9151
H	0.60269	3.65576	1.99718			
O	-1.56047	1.46159	2.39643			
C	5.66480	-1.83601	0.93736			
H	6.51717	-1.23195	0.60141			
H	5.62297	-1.76987	2.02950			
H	5.89241	-2.87833	0.67846			
C	-3.18164	-0.68887	-0.69599			
C	-4.16135	0.14311	-0.13037			
C	-3.58554	-1.74568	-1.53671			
C	-5.51687	-0.03227	-0.36126			
H	-3.82610	0.95771	0.51450			
C	-4.94823	-1.93085	-1.77634			
C	-5.88741	-1.09049	-1.19954			
H	-5.26915	-2.74517	-2.42591			
H	-6.94415	-1.25844	-1.40615			
O	-2.65484	-2.54543	-2.08767			
H	-3.09511	-3.22033	-2.61740			
C	-6.55053	0.85833	0.25923			
H	-6.08738	1.70031	0.78297			
H	-7.23316	1.26832	-0.49438			
H	-7.16446	0.31377	0.98712			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.485726 Electronic Energy = -1521.42825650
Internal Energy (E)= -1520.9072145 Enthalpy (H)= -1520.9062695
Gibbs Free Energy (G)=-1521.0070655 Gibbs Free Energy of Solvation=-1521.04472774

St.Pt.	General Structure	Ball & Stick model
VII-2		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.16042	-2.30792	0.56907
C	-1.95378	-1.37970	1.35126
C	-2.91322	-0.77824	0.46972
C	-2.76099	-1.40499	-0.83930
C	-1.72376	-2.36827	-0.77587
C	2.40841	-0.20196	0.66137
Ir	-0.86397	-0.38471	-0.22304
C	2.13622	-0.74674	-0.61765
C	3.20065	-1.38075	-1.29492
C	3.68367	-0.35082	1.22567
C	4.45365	-1.48396	-0.72149
C	4.72523	-0.97385	0.55884
H	3.83595	0.06394	2.22193
H	5.25155	-1.98589	-1.27110
H	2.99091	-1.79872	-2.27791

Frequencies

27.0374	38.0242	45.3514
56.0190	62.4824	73.3168
77.6217	83.7397	85.8105
93.1465	99.4151	104.6044
111.0311	120.3129	126.9880
127.2452	149.0391	155.2796
164.4961	166.8989	169.9657
175.0339	178.5033	182.4628
187.4830	202.6102	207.8628
216.3317	221.9281	224.2971
238.2032	242.4485	255.2940
264.8283	268.3674	275.8335
282.0753	286.0490	301.0501
306.0386	322.0609	341.7033
355.0522	366.3891	368.2684
392.7874	401.8132	420.4833
422.4638	451.6623	473.7694
492.4650	503.1157	525.8364
536.5224	540.3312	548.2169

C	0.24522	1.16589	0.72532
C	-0.51647	2.11144	1.66102
C	0.43609	1.76239	-0.62112
C	1.92008	2.53802	-2.29519
H	1.42168	1.75322	-2.87444
H	1.52865	3.50911	-2.62030
C	3.42065	2.45196	-2.37658
H	3.74962	2.57198	-3.41368
H	3.89340	3.23172	-1.77125
H	3.76155	1.47531	-2.01220
O	1.57202	2.35588	-0.90209
O	-0.48856	1.60226	-1.43751
C	-3.99512	0.16223	0.86727
H	-4.39632	0.70017	0.00186
H	-4.82784	-0.38103	1.33405
H	-3.61156	0.89823	1.57936
C	-1.78282	-1.13609	2.80959
H	-2.34119	-0.25538	3.13289
H	-2.12811	-2.01040	3.37691
H	-0.73059	-0.96066	3.06425
C	-0.04960	-3.15706	1.07901
H	0.45210	-2.67688	1.92639
H	-0.42405	-4.13457	1.41111
H	0.70612	-3.32382	0.30301
C	-1.14182	-3.17607	-1.88206
H	-0.09642	-2.88063	-2.05080
H	-1.16143	-4.24662	-1.64282
H	-1.68640	-3.03034	-2.81963
C	-3.54718	-1.01006	-2.03960
H	-4.57012	-1.40414	-1.98388
H	-3.61501	0.08181	-2.11282
H	-3.08852	-1.37725	-2.96227
C	1.40820	0.55570	1.43728
O	0.96101	-0.71020	-1.21492
O	1.48282	0.67092	2.66051
N	-2.49982	3.43152	-0.41414
N	-3.32581	2.93483	-0.95432
C	0.18364	3.41028	1.95168
H	0.15774	4.04040	1.05208
H	-0.32655	3.93335	2.76356
H	1.23341	3.23685	2.20685
O	-1.60976	1.86423	2.11949
C	6.09141	-1.10416	1.16467
H	6.85357	-0.58368	0.57004
H	6.11824	-0.68290	2.17513
H	6.40669	-2.15327	1.23535
C	-3.18164	-0.68887	-0.69599
C	-4.16135	0.14311	-0.13037
C	-3.58554	-1.74568	-1.53671
C	-5.51687	-0.03227	-0.36126
H	-3.82610	0.95771	0.51450
C	-4.94823	-1.93085	-1.77634
C	-5.88741	-1.09049	-1.19954
H	-5.26915	-2.74517	-2.42591
H	-6.94415	-1.25844	-1.40615
O	-2.65484	-2.54543	-2.08767
H	-3.09511	-3.22033	-2.61740
C	-6.55053	0.85833	0.25923
H	-6.08738	1.70031	0.78297
H	-7.23316	1.26832	-0.49438
H	-7.16446	0.31377	0.98712

553.9186	563.6388	587.0410
598.3832	608.5899	637.2789
657.9873	673.7416	728.8159
741.3105	778.8378	800.3510
806.9108	813.4168	824.0670
833.7274	843.3975	864.3317
894.3725	924.1010	939.8879
955.2932	962.1385	970.9599
996.8634	1002.3543	1022.0531
1035.3642	1039.0454	1042.5985
1044.1345	1046.3444	1049.1245
1059.6760	1084.1646	1091.0992
1095.2066	1111.0199	1126.6551
1137.7976	1146.9939	1174.8059
1181.4574	1187.5396	1205.4045
1231.6208	1250.7742	1274.3857
1286.8767	1337.8037	1343.2343
1367.4080	1376.5016	1383.3219
1384.5775	1394.2917	1396.6446
1397.3547	1400.7598	1404.4098
1427.5444	1436.6941	1439.3905
1443.6034	1444.6050	1446.1633
1452.6721	1454.5604	1456.5426
1458.2719	1459.0212	1459.2038
1462.3455	1468.8299	1471.5616
1472.5130	1479.3900	1485.0932
1486.1723	1487.7009	1505.7402
1512.3302	1519.4863	1529.1626
1554.1698	1609.3607	1673.6999
1686.4142	1735.7713	1848.7216
2461.5187	3022.3279	3026.1040
3030.0800	3036.3246	3037.8102
3040.2359	3041.6788	3046.2118
3059.2618	3094.1644	3099.2551
3111.4683	3113.2453	3117.3595
3118.2692	3125.3325	3129.9608
3131.3988	3133.0213	3141.4628
3142.2107	3145.7040	3147.9008
3149.8029	3165.3143	3170.0410
3174.6031	3175.7327	3186.1035

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.486913 Electronic Energy = -1521.46594684
Internal Energy (E)= -1520.94323484 Enthalpy (H)= -1520.94229084
Gibbs Free Energy (G)=-1521.04488184 Gibbs Free Energy of Solvation=-1521.0825957

St.Pt.	General Structure	Ball & Stick model
VII'-2		

Cartesian co-ordinate

Atoms	X	Y	Z
C	2.81326	-0.62524	-1.89362
C	2.29675	0.70690	-1.83911
C	2.57491	1.26786	-0.51931
C	3.20004	0.25332	0.26409
C	3.30090	-0.93785	-0.57451
O	-1.34180	0.97713	-1.53414
C	-1.74357	2.24082	-1.31113
O	-0.91822	3.12629	-1.30405
C	-3.23779	2.51059	-1.13472
C	-1.16936	-2.26953	-0.63266
H	-2.06786	0.34276	-1.43233
C	1.61673	1.45368	-2.92696
H	0.87678	2.14661	-2.51054
H	2.35071	2.03179	-3.50479
H	1.09510	0.77676	-3.61064
C	2.31523	2.68288	-0.14899
H	2.95070	3.34825	-0.74826
H	1.26728	2.95169	-0.33071
H	2.54116	2.86218	0.90618
C	3.86574	-2.23940	-0.13370
H	3.71024	-3.01419	-0.89031
H	4.94430	-2.14491	0.04970
H	3.38483	-2.56735	0.79438
C	2.70052	-1.58981	-3.02267
H	2.18747	-1.13645	-3.87589
H	3.68785	-1.92407	-3.36364
H	2.12015	-2.47124	-2.72280
C	3.73144	0.36579	1.64821
H	4.81843	0.51986	1.62630
H	3.27152	1.19301	2.19682
H	3.52146	-0.54202	2.22233
Ir	1.23567	-0.44988	-0.33683
C	-3.65964	3.39153	-2.31545
H	-3.57018	2.85588	-3.26943
H	-4.70768	3.69207	-2.19430

Frequencies

28.0081	38.8480	44.4947
57.0181	60.5211	67.8646
76.3602	78.5430	91.3699
96.5762	97.9606	99.9269
104.2754	110.0525	113.0671
123.4579	132.9219	133.9397
142.4114	146.3367	150.0442
151.5461	158.4699	161.0820
167.4570	177.1434	181.1870
187.6267	195.4322	199.7159
202.1296	218.1391	227.4732
243.3413	244.9557	251.9508
255.3678	263.9309	277.3727
285.5518	288.6292	294.9940
297.3137	304.9096	309.0043
322.6322	334.2567	341.9017
363.4994	364.9953	370.5794
372.6987	391.1825	397.0401
398.6695	407.2150	422.1411
425.1035	442.1200	444.7566
454.9700	489.0453	513.7018
521.8276	532.2608	533.4803
540.8585	548.4036	549.2607
552.5155	576.2030	584.7761
588.7045	604.4592	642.1674
649.5177	690.4450	712.9099
738.1201	752.6448	770.4208
782.1454	799.3474	805.8715
811.8591	814.3259	822.4829
836.6902	873.2556	885.0110
890.1125	899.9253	917.0604
948.5143	956.2870	957.5308
960.6384	964.7134	968.7209
969.7033	993.4932	1003.7965
1012.0664	1025.6560	1030.0659
1037.6244	1041.5172	1044.3048
1049.1828	1050.0286	1052.4167
1052.9623	1092.0931	1096.1435
1101.0400	1112.0863	1118.5315

H	-3.03999	4.29254	-2.36657	1140.6374	1145.6957	1170.0113
C	-4.09257	1.24714	-1.09756	1179.3036	1185.2926	1189.7475
H	-3.84682	0.62316	-0.22878	1194.4679	1213.7645	1232.4104
H	-5.14805	1.52942	-1.00667	1242.8830	1255.7780	1273.0333
H	-4.00817	0.65648	-2.02161	1276.0894	1291.2874	1304.2200
C	-3.40376	3.28188	0.17593	1332.8598	1368.9915	1372.3023
H	-3.01248	2.70020	1.02121	1374.0665	1380.2033	1382.6428
H	-2.86806	4.23542	0.12342	1386.2074	1387.5710	1389.3462
H	-4.46724	3.48753	0.35055	1391.9380	1396.5995	1401.5185
O	-0.00298	-1.85129	-1.08523	1406.8085	1417.8882	1423.1116
C	-1.95245	-1.60337	0.33787	1429.5856	1435.5971	1436.2617
C	-3.23391	-2.09647	0.64970	1441.0169	1447.5434	1448.0831
C	-1.71137	-3.42978	-1.22833	1450.6194	1452.1479	1455.5812
C	-3.75755	-3.23783	0.07062	1455.9604	1456.5388	1462.6732
C	-2.96086	-3.89749	-0.88182	1464.6752	1468.2260	1468.8701
C	-1.49300	-0.41301	1.09291	1469.9633	1471.4117	1476.1911
O	-2.31590	0.37982	1.54074	1479.6138	1482.6440	1483.9517
H	-1.10654	-3.93249	-1.97938	1492.1703	1497.0509	1497.9230
H	-3.34438	-4.80047	-1.35841	1501.8399	1516.3159	1518.3574
H	-3.80661	-1.54922	1.39922	1520.4456	1527.2851	1547.4111
C	-0.02093	-0.31859	1.40430	1607.2168	1680.3182	1743.6719
C	0.35228	-1.52939	2.29840	1789.8994	1819.5792	1859.8981
C	0.35404	0.89355	2.19249	3018.9509	3028.8775	3030.8416
C	0.22263	3.20789	2.47744	3031.6258	3031.8414	3036.1587
H	1.31475	3.30553	2.54889	3040.1692	3041.3847	3041.6445
H	-0.14144	3.04787	3.49959	3046.9291	3049.0721	3056.2307
C	-0.40848	4.40882	1.82622	3095.4069	3097.9311	3106.0487
H	-0.06825	5.32492	2.32036	3113.6294	3114.8631	3116.5583
H	-0.15062	4.46051	0.76220	3119.4018	3129.6340	3130.2019
H	-1.49887	4.36438	1.90146	3130.5284	3133.7354	3134.2387
O	-0.09273	2.05322	1.68702	3139.1955	3142.0526	3143.5052
O	1.04688	0.84580	3.19502	3144.6264	3145.0441	3146.7846
O	1.32558	-2.22668	2.09444	3149.0380	3156.1700	3156.5996
C	-0.57190	-1.80193	3.45489	3160.6974	3164.8120	3172.3886
H	-0.07226	-2.44714	4.18051	3181.0301	3201.8792	3800.4504
H	-0.90265	-0.87257	3.92794			
H	-1.46569	-2.31774	3.07897			
C	-5.10882	-3.76948	0.44413			
H	-5.76859	-3.85089	-0.42906			
H	-5.04141	-4.77214	0.88549			
H	-5.60300	-3.12006	1.17419			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.629696 Electronic Energy = -1758.83708295
Internal Energy (E)= -1758.16590795 Enthalpy (H)= -1758.16496295
Gibbs Free Energy (G)=-1758.27801795 Gibbs Free Energy of Solvation=-1758.3348937

St.Pt.	General Structure	Ball & Stick model
TS_2-7		
Cartesian co-ordinate		**Frequencies**

Atoms	X	Y	Z
C	1.67468	-2.00349	-1.94067
C	2.63544	-1.13147	-1.37597
C	2.68538	-1.36819	0.06466
C	1.79892	-2.46674	0.36307
C	1.10265	-2.79926	-0.85775
O	0.34172	1.39349	-0.89520
C	0.92300	2.59081	-0.98344
O	2.09625	2.73533	-0.71741
C	-0.00868	3.74307	-1.34831
C	-2.34862	-0.30953	-1.06754
H	-0.52747	0.96061	-1.39702
C	3.42196	-0.07332	-2.06384
H	3.27932	0.89703	-1.57259
H	4.49218	-0.31559	-2.03104
H	3.13056	0.03011	-3.11335
C	3.62642	-0.69572	1.00042
H	4.62945	-1.13884	0.93804
H	3.70684	0.37043	0.75296
H	3.27512	-0.77862	2.03442
C	0.07882	-3.85902	-1.05294
H	-0.64672	-3.55208	-1.81565
H	0.55070	-4.79178	-1.39028
H	-0.47643	-4.04528	-0.13204
C	1.21717	-2.06715	-3.35492
H	1.65933	-1.26738	-3.95635
H	1.48805	-3.02715	-3.81248
H	0.12720	-1.96091	-3.41222
C	1.69104	-3.16023	1.67338
H	2.55754	-3.82224	1.80171
H	1.68081	-2.44423	2.50305
H	0.78201	-3.76337	1.73354
Ir	0.67716	-0.76568	-0.37612
C	0.75045	4.71540	-2.24735
H	0.97738	4.26499	-3.22206
H	0.14333	5.61198	-2.42261
H	1.69485	5.01496	-1.78326
C	-1.29211	3.28036	-2.03327
H	-1.92242	2.67819	-1.36556
H	-1.88142	4.15726	-2.32694
H	-1.08981	2.70068	-2.94399
C	-0.36020	4.42323	-0.01761
H	-0.82770	3.71761	0.68255
H	0.53884	4.83664	0.45392
H	-1.06349	5.24477	-0.20450
O	-1.10190	-0.25176	-1.57553
C	-2.65489	0.24299	0.18610
C	-3.98821	0.30625	0.60566
C	-3.38259	-0.83936	-1.84481
C	-5.02241	-0.21709	-0.16003
C	-4.69068	-0.80094	-1.38949
C	-1.61231	0.71639	1.13472
O	-1.78312	1.73685	1.78259
H	-3.13020	-1.26194	-2.81527
H	-5.48449	-1.22470	-2.00514
H	-4.19701	0.76231	1.57382

-892.2231	-116.0005	-83.2172
-47.1077	-38.6385	31.4624
46.8324	59.6524	66.1514
69.1895	80.6594	86.8099
93.8134	105.0165	109.1578
115.5822	120.6053	122.4015
127.3210	132.4672	136.1519
141.9003	153.5861	159.5331
160.9744	168.3657	172.6953
184.1679	192.2777	201.7683
210.5753	215.6963	219.3265
225.2251	232.9466	256.5025
258.7861	266.5017	274.8005
276.1285	279.2473	288.8830
294.4038	298.1027	305.1043
315.2676	317.7048	325.2554
326.0116	348.3050	361.0656
366.6535	376.7370	385.1344
387.9299	401.9515	408.3520
414.8627	431.8559	434.2876
446.4299	457.7480	488.9051
501.5116	533.5489	535.0620
538.9496	546.0393	557.5277
560.5730	582.0235	587.8719
588.4344	602.4504	609.2257
635.3446	656.8817	689.8195
727.2756	744.7278	771.8782
783.1009	798.3953	803.9665
810.6440	812.2494	834.5457
837.0976	873.9787	882.8331
893.3533	908.4467	937.3052
945.5791	947.1461	951.2571
953.5845	956.8164	963.3446
971.0747	990.7583	1013.4066
1021.8799	1027.7199	1029.9047
1036.0609	1037.6715	1040.1982
1044.0186	1045.7995	1048.8850
1051.0911	1089.0014	1089.8520
1096.6696	1108.3926	1120.9471
1134.2720	1145.8085	1171.1954
1179.9501	1183.4479	1185.5238
1200.6856	1211.9901	1223.8895
1235.4861	1251.3195	1264.0903
1281.5064	1288.2229	1308.8650
1317.4142	1344.9942	1366.0598
1371.3876	1371.5113	1374.3135
1379.4388	1380.0169	1384.5892
1385.4582	1394.4209	1397.9713
1402.9393	1415.8969	1418.8414
1427.0652	1435.9256	1438.5660
1441.8972	1442.5331	1445.3080
1445.6415	1445.9713	1453.6343
1453.9411	1455.5307	1456.2598
1460.9280	1463.5607	1464.5487
1465.6564	1467.8715	1471.6833
1475.5203	1477.4663	1480.0512
1483.0819	1483.8459	1486.3717
1496.6439	1503.0693	1506.9049
1511.0148	1530.0538	1558.2843
1628.4435	1675.7250	1771.2772
1781.2211	1826.6945	1831.4997

C	-0.46098	-0.24689	1.40183	2070.6286	3024.0207	3027.0684
C	-1.15515	-1.47532	2.02017	3031.1496	3031.2595	3031.7498
C	0.58641	0.29029	2.32475	3035.1985	3035.8339	3037.0382
C	1.97409	2.09503	2.89919	3037.6523	3049.0018	3050.9509
H	2.91714	1.55785	2.73070	3051.8281	3101.1154	3103.2338
H	1.68815	1.92471	3.94399	3107.4196	3108.3593	3111.6395
C	2.09733	3.55826	2.56989	3112.8119	3115.8171	3116.0585
H	2.85285	4.02477	3.21082	3117.7603	3119.2308	3122.9524
H	2.39135	3.69298	1.52338	3133.3769	3136.0416	3137.0264
H	1.14167	4.06822	2.73447	3138.5938	3139.6998	3144.0435
O	0.96442	1.54113	2.04622	3144.6648	3150.3015	3161.1196
O	1.11271	-0.36384	3.21376	3164.2404	3164.2621	3167.2724
O	-1.34259	-2.50497	1.40430	3173.2433	3191.5842	3211.0222
C	-1.67899	-1.31562	3.42397			
H	-2.47210	-2.04597	3.60050			
H	-0.85436	-1.49608	4.12178			
H	-2.03677	-0.29696	3.61382			
C	-6.44825	-0.16184	0.30199			
H	-7.04779	0.51633	-0.31877			
H	-6.92655	-1.14766	0.25166			
H	-6.51928	0.19064	1.33611			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.622812 Electronic Energy = -1758.82699130
Internal Energy (E)= -1758.1659303 Enthalpy (H)= -1758.1649863
Gibbs Free Energy (G)=-1758.2699963 Gibbs Free Energy of Solvation=-1758.31872946

St.Pt.	General Structure	Ball & Stick model
VIII-2		

Cartesian co-ordinate

Atoms	X	Y	Z
C	1.13549	-2.56228	-1.57369
C	2.26642	-1.93985	-0.99353
C	2.09886	-1.97065	0.45739
C	0.90326	-2.74909	0.75230
C	0.26966	-3.03656	-0.49522
O	0.73811	1.03970	-1.10637
C	1.79365	1.79622	-0.98433
O	2.81583	1.48210	-0.38573
C	1.64698	3.17421	-1.64616
C	-2.53304	0.20373	-1.25852
H	-0.74690	0.55856	-1.93821
C	3.40835	-1.31380	-1.70903
H	3.73809	-0.40820	-1.19322
H	4.24741	-2.01972	-1.76728

Frequencies

35.1438	54.9639	62.3042
64.0574	68.4333	78.1437
82.2259	91.2906	94.5255
101.4387	103.4915	110.5772
116.4562	118.0715	126.3978
132.0394	138.1678	140.2117
143.5743	147.9218	153.4864
154.4846	167.8784	176.3248
188.0045	191.6878	198.0812
206.9178	210.2304	217.8573
220.4319	228.1678	240.6564
249.8217	253.5542	256.8415
268.9509	281.4357	288.4418
290.4920	296.6641	313.3992
323.2311	329.9390	333.6835
334.0758	343.9135	347.6790
361.3141	362.9038	373.2353
382.5421	387.1841	394.7455

H	3.13359	-1.03223	-2.73118	404.5032	405.9866	408.8683
C	3.10003	-1.47600	1.43803	426.6249	433.4941	442.8987
H	3.93694	-2.18133	1.53016	468.1451	477.2769	482.1312
H	3.49017	-0.50549	1.10863	518.3172	533.4434	539.2370
H	2.64378	-1.34766	2.42546	544.4883	553.0329	563.8677
C	-1.00657	-3.76490	-0.72329	576.7262	585.4469	595.2534
H	-1.57795	-3.28776	-1.52851	596.9753	605.2358	631.5624
H	-0.80721	-4.80331	-1.02050	651.4780	683.5213	718.3181
H	-1.63863	-3.75883	0.16643	734.7126	776.1087	786.7900
C	0.81802	-2.69238	-3.02146	802.4643	808.1202	810.5087
H	1.47836	-2.07117	-3.63410	813.4238	814.9915	828.0386
H	0.92583	-3.73272	-3.35502	834.3563	871.9261	882.4334
H	-0.21362	-2.38240	-3.22224	895.6899	916.3418	922.6396
C	0.47555	-3.19787	2.10312	948.5377	949.3228	954.3049
H	1.06909	-4.07252	2.40061	954.7711	960.1832	970.1466
H	0.62509	-2.40957	2.84861	986.5939	991.0563	1014.2486
H	-0.58146	-3.47536	2.11502	1020.5822	1021.6384	1034.2622
Ir	0.44172	-0.88575	-0.29230	1037.0506	1038.0188	1039.5391
C	2.88698	3.43423	-2.49950	1048.0663	1048.1809	1054.5669
H	2.94489	2.73687	-3.34626	1058.2637	1092.7959	1099.2537
H	2.85850	4.45358	-2.90629	1106.0788	1119.5297	1119.9837
H	3.79635	3.32045	-1.90101	1137.4751	1149.5297	1182.8426
C	0.38996	3.28001	-2.50306	1188.2052	1190.1377	1190.3613
H	-0.51557	3.15088	-1.89764	1211.9434	1237.3424	1244.0695
H	0.34245	4.27250	-2.97000	1247.4222	1260.7989	1268.9485
H	0.38349	2.53213	-3.30692	1286.6907	1293.3711	1319.8608
C	1.57028	4.20364	-0.51474	1345.6681	1365.2300	1365.8329
H	0.76432	3.95482	0.18817	1376.6947	1377.7978	1378.4297
H	2.51338	4.24126	0.04044	1381.2457	1382.0370	1382.8250
H	1.37769	5.20051	-0.93305	1396.0644	1400.6302	1402.5866
O	-1.31963	-0.22599	-1.77056	1404.5194	1416.4727	1419.5462
C	-2.57953	1.04544	-0.15008	1431.1451	1432.2067	1440.1834
C	-3.82318	1.52051	0.27103	1440.7069	1443.5112	1447.6371
C	-3.69587	-0.20641	-1.89306	1450.1711	1451.3205	1452.4916
C	-5.00773	1.12578	-0.34640	1454.8259	1459.3091	1463.0280
C	-4.92413	0.24140	-1.42512	1463.7891	1468.2142	1469.4317
C	-1.38506	1.39136	0.69524	1472.2864	1474.1532	1479.8153
O	-1.17536	2.55329	0.98657	1483.7691	1485.6348	1490.2404
H	-3.61924	-0.86430	-2.75529	1492.8240	1496.7942	1499.8715
H	-5.83885	-0.08848	-1.91636	1510.7249	1523.6576	1530.3985
H	-3.84990	2.19574	1.12642	1532.3549	1538.3383	1559.6099
C	-0.65277	0.19664	1.27095	1651.8322	1680.1466	1764.0861
C	-1.74416	-0.69784	1.88733	1768.6223	1796.1435	1829.1818
C	0.38995	0.49739	2.30150	3023.8936	3027.7114	3036.2331
C	2.19463	1.80073	3.00974	3036.8991	3038.0941	3038.3591
H	2.83245	0.90860	3.04312	3038.6620	3041.2024	3044.5336
H	1.75926	1.92224	4.00982	3047.0004	3048.2784	3056.1348
C	2.96268	3.01281	2.56120	3104.2967	3107.8406	3111.0416
H	3.77937	3.21538	3.26235	3117.0202	3117.0651	3120.9465
H	3.38044	2.84026	1.56332	3122.6487	3124.3562	3128.9216
H	2.31292	3.89362	2.52385	3130.1793	3137.4138	3138.4942
O	1.13184	1.57750	2.07147	3138.9908	3140.8164	3143.5874
O	0.58765	-0.23417	3.26376	3148.3739	3152.3630	3157.7383
O	-2.16357	-1.70088	1.34571	3159.6963	3164.5575	3164.6876
C	-2.34746	-0.22554	3.18706	3171.8997	3172.9622	3175.7981
H	-3.36614	-0.61210	3.27472	3188.9344	3200.6236	3499.1747
H	-1.74083	-0.61596	4.01083			
H	-2.33889	0.86757	3.27377			
C	-6.33674	1.63540	0.12540			
H	-6.75411	2.37041	-0.57426			
H	-7.06843	0.82400	0.21337			

H	-6.25437	2.12232	1.10230	

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.631281 Electronic Energy = -1758.84125177
Internal Energy (E)= -1758.16938677 Enthalpy (H)= -1758.16844277
Gibbs Free Energy (G)=-1758.27797777 Gibbs Free Energy of Solvation=-1758.32831181

St.Pt.	General Structure	Ball & Stick model
VIII'-2		

Cartesian co-ordinate

Atoms	X	Y	Z
H	0.97884	1.32646	0.35925
C	-1.98705	-2.44583	-1.56000
C	-1.59155	-2.90684	-0.27039
C	-2.53737	-2.38836	0.71144
C	-3.53465	-1.62359	0.01002
C	-3.16692	-1.60167	-1.39689
C	-2.76088	1.97487	0.12516
O	-1.88122	1.15034	0.61207
O	-3.63216	1.69256	-0.69190
C	-2.56915	3.42370	0.60124
O	0.06935	-0.57709	1.36139
C	0.52059	0.40975	1.94600
O	0.98695	1.46997	1.33997
C	0.60159	0.44380	3.45989
C	-4.71581	-0.95434	0.61268
H	-5.59994	-1.59846	0.52047
H	-4.55467	-0.75002	1.67629
H	-4.90691	0.00018	0.11536
C	-3.91130	-0.93686	-2.49695
H	-4.62060	-1.63455	-2.96152
H	-4.44521	-0.05882	-2.12603
H	-3.21585	-0.58696	-3.26630
C	-2.50212	-2.69226	2.16580
H	-1.48107	-2.60598	2.55269
H	-3.13325	-2.00072	2.73284
H	-2.85454	-3.71331	2.36163
C	-0.40480	-3.73986	0.05870
H	-0.01529	-3.48248	1.05003
H	-0.67413	-4.80414	0.06467
H	0.40562	-3.56892	-0.65374
C	-1.30992	-2.72373	-2.85272
H	-0.26124	-2.98790	-2.70132
H	-1.81603	-3.54684	-3.37385
H	-1.33320	-1.84436	-3.50378
C	-0.83140	0.31019	3.98318
H	-0.82656	0.30903	5.08002

Frequencies

-26.0554	-10.4801	31.7417
40.0619	45.2716	56.5993
64.7154	67.4413	76.4374
78.4569	83.9817	87.3911
92.1241	96.7850	98.3300
104.9099	112.1095	120.1644
120.8557	125.7439	129.8184
135.8738	140.6916	145.5828
149.8269	158.7139	163.3851
167.6110	177.8825	181.1554
183.0823	190.7116	191.9295
195.8416	203.1842	207.0396
213.3808	218.9292	221.9433
224.0592	233.4488	238.0107
246.2097	248.6390	249.9629
253.9603	266.0060	273.6761
286.7023	299.8459	304.9784
309.3162	310.5881	317.3231
318.5061	319.7177	320.3180
321.6071	328.9227	332.4507
338.2895	340.1862	341.9541
351.1595	356.0243	374.9176
393.4142	395.0072	399.1456
401.7959	406.5081	420.2154
427.1699	433.5910	442.2124
448.8826	459.9567	473.0403
475.3021	504.3397	535.0865
536.5423	540.1851	543.4631
546.4498	569.9466	584.6361
586.8183	591.0729	593.6780
601.7770	621.8789	628.9774
633.2279	674.1292	686.7254
719.5650	752.7730	767.2754
781.3353	792.8306	798.2469
805.7943	807.2204	807.7719
811.5869	818.0707	819.4221
832.3243	865.7984	899.5489
906.1731	914.0707	916.5177
938.2126	948.7576	953.4661
956.6529	957.2979	962.8339

H	-1.45406	1.14356	3.63529	965.9464	973.6535	974.0432
H	-1.28935	-0.62010	3.63092	984.3218	996.8644	1020.3466
C	1.23176	1.73113	3.97811	1032.4145	1032.5815	1036.2505
H	1.27048	1.70026	5.07395	1038.8396	1042.8864	1045.2632
H	2.25185	1.86078	3.60094	1045.9022	1046.6854	1048.0500
H	0.64933	2.61063	3.68140	1053.5737	1056.1133	1059.4703
C	1.44203	-0.76190	3.89259	1094.7609	1100.6118	1107.9354
H	1.00325	-1.70161	3.53582	1108.3067	1139.5348	1146.8034
H	2.46370	-0.69142	3.49442	1162.9014	1179.8293	1185.4439
H	1.50282	-0.79835	4.98704	1189.0587	1191.3619	1234.8760
C	-3.87437	4.19466	0.44634	1237.1779	1239.6669	1243.3690
H	-4.64945	3.79647	1.11321	1249.8229	1269.6097	1271.3457
H	-3.72221	5.25316	0.69546	1279.5397	1282.7310	1291.2346
H	-4.25004	4.12021	-0.57835	1306.5621	1315.3823	1323.4474
C	-1.50290	4.01999	-0.32409	1364.5701	1371.2875	1372.0319
H	-1.30012	5.06467	-0.05327	1374.1779	1377.5474	1379.6025
H	-0.56185	3.45734	-0.24889	1381.2456	1383.8363	1386.9681
H	-1.83878	3.99394	-1.36835	1389.2328	1391.4958	1393.4970
C	-2.08438	3.49928	2.04569	1395.2224	1401.2364	1411.6910
H	-1.99051	4.54980	2.35233	1416.1966	1417.2321	1424.5430
H	-2.79235	3.01427	2.73131	1428.2838	1430.7600	1437.0362
H	-1.10522	3.02063	2.16118	1437.6945	1441.0973	1444.4273
Ir	-1.60858	-0.73555	-0.28125	1448.5531	1449.4067	1450.0668
C	1.50056	0.89079	-1.55437	1451.2391	1455.4582	1455.8692
C	1.81797	-0.48281	-1.19973	1458.3959	1460.1828	1460.8015
O	0.99656	-1.40436	-1.26932	1463.7517	1467.4235	1469.4788
C	3.18974	-0.88319	-0.72184	1469.9855	1472.5008	1475.6086
C	4.35931	-0.70025	-1.46487	1477.9492	1479.4508	1479.7007
C	3.26818	-1.57352	0.48499	1482.3057	1482.6168	1483.9473
C	5.57406	-1.17646	-0.98163	1487.5890	1488.6406	1493.7315
C	4.47831	-2.03817	1.00201	1502.5042	1512.4467	1513.4451
H	2.33810	-1.74654	1.03084	1515.5683	1517.0490	1539.9297
C	5.63076	-1.83156	0.24456	1552.9664	1579.9754	1661.0117
H	6.47954	-1.03768	-1.57356	1678.3960	1706.7468	1759.3303
H	6.58879	-2.19897	0.61146	1766.6549	1832.0011	3018.5153
O	4.25573	-0.05033	-2.65532	3020.2281	3023.9499	3028.7006
H	5.12507	0.01739	-3.06359	3032.0365	3037.1065	3037.8376
C	0.21835	1.18753	-2.11655	3039.3753	3039.6641	3040.4764
C	2.55756	1.91815	-1.63112	3041.2124	3043.8719	3044.6488
C	4.56443	2.61041	-0.59712	3046.3903	3054.5404	3088.5025
H	4.30980	3.67549	-0.66644	3098.8549	3102.0298	3106.5117
H	5.11842	2.35153	-1.51174	3111.5784	3113.1677	3114.8025
C	5.34561	2.28152	0.64928	3120.4414	3124.4684	3124.8540
H	6.29675	2.82384	0.66440	3125.4694	3127.0959	3127.7982
H	4.77758	2.55699	1.54408	3128.6285	3129.4319	3130.4160
H	5.55328	1.20544	0.69502	3135.9094	3136.8635	3138.7666
O	3.37126	1.83398	-0.55110	3141.0943	3146.6514	3148.7779
O	2.70423	2.77923	-2.47372	3149.5975	3153.3702	3154.1347
C	0.03234	2.32769	-3.07869	3154.6103	3163.0449	3164.7984
H	-1.02828	2.39194	-3.33497	3168.5406	3170.8096	3171.7306
H	0.38042	3.27357	-2.65298	3176.8331	3381.8933	3897.7677
H	0.64301	2.17344	-3.97399			
O	-0.83930	0.54566	-1.86585			
C	4.53895	-2.73472	2.32991			
H	5.26491	-3.55605	2.32172			
H	4.83981	-2.05140	3.13576			
H	3.56391	-3.15269	2.60580			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.777792 Electronic Energy = -2105.66317227
Internal Energy (E)= -2104.83645427 Enthalpy (H)= -2104.83551027
Gibbs Free Energy (G)=-2104.96181227 Gibbs Free Energy of Solvation=-2105.03088256

St.Pt.	General Structure	Ball & Stick model
TS_2-8		

Cartesian co-ordinate

Atoms	X	Y	Z
H	1.14898	1.16800	-0.06184
C	-1.99547	-2.27966	-1.69224
C	-1.55097	-2.86434	-0.47043
C	-2.48685	-2.47070	0.57790
C	-3.52758	-1.66932	-0.02988
C	-3.19957	-1.50265	-1.42699
C	-2.84393	1.95072	0.23709
O	-2.01027	1.09791	0.75372
O	-3.70917	1.69421	-0.59518
C	-2.58280	3.39628	0.68739
O	0.02375	-0.64460	1.22409
C	0.49892	0.38207	1.80239
O	0.93056	1.40570	1.21186
C	0.59115	0.32313	3.32605
C	-4.68704	-1.06352	0.67558
H	-5.56384	-1.71928	0.60032
H	-4.46318	-0.91198	1.73686
H	-4.92184	-0.08520	0.24606
C	-3.98239	-0.77586	-2.46153
H	-4.54815	-1.48152	-3.08471
H	-4.66546	-0.05708	-2.00550
H	-3.31331	-0.20230	-3.11245
C	-2.40146	-2.91290	1.99498
H	-1.38488	-2.76969	2.37867
H	-3.08196	-2.34252	2.63453
H	-2.65664	-3.97638	2.08905
C	-0.33590	-3.69479	-0.25431
H	0.06118	-3.53577	0.75565
H	-0.56767	-4.76247	-0.36095
H	0.45516	-3.42454	-0.95974
C	-1.37650	-2.40968	-3.03649
H	-0.36402	-2.81163	-2.98179
H	-1.99329	-3.07239	-3.65811
H	-1.32284	-1.43755	-3.53731
C	-0.83110	0.20353	3.87870
H	-0.79825	0.08929	4.97009
H	-1.42423	1.09496	3.64210
H	-1.34526	-0.66281	3.44758
C	1.26851	1.56756	3.88496
H	1.33408	1.49513	4.97837

Frequencies

-1460.5629	-85.0322	29.4182
32.7415	38.0021	44.1669
52.9975	59.7711	67.2918
74.0594	76.6495	79.9012
83.5646	92.4229	95.6480
104.1104	108.4854	111.5102
114.3929	116.3070	120.3718
126.4208	132.6780	139.3049
141.4048	146.4381	153.2072
158.4680	164.6894	171.8692
180.5918	193.5591	196.6040
201.4680	204.4035	210.1287
216.0357	218.3752	224.6195
228.0019	230.8523	233.5380
237.3333	248.4446	251.2287
253.9035	262.8106	272.7194
279.1581	286.1258	300.3066
304.8660	305.9301	310.4398
318.6329	323.4546	324.3647
327.7090	330.7103	336.9560
341.5723	344.5034	346.6667
349.3246	358.2168	372.5515
387.2421	393.5282	397.8626
404.2500	407.4511	413.2196
421.8572	433.1174	441.8789
446.6683	458.3330	463.2696
468.4766	471.1499	519.8935
536.7641	538.7233	540.5044
548.2193	567.5238	572.1974
587.6507	591.5429	595.7860
605.3477	614.7276	623.0608
634.9473	677.6173	692.1958
712.9266	750.0867	779.2624
789.6959	801.5417	804.0612
805.4656	807.7001	813.7524
814.1049	817.5157	822.7114
854.9180	872.2660	907.0385
911.6078	916.4916	920.9324
931.2620	945.1560	947.4302
948.5103	952.6498	958.1701
962.6456	962.9565	972.2108
974.6861	995.1744	1013.9505
1029.5558	1032.1088	1036.4055
1037.9099	1041.1425	1041.4452

H	2.28052	1.68316	3.48152	1042.6168	1048.0489	1048.8318
H	0.70637	2.47337	3.63217	1050.1743	1051.5731	1055.9491
C	1.40240	-0.91990	3.70169	1090.9562	1096.0842	1097.9240
H	0.92889	-1.83396	3.32262	1109.5058	1138.6268	1143.4030
H	2.41880	-0.86397	3.28701	1154.1423	1173.6972	1176.3607
H	1.48466	-0.99761	4.79338	1186.2959	1189.3450	1216.5441
C	-3.84557	4.23037	0.51373	1235.0614	1240.6852	1250.1240
H	-4.64288	3.88222	1.18250	1251.9497	1268.1059	1270.4789
H	-3.64073	5.28334	0.74841	1273.4730	1281.5284	1291.8366
H	-4.22010	4.16047	-0.51190	1296.2743	1311.6340	1326.0593
C	-1.48201	3.91149	-0.24899	1357.2065	1368.6977	1370.7660
H	-1.25021	4.96084	-0.02287	1372.4071	1374.2365	1375.1190
H	-0.56402	3.32073	-0.11917	1377.9047	1379.0552	1381.3295
H	-1.80195	3.84547	-1.29734	1385.9688	1386.9689	1393.8409
C	-2.08519	3.47541	2.12688	1397.6764	1400.5026	1403.0143
H	-1.93944	4.52594	2.41281	1403.5878	1404.2399	1413.1069
H	-2.80723	3.03457	2.82723	1417.2033	1429.2696	1431.7813
H	-1.12865	2.95229	2.23821	1435.9229	1439.6260	1443.8620
Ir	-1.62242	-0.71209	-0.22088	1446.2110	1447.1648	1447.9637
C	1.50609	1.01913	-1.31299	1450.8943	1452.9541	1455.1525
C	1.89134	-0.42823	-1.33823	1456.4054	1457.7980	1460.3941
O	1.13893	-1.29143	-1.76246	1461.7886	1464.6566	1466.4172
C	3.19881	-0.88138	-0.75369	1470.1819	1472.1501	1473.5740
C	4.42027	-0.64785	-1.38497	1476.5494	1477.3114	1477.5003
C	3.16413	-1.67547	0.38787	1479.3171	1482.2307	1486.3538
C	5.58996	-1.17829	-0.85158	1489.0185	1490.2393	1493.9191
C	4.32635	-2.21042	0.94659	1498.5048	1504.0104	1506.9680
H	2.19279	-1.86841	0.84632	1510.2858	1513.1405	1529.6051
C	5.53742	-1.94779	0.30664	1545.3174	1554.9921	1667.8824
H	6.54225	-0.99817	-1.35146	1682.5280	1692.7252	1707.2595
H	6.45925	-2.36416	0.71186	1764.3546	1786.5202	1851.3055
O	4.39636	0.10179	-2.52096	3013.6621	3017.7118	3025.8101
H	5.28678	0.18305	-2.87832	3025.9601	3031.1546	3032.9601
C	0.24476	1.31196	-2.02748	3037.0904	3037.3624	3038.4056
C	2.61177	2.02592	-1.41731	3039.2956	3040.6350	3040.7290
C	4.63632	2.66798	-0.39588	3042.7029	3047.7378	3055.9657
H	4.36684	3.73086	-0.42332	3093.3679	3095.4888	3100.9271
H	5.18837	2.44875	-1.32116	3101.9476	3106.6573	3110.6982
C	5.41807	2.29770	0.83764	3113.0505	3116.3737	3120.7190
H	6.37386	2.83088	0.86417	3121.5023	3122.7575	3122.8669
H	4.85479	2.55197	1.74109	3124.5406	3124.6311	3124.9692
H	5.61536	1.21892	0.85184	3127.6623	3137.0881	3139.7433
O	3.44783	1.87770	-0.37798	3141.3251	3141.4870	3143.4050
O	2.74580	2.89427	-2.25066	3145.8717	3147.7257	3153.9923
C	0.16062	2.33075	-3.11767	3154.7797	3155.9669	3163.1955
H	-0.84895	2.31718	-3.53535	3172.5875	3173.9566	3174.9171
H	0.38875	3.32375	-2.71533	3184.5201	3192.9693	3897.0632
H	0.91912	2.14661	-3.88415			
O	-0.81444	0.74481	-1.71878			
C	4.27806	-3.04984	2.18955			
H	4.94465	-3.91690	2.11373			
H	4.58965	-2.48345	3.07736			
H	3.26534	-3.42275	2.37962			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm

Zero-point correction= 0.772620 Electronic Energy = -2105.65122227

Internal Energy (E)= -2104.82917627	Enthalpy (H)= -2104.82823127
Gibbs Free Energy (G)=-2104.95693327	Gibbs Free Energy of Solvation=-2105.02334442

St.Pt.	General Structure	Ball & Stick model
IX-2		

Cartesian co-ordinate

Atoms	X	Y	Z
H	1.21081	1.02093	-0.20598
C	-2.06648	-1.90714	-1.94951
C	-1.70330	-2.69807	-0.82068
C	-2.65893	-2.41031	0.24052
C	-3.63975	-1.46712	-0.28065
C	-3.25252	-1.12659	-1.62103
C	-2.74212	2.06602	0.47573
O	-1.97343	1.09916	0.88848
O	-3.65226	1.96436	-0.34065
C	-2.32571	3.42678	1.05063
O	0.03741	-0.77210	1.02163
C	0.45782	0.12098	1.87477
O	0.86484	1.24361	1.58169
C	0.43575	-0.33495	3.34027
C	-4.79610	-0.92273	0.47758
H	-5.67394	-1.57032	0.35613
H	-4.56197	-0.86093	1.54635
H	-5.03420	0.08893	0.13869
C	-3.95206	-0.21032	-2.55841
H	-4.61770	-0.77314	-3.22649
H	-4.52265	0.54233	-2.01190
H	-3.22666	0.33173	-3.17428
C	-2.68949	-3.08586	1.56423
H	-1.68189	-3.15627	1.98795
H	-3.31693	-2.54387	2.27834
H	-3.09013	-4.10343	1.46555
C	-0.52830	-3.60248	-0.69910
H	-0.15299	-3.60636	0.33030
H	-0.79124	-4.63388	-0.96720
H	0.29305	-3.26702	-1.34035
C	-1.39408	-1.87414	-3.27413
H	-0.39306	-2.30682	-3.23658
H	-2.00046	-2.43268	-3.99955
H	-1.29883	-0.84699	-3.64165
C	-1.03147	-0.35385	3.78266
H	-1.11005	-0.73167	4.81122
H	-1.46597	0.65268	3.75072
H	-1.63293	-0.99260	3.12459
C	1.22238	0.63553	4.21230

Frequencies

25.9922	30.7813	37.6946
48.6267	52.8946	56.2014
63.3247	67.1827	71.7243
75.6540	81.9482	84.8428
89.3752	92.7026	104.7246
107.5166	114.4212	119.9627
124.0809	127.5273	134.0952
139.7160	145.5510	150.9619
155.7961	161.6810	166.3695
170.7831	184.7615	185.6451
187.3977	197.7223	199.9065
202.3551	206.9121	211.9173
215.5939	224.3279	231.2881
233.8324	244.1743	248.7046
255.5533	261.6120	264.4716
277.6333	278.9827	293.0339
298.6323	301.4830	309.9743
313.6370	313.7251	315.9768
324.1993	327.8381	329.8394
338.8783	340.0629	345.5170
348.7352	354.5008	369.7388
371.6989	379.0100	386.9194
388.9454	390.2732	393.6869
398.8835	411.3071	417.0094
421.1668	425.3341	436.5740
451.8814	453.3633	470.1194
470.8791	517.9525	531.7076
537.0250	538.4676	546.7864
557.3636	572.5249	574.2374
578.5488	588.4110	603.0492
603.9976	608.2922	628.8417
641.0975	675.4066	687.7899
742.9557	765.0090	789.8764
796.0133	799.1315	802.6475
805.2956	811.2210	812.4774
813.3024	816.6427	855.4465
859.7276	902.1528	908.5440
913.0563	921.6774	924.4943
941.6996	949.5542	953.6972
954.4455	959.0578	961.3826
970.3871	980.7967	986.9962
997.7417	1012.7788	1015.7244
1032.1199	1034.8993	1038.5849

H	1.18465	0.31466	5.26208	1042.8670	1044.1937	1045.0791
H	2.27325	0.68105	3.90217	1046.0472	1047.4414	1048.2550
H	0.81548	1.64941	4.14255	1048.6578	1053.6351	1073.1496
C	1.03469	-1.73436	3.46396	1094.2180	1099.6887	1106.5196
H	0.49235	-2.45533	2.84183	1110.7088	1133.6939	1141.3498
H	2.08704	-1.73908	3.14663	1166.0404	1169.9634	1184.5745
H	0.99711	-2.07322	4.50789	1190.0922	1208.0302	1233.6114
C	-3.46590	4.42591	0.90727	1237.0583	1242.7250	1247.1527
H	-4.33473	4.12326	1.50525	1253.1462	1260.7575	1264.5018
H	-3.14336	5.41743	1.25185	1273.2063	1279.3423	1280.5088
H	-3.79230	4.50177	-0.13453	1283.2629	1307.7376	1323.9568
C	-1.12429	3.87184	0.20419	1355.3801	1359.9884	1364.1392
H	-0.76030	4.84816	0.55173	1369.0868	1373.7157	1375.2760
H	-0.30707	3.14354	0.29259	1375.3051	1379.1528	1385.2527
H	-1.40732	3.96957	-0.85253	1387.2210	1389.2639	1390.7630
C	-1.89144	3.31845	2.51056	1395.7026	1398.3079	1400.1942
H	-1.63796	4.31555	2.89580	1401.0410	1412.5959	1416.2201
H	-2.69698	2.91378	3.13848	1425.6055	1426.8423	1428.7371
H	-1.01026	2.67447	2.60758	1433.8652	1439.7868	1443.7313
Ir	-1.68357	-0.60919	-0.22873	1444.0612	1448.5818	1449.1239
C	1.58481	1.02480	-1.26055	1451.6001	1454.3833	1458.6417
C	2.04236	-0.41256	-1.46545	1461.2147	1461.6047	1462.7769
O	1.33100	-1.18220	-2.08384	1463.1672	1467.5263	1469.9535
C	3.28379	-0.90451	-0.80330	1471.8671	1476.4656	1477.1195
C	4.54712	-0.53001	-1.26052	1478.1917	1479.8134	1481.0666
C	3.16726	-1.82830	0.23083	1482.0817	1487.3840	1488.5295
C	5.68250	-1.05253	-0.65209	1490.4629	1494.6811	1496.3396
C	4.29492	-2.35939	0.85859	1501.3910	1506.6580	1508.6544
H	2.16329	-2.11433	0.55019	1511.0107	1517.4428	1545.0363
C	5.54870	-1.95231	0.40076	1550.9426	1664.2904	1679.2230
H	6.67092	-0.76745	-1.01319	1734.7887	1763.3940	1772.9489
H	6.44490	-2.36025	0.86714	1805.2648	1859.7664	2801.5703
O	4.59283	0.32445	-2.31936	3013.5582	3021.6104	3023.1880
H	5.50825	0.51100	-2.55282	3026.9100	3029.4882	3030.9666
C	0.38460	1.25749	-2.14632	3031.8978	3038.5758	3039.9722
C	2.64064	2.10658	-1.26505	3040.2594	3041.6230	3042.5152
C	4.52252	2.86715	-0.07803	3043.4370	3048.8677	3053.9361
H	4.11823	3.88059	0.03415	3096.0848	3099.1707	3099.7593
H	5.11010	2.85456	-1.00657	3103.2059	3105.6335	3108.2570
C	5.32144	2.42505	1.11935	3110.6300	3112.2938	3114.7794
H	6.18311	3.08285	1.27079	3119.1496	3119.8043	3121.7038
H	4.70241	2.44759	2.02169	3126.8025	3128.5985	3130.8620
H	5.68135	1.39829	0.98164	3132.2729	3133.5745	3134.0969
O	3.43522	1.94620	-0.20734	3135.6348	3144.0861	3147.7810
O	2.73699	3.01747	-2.05461	3149.2653	3150.3816	3151.8112
C	0.57962	1.73543	-3.54318	3161.2674	3164.6138	3167.4263
H	-0.36658	1.69871	-4.08817	3170.2362	3179.2762	3182.7018
H	0.99096	2.74930	-3.53475	3188.7344	3191.7598	3897.5632
H	1.33491	1.10343	-4.02905			
O	-0.73812	0.98837	-1.73385			
C	4.16603	-3.33530	1.99074			
H	4.92269	-4.12569	1.92647			
H	4.29339	-2.84557	2.96543			
H	3.17914	-3.81126	1.99546			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm

Zero-point correction= 0.778500	Electronic Energy = -2105.66028380
Internal Energy (E)= -2104.8317118	Enthalpy (H)= -2104.8307678
Gibbs Free Energy (G)=-2104.9610008	Gibbs Free Energy of Solvation=-2105.03228424

St.Pt.	General Structure	Ball & Stick model
X-2		

Cartesian co-ordinate

Atoms	X	Y	Z
C	1.74593	1.03496	0.11820
C	1.46960	-0.31232	-0.06977
C	0.07974	-0.77208	-0.26136
C	-0.53388	1.60992	-0.03469
O	0.75079	1.97319	0.13177
C	2.53561	-1.21804	-0.08456
C	3.04796	1.49575	0.29447
C	3.84362	-0.79538	0.08694
C	4.08039	0.57768	0.27744
H	2.29262	-2.26785	-0.23996
H	5.10437	0.92371	0.41255
H	3.22094	2.55874	0.43767
O	-0.17853	-1.94378	-0.48691
C	-0.91685	0.30985	-0.19642
C	-1.41353	2.81004	-0.01060
H	-1.68166	3.09932	-1.03196
H	-2.35360	2.61353	0.50737
H	-0.88224	3.63626	0.46780
C	-2.36469	0.03299	-0.38173
C	-4.10214	-1.50402	0.00946
H	-4.09399	-2.59369	0.10253
H	-4.42407	-1.23413	-1.00194
C	-4.98088	-0.85978	1.05398
H	-6.00527	-1.23835	0.97326
H	-4.61182	-1.08292	2.06034
H	-5.00601	0.22557	0.91881
O	-3.13388	0.78056	-0.95174
O	-2.73004	-1.12033	0.18016
C	4.98944	-1.76142	0.06818
H	4.64167	-2.78836	-0.07756
H	5.69451	-1.52887	-0.73900
H	5.55589	-1.72895	1.00667

Frequencies

33.0831	36.0553	50.8845
70.6132	86.6112	109.4053
135.3970	148.2641	162.0790
190.1080	206.4316	240.9165
251.0911	286.6228	333.5210
354.6506	359.3151	372.7512
394.4351	431.2323	437.9034
474.4640	539.4242	545.6281
569.5057	592.7356	611.8086
674.7863	691.7016	739.8842
770.9361	788.8425	816.7880
827.2189	838.7873	888.5964
897.1287	919.9141	962.8006
964.8446	1002.0408	1025.3518
1037.5120	1048.9945	1050.7194
1113.2638	1127.0019	1134.5496
1146.6475	1186.4310	1216.2548
1243.9799	1276.7125	1281.9143
1312.8835	1340.5684	1381.7855
1387.6541	1394.1225	1399.9689
1404.9442	1420.8335	1449.7182
1449.9800	1463.3099	1467.0005
1468.4666	1469.7799	1487.2120
1497.3597	1530.9089	1631.7214
1672.7141	1687.7574	1800.9265
1827.7476	3035.7713	3049.6574
3064.2847	3072.3806	3108.1507
3130.4010	3139.9740	3142.6535
3149.0934	3155.9771	3172.4759
3179.2879	3193.1301	3208.3000

Statistical Thermodynamic Analysis

Temperature=298 K	Pressure=1 atm
Zero-point correction= 0.253896	Electronic Energy = -842.320820182
Internal Energy (E)= -842.049950182	Enthalpy (H)= -842.049006182
Gibbs Free Energy (G)=-842.112753182	Gibbs Free Energy of Solvation=-842.132981798

St.Pt.	General Structure	Ball & Stick model
S3		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.18546	0.90192	0.00014
O	-2.46478	1.30913	0.00035
C	-0.12431	1.81072	-0.00016
C	1.19134	1.37309	-0.00032
C	-0.90720	-0.47973	0.00029
C	1.46252	0.00916	-0.00014
C	0.42373	-0.90361	0.00021
H	0.63630	-1.97190	0.00041
H	2.00908	2.08874	-0.00058
C	-1.94216	-1.53035	0.00051
H	-1.49814	-2.55792	0.00152
O	-3.13858	-1.37061	-0.00028
H	-0.33715	2.87914	-0.00028
H	-2.49259	2.27319	0.00070
Cl	3.11757	-0.54745	-0.00032

Frequencies

71.0183	118.2841	176.3764
212.0578	261.0385	336.7142
381.1652	397.0581	414.7774
444.0264	448.9050	553.4818
655.0650	713.7400	736.7306
780.5222	814.2674	900.9222
909.0308	938.8747	1016.7546
1113.9573	1129.7446	1173.8617
1218.1126	1299.1763	1339.1466
1377.8481	1412.9873	1463.3934
1534.2871	1646.0001	1671.6174
1857.6825	2837.5932	3166.9990
3179.8043	3209.0734	3874.3383

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.104309 Electronic Energy = -880.092861874
Internal Energy (E)= -879.979774874 Enthalpy (H)= -879.978831874
Gibbs Free Energy (G)=-880.023000874 Gibbs Free Energy of Solvation=-880.044173978

St.Pt.	General Structure	Ball & Stick model
I-3		

Cartesian co-ordinate

Atoms	X	Y	Z

Frequencies

14.1280	26.5273	39.3348
45.9899	55.1949	59.8145
62.7488	71.6084	79.1086
80.4292	86.3813	99.9530

C	-2.18908	-1.90296	1.19301	112.7085	121.3215	124.2939
C	-3.28995	-0.99216	1.05706	129.7300	133.6954	142.8251
C	-3.61374	-0.87223	-0.35882	146.6173	155.2572	159.4142
C	-2.68202	-1.69335	-1.08449	170.8136	172.1245	179.1413
C	-1.78071	-2.31585	-0.13187	185.7551	196.4000	203.5604
C	1.48108	-0.75535	-1.98854	208.6878	213.1215	216.0054
C	-0.63092	3.53934	-1.33327	238.9838	245.1921	246.6983
C	-1.10423	2.17961	-0.86488	272.6589	278.7617	283.6051
O	-1.76228	2.02596	0.20356	293.3327	303.3205	307.5627
O	-0.83785	1.14369	-1.55641	310.8538	312.2610	317.7921
C	-4.70252	-0.03213	-0.92837	321.9655	331.7462	336.5468
H	-4.77249	0.92536	-0.40050	338.5197	343.6001	350.4297
H	-4.51481	0.19172	-1.98317	372.8444	378.9611	380.7300
H	-5.67624	-0.53320	-0.85616	390.4420	397.7449	405.9297
C	-2.57122	-1.82539	-2.56144	407.4044	410.0462	421.3148
H	-1.51955	-1.76946	-2.86752	426.8623	439.1625	448.9617
H	-2.98381	-2.78650	-2.89404	451.3053	458.0022	462.0827
H	-3.11434	-1.02552	-3.07416	470.4525	534.9154	538.5961
C	-0.68617	-3.28539	-0.40790	547.6643	555.0105	561.2885
H	-0.39905	-3.29396	-1.46118	573.4737	583.2172	587.5953
H	0.21376	-3.01092	0.15763	605.8118	621.5180	639.9223
H	-0.98542	-4.29810	-0.10558	654.8071	717.4803	734.8882
C	-1.57348	-2.37582	2.46075	781.5384	791.2251	793.9646
H	-0.49531	-2.53097	2.33850	808.6365	816.0182	820.1089
H	-1.70883	-1.65242	3.26711	820.7711	831.7807	907.4781
H	-2.01858	-3.33614	2.75419	910.2126	922.0084	937.2410
C	-3.92625	-0.25424	2.18039	944.4474	949.2929	950.1186
H	-4.50385	0.60097	1.81676	953.9674	957.6183	960.2568
H	-4.59999	-0.90768	2.74904	964.7968	972.8701	993.9317
H	-3.14752	0.12796	2.85063	1028.5022	1040.4083	1041.2699
C	0.31318	0.48723	2.10106	1041.6105	1042.0430	1045.7221
O	0.28231	0.21365	0.82581	1046.2823	1047.3033	1054.8589
O	-0.65957	0.51745	2.84860	1060.8400	1097.4526	1100.1239
C	1.73208	0.75120	2.62613	1117.5156	1131.9744	1135.9326
O	0.72589	-1.57044	-2.47560	1181.2387	1189.3912	1193.5893
C	2.54681	-0.53524	2.46536	1219.5814	1243.3331	1243.6818
H	2.56932	-0.86524	1.42012	1246.7890	1256.2184	1266.8141
H	3.58148	-0.37616	2.80113	1269.0026	1306.8685	1333.9563
H	2.11680	-1.34390	3.07300	1367.9748	1376.2323	1376.2652
C	1.67538	1.14240	4.09675	1378.5767	1383.3358	1384.3487
H	2.69102	1.29829	4.48450	1386.6553	1389.6609	1393.9372
H	1.10332	2.06606	4.23767	1400.8139	1410.6543	1411.9848
H	1.18725	0.36307	4.69130	1414.5995	1417.8102	1427.3058
C	2.36865	1.87925	1.81608	1435.2188	1439.3182	1441.8644
H	1.76572	2.79606	1.87769	1447.2663	1448.3411	1452.3180
H	3.37138	2.10897	2.20111	1457.6321	1459.2446	1460.7404
H	2.45948	1.59861	0.76105	1462.0227	1464.2085	1465.9164
C	0.86323	3.44252	-1.64920	1470.3068	1470.8920	1473.9346
H	1.05065	2.71318	-2.44580	1475.9538	1477.2717	1485.4651
H	1.23982	4.41928	-1.97855	1486.2544	1487.6100	1490.6045
H	1.43421	3.14180	-0.75950	1493.7906	1500.1908	1507.2857
C	-0.87500	4.58937	-0.25722	1513.3020	1518.6120	1531.1873
H	-0.52841	5.56926	-0.60942	1533.0860	1541.7069	1612.9679
H	-1.93868	4.66456	-0.00811	1649.4168	1672.6091	1760.7297
H	-0.33742	4.34103	0.66509	1827.8705	2932.3109	3020.0641
C	-1.40550	3.89018	-2.60705	3023.2492	3024.8681	3030.0639
H	-2.48092	3.97252	-2.40530	3033.6117	3034.7552	3036.2355
H	-1.06024	4.85594	-2.99765	3037.9768	3038.4253	3041.0758
H	-1.25517	3.12824	-3.37976	3041.4056	3098.2934	3100.0577
Ir	-1.60333	-0.18888	0.01862	3103.7969	3109.3525	3115.8354
H	1.19971	0.31949	-1.93877	3116.0385	3118.4066	3122.3440

C	2.81027	-1.04060	-1.41600	3122.6179	3127.0290	3128.2849
C	3.58575	0.07043	-1.07434	3129.7129	3136.2020	3140.5326
C	3.33040	-2.32991	-1.19069	3141.0811	3141.5261	3143.7240
C	4.84361	-0.07960	-0.51849	3145.2121	3150.9524	3158.1908
H	3.18095	1.06640	-1.25304	3164.7008	3173.7728	3185.3642
C	4.59826	-2.46460	-0.61967	3195.5659	3202.8965	3877.8836
C	5.35484	-1.35122	-0.28365			
H	4.99854	-3.46185	-0.43748			
H	6.33977	-1.46694	0.16095			
O	2.59335	-3.40745	-1.52203			
H	3.08325	-4.20525	-1.29213			
Cl	5.78467	1.32724	-0.08879			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.603838 Electronic Energy = -2067.06296607
Internal Energy (E)= -2066.41886407 Enthalpy (H)= -2066.41792007
Gibbs Free Energy (G)=-2066.52998907 Gibbs Free Energy of Solvation=-2066.59266073

St.Pt.	General Structure	Ball & Stick model
TS_3-1		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-2.37632	-2.00556	0.93702
C	-3.22573	-0.82815	0.98166
C	-3.53528	-0.44312	-0.39117
C	-2.85245	-1.35915	-1.25952
C	-2.12755	-2.32372	-0.44924
C	1.31346	-0.33354	-1.77214
C	-0.80563	3.70473	-0.91334
C	-1.04198	2.21613	-0.70224
O	-1.20332	1.77292	0.48508
O	-1.04204	1.42844	-1.68453
C	-4.35341	0.73095	-0.80194
H	-4.22001	1.56148	-0.09909
H	-4.04757	1.09169	-1.78917
H	-5.42165	0.48377	-0.83901
C	-2.81852	-1.30712	-2.74394
H	-1.84013	-1.62363	-3.11562
H	-3.58575	-1.96933	-3.16560
H	-2.99381	-0.29207	-3.11064
C	-1.31847	-3.46387	-0.95785
H	-0.76751	-3.19016	-1.86218
H	-0.57024	-3.76379	-0.21674
H	-1.95543	-4.33193	-1.17391
C	-1.86858	-2.74540	2.12191

Frequencies

-82.8000	25.6550	35.4635
41.6378	44.6888	51.8060
69.9060	73.1808	81.4588
83.9267	96.8724	101.3604
103.1918	109.7774	119.2958
122.3729	131.6074	133.0473
148.5573	151.3407	161.0149
164.7474	175.6581	182.4817
188.8226	198.2932	205.0086
218.8111	221.1560	225.7348
233.6460	241.3677	253.6392
268.5172	277.9495	278.8506
283.8601	289.1599	291.6040
300.9153	306.8216	314.1547
328.5983	332.3632	334.5055
342.2043	350.5267	358.6774
368.2978	373.8664	379.9051
383.2480	392.8903	398.0420
414.9858	426.3216	432.4676
440.3753	455.2921	456.6685
458.7098	462.4468	472.8373
475.9476	533.8791	538.2109
545.5800	550.5654	557.5915
566.0640	582.7517	589.3452
602.8514	620.7649	627.5788
654.4802	717.9553	738.0345
786.7216	790.3726	800.5514

H	-0.98074	-3.33155	1.86412	806.1388	812.5422	813.9885
H	-1.58599	-2.04510	2.91375	814.2200	825.9026	906.3726
H	-2.63520	-3.43571	2.49784	912.6073	916.1217	925.8414
C	-3.68002	-0.15644	2.22605	939.5959	947.7591	949.0830
H	-4.07585	0.84213	2.01880	950.4452	951.2820	955.4571
H	-4.46773	-0.74461	2.71491	962.0083	966.4792	981.8917
H	-2.83219	-0.04926	2.91269	1034.7580	1035.7977	1041.6325
C	0.45702	-0.04278	2.26182	1044.3403	1045.4940	1045.6480
O	0.42744	-0.37755	1.00553	1046.4616	1048.7128	1053.4953
O	-0.50168	-0.03886	3.02871	1056.1052	1095.7803	1102.5688
C	1.85196	0.41075	2.72094	1114.9105	1118.7828	1134.7226
O	0.36003	-1.04841	-2.01365	1181.0706	1183.8306	1189.3630
C	2.89186	-0.66150	2.39669	1224.0387	1239.7950	1241.7967
H	2.89211	-0.90622	1.32968	1248.3935	1256.4231	1267.1227
H	3.89630	-0.30894	2.67134	1270.0145	1309.8589	1334.2584
H	2.69477	-1.58314	2.96016	1367.0382	1370.1854	1373.1870
C	1.84797	0.69363	4.21671	1373.8981	1377.7214	1382.4718
H	2.83972	1.03990	4.53752	1385.2040	1387.4318	1392.9864
H	1.10895	1.46078	4.46954	1395.6454	1402.2171	1407.5607
H	1.59280	-0.20622	4.78819	1409.3673	1414.1009	1422.1329
C	2.17183	1.69541	1.95066	1433.4894	1437.7698	1443.9696
H	1.44078	2.48126	2.18597	1448.3581	1449.5047	1457.4289
H	3.17439	2.06302	2.20943	1457.8057	1460.7486	1462.3114
H	2.12919	1.51110	0.87057	1465.5409	1466.3537	1468.1476
C	0.69110	3.87671	-1.19666	1468.3514	1471.6085	1474.5266
H	0.98552	3.31706	-2.09353	1477.3359	1478.6058	1481.8982
H	0.92434	4.93657	-1.36192	1488.0217	1489.1622	1492.4082
H	1.29481	3.52500	-0.34833	1497.8284	1502.2114	1506.0930
C	-1.19641	4.50624	0.32215	1511.8642	1515.9257	1520.7273
H	-1.01694	5.57492	0.14595	1527.6282	1532.9946	1629.3790
H	-2.25848	4.37111	0.56042	1648.9735	1669.0921	1761.3787
H	-0.62030	4.19453	1.19935	1810.4072	2929.7679	3016.4094
C	-1.61563	4.16824	-2.12271	3022.7592	3024.8067	3027.9817
H	-2.69215	4.03946	-1.94753	3032.6469	3034.3234	3035.6813
H	-1.43049	5.23316	-2.31366	3038.1475	3039.0192	3041.0512
H	-1.34758	3.59793	-3.01751	3047.2218	3100.2470	3102.5769
Ir	-1.42798	-0.34335	-0.00373	3105.4055	3108.2298	3116.1187
H	1.18279	0.77291	-1.75300	3117.0874	3117.7903	3118.1818
C	2.68092	-0.76381	-1.45740	3118.5087	3125.7779	3130.1138
C	3.59196	0.25232	-1.15474	3139.1070	3139.6419	3140.8439
C	3.09960	-2.10595	-1.37802	3141.5368	3145.9775	3146.8354
C	4.88557	-0.04453	-0.76720	3149.7505	3153.9966	3159.4568
H	3.26067	1.28948	-1.20551	3161.7109	3166.5948	3170.1092
C	4.41458	-2.38821	-1.00055	3182.1377	3210.4243	3876.4090
C	5.30391	-1.36900	-0.69120			
H	4.74235	-3.42572	-0.93973			
H	6.32091	-1.59952	-0.38582			
O	2.22286	-3.08501	-1.66834			
H	2.65666	-3.93846	-1.55422			
Cl	5.98485	1.24144	-0.33807			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.603387 Electronic Energy = -2067.04796691
Internal Energy (E)= -2066.40515191 Enthalpy (H)= -2066.40420791
Gibbs Free Energy (G)=-2066.51332891 Gibbs Free Energy of Solvation=-2066.58172528

St.Pt.	General Structure	Ball & Stick model
II-3		

Cartesian co-ordinate

Atoms	X	Y	Z
C	3.12513	0.12025	-1.60469
C	3.53151	-0.00216	-0.21312
C	3.18504	-1.34407	0.22554
C	2.51111	-2.00946	-0.84406
C	2.47487	-1.09682	-1.98428
C	-1.61386	-0.40369	-0.44810
C	-0.43024	-0.79545	3.59617
C	0.20660	-1.10305	2.23106
O	0.51140	-0.02903	1.56488
O	0.35965	-2.25854	1.84274
C	3.45937	-1.88912	1.58136
H	3.30390	-1.11910	2.34575
H	2.79341	-2.72177	1.81672
H	4.50175	-2.22646	1.64916
C	1.92396	-3.37640	-0.80114
H	1.14177	-3.48842	-1.55967
H	2.68964	-4.14089	-0.98609
H	1.45866	-3.55397	0.17391
C	1.85917	-1.40825	-3.30306
H	0.89811	-1.91997	-3.17844
H	1.67521	-0.49611	-3.87871
H	2.51475	-2.05869	-3.89652
C	3.32351	1.33063	-2.44522
H	2.56935	1.39614	-3.23637
H	3.24122	2.23321	-1.83225
H	4.31345	1.30825	-2.91941
C	4.31395	1.00114	0.55627
H	4.24758	0.80791	1.63164
H	5.37404	0.96557	0.27048
H	3.91887	2.00521	0.37771
C	0.77829	2.72796	-0.26198
O	0.32525	1.55525	-0.57723
O	1.94588	3.01363	-0.01534
C	-0.33700	3.78264	-0.15354
O	-0.61210	-0.94154	-0.91416
C	-1.36853	3.62144	-1.26729
H	-1.83043	2.62807	-1.24199
H	-2.15935	4.37616	-1.15930
H	-0.91161	3.75337	-2.25638
C	0.26465	5.18146	-0.19724
H	-0.52411	5.93741	-0.08584
H	1.00035	5.31756	0.60107
H	0.77775	5.35899	-1.15012
C	-1.00965	3.55112	1.20333
H	-0.27897	3.61667	2.01966
H	-1.79101	4.30325	1.37714

Frequencies

28.4051	30.2938	35.4825
37.8937	42.1243	55.8950
62.8228	64.3153	76.3170
82.0011	93.1934	95.8021
99.4604	105.0668	111.8235
121.6146	129.0071	138.5695
147.0001	152.4495	158.1344
167.3238	176.2675	182.8488
194.5227	197.8054	200.4870
208.1822	217.6073	235.1388
241.9930	247.7907	254.4252
262.4761	270.3727	276.7538
287.1788	297.8630	303.6103
311.1143	317.8095	319.2063
321.0963	322.0578	329.0785
337.0152	341.1404	343.5541
345.5955	361.4628	378.2780
382.0929	384.1725	392.1755
393.7705	429.5740	432.2022
435.9567	444.1159	447.8830
457.2727	467.3497	468.4219
471.4468	537.1193	539.7045
544.7566	560.2768	569.3690
573.9024	583.8007	594.0339
602.8772	633.0357	640.7773
655.2514	722.6833	744.2937
786.0806	792.9382	794.4291
806.8659	810.5879	816.5072
817.2208	819.2464	913.1636
914.8414	918.1994	919.2065
945.3062	946.4647	949.1447
949.7207	950.6065	953.0846
963.2458	970.2398	976.0563
1003.4602	1038.1915	1040.4557
1040.4916	1043.0024	1043.5726
1045.6149	1046.2434	1049.3397
1050.1575	1095.0744	1100.9297
1109.4872	1124.8157	1137.2415
1183.3969	1187.2349	1188.2561
1235.0838	1238.2363	1243.4293
1247.9726	1253.4794	1265.0610
1268.2480	1319.8280	1337.8598
1364.6213	1367.2305	1375.1124
1376.4858	1376.8862	1380.1723
1388.7165	1390.8341	1393.7130
1395.1496	1396.7018	1400.1300
1413.1136	1419.1084	1419.8846
1429.4641	1432.2167	1438.9726
1447.1261	1447.3828	1450.3875
1454.2851	1460.9461	1461.3410

H	-1.47176	2.55573	1.24506
C	-1.78929	-0.14066	3.34038
H	-2.43905	-0.80127	2.74792
H	-2.30026	0.06620	4.29014
H	-1.66583	0.80771	2.80277
C	0.46501	0.16828	4.37423
H	0.02725	0.37977	5.35919
H	1.46016	-0.26708	4.53883
H	0.59283	1.11319	3.83632
C	-0.61816	-2.08553	4.38326
H	0.34324	-2.58084	4.56173
H	-1.08247	-1.87037	5.35490
H	-1.25297	-2.79232	3.83883
Ir	1.41694	-0.21556	-0.32137
H	-1.49980	0.37953	0.32274
C	-2.97946	-0.72280	-0.83640
C	-3.99363	0.00621	-0.20013
C	-3.32706	-1.69968	-1.79362
C	-5.32310	-0.22802	-0.49568
H	-3.72011	0.76531	0.53161
C	-4.67627	-1.92142	-2.07765
C	-5.66829	-1.19566	-1.43610
H	-4.95046	-2.67602	-2.81397
H	-6.71538	-1.37713	-1.66349
O	-2.35238	-2.39011	-2.40731
H	-2.74769	-3.02473	-3.01655
Cl	-6.57374	0.68394	0.30640

1462.0213	1463.1249	1464.6202
1466.6489	1472.4399	1472.8560
1475.7965	1477.2950	1480.3284
1481.1048	1483.9483	1485.7323
1491.9712	1497.7474	1500.7337
1501.8471	1514.2635	1523.2243
1535.5122	1538.7577	1645.9526
1671.7617	1748.0085	1761.5232
1770.8373	3009.6291	3021.0505
3024.1390	3025.1071	3032.2358
3032.7888	3033.5895	3033.9336
3037.7574	3039.8856	3041.1992
3042.4883	3092.4095	3101.3731
3104.0555	3110.1500	3113.2992
3117.1661	3117.2280	3118.0231
3119.4545	3119.8547	3122.0541
3124.2298	3126.7258	3131.4349
3140.2259	3141.7072	3144.1100
3144.1937	3144.9483	3160.2670
3166.6326	3172.5149	3173.3140
3185.6004	3209.8790	3871.8524

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.603236 Electronic Energy = -2067.05972637
Internal Energy (E)= -2066.41602937 Enthalpy (H)= -2066.41508637
Gibbs Free Energy (G)=-2066.52768637 Gibbs Free Energy of Solvation=-2066.58993137

St.Pt.	General Structure	Ball & Stick model
II'-3		

Cartesian co-ordinate

Atoms	X	Y	Z
C	1.26727	-2.65685	-0.55390
C	2.45647	-1.83740	-0.39606
C	2.44618	-1.29872	0.95091
C	1.23962	-1.75917	1.59093
C	0.51168	-2.60520	0.66356
O	0.95842	1.41627	-0.50775
C	2.13445	2.02981	-0.53117
O	3.17332	1.45756	-0.80317

Frequencies

15.4373	19.7758	37.6368
49.0961	62.0702	72.4820
78.8569	88.9554	106.4554
115.9816	126.8402	137.1037
145.7970	152.2589	161.5861
174.2542	178.7119	189.5610
200.6205	202.2349	202.4968
206.4525	215.2932	223.2893
232.2276	246.9801	259.9818
277.4107	284.4637	294.5356
304.0026	313.4962	321.6674
324.8965	329.8291	342.6581

C	2.07707	3.48856	-0.09040
C	-2.32779	0.67039	0.56032
H	-0.52387	1.49600	0.35603
C	3.54236	-1.65182	-1.38849
H	3.85202	-0.60287	-1.41253
H	4.40529	-2.27088	-1.11023
H	3.22762	-1.94504	-2.39365
C	3.52125	-0.48227	1.57022
H	3.96119	0.20576	0.84132
H	3.14327	0.10637	2.41260
H	4.30951	-1.14267	1.95398
C	-0.79253	-3.27237	0.92661
H	-1.36996	-3.39569	0.00440
H	-0.64429	-4.26758	1.36289
H	-1.40575	-2.69271	1.62488
C	0.89225	-3.36910	-1.80120
H	-0.17015	-3.62670	-1.81977
H	1.10935	-2.75929	-2.68427
H	1.46627	-4.29981	-1.88755
C	0.80294	-1.39772	2.96291
H	1.25946	-2.07640	3.69424
H	1.10301	-0.37609	3.21840
H	-0.28335	-1.46667	3.07357
Ir	0.72268	-0.60267	-0.14274
C	0.84634	4.20970	-0.63593
H	-0.09082	3.78736	-0.25420
H	0.87713	5.26357	-0.33471
H	0.81418	4.17701	-1.73117
C	2.01728	3.43185	1.44409
H	2.91819	2.95372	1.85055
H	1.95808	4.44589	1.85728
H	1.13851	2.87043	1.79219
C	3.34370	4.21200	-0.53092
H	4.23914	3.70358	-0.16195
H	3.41387	4.25830	-1.62346
H	3.33920	5.23845	-0.14557
O	-0.99796	0.78150	0.85811
C	-3.24130	0.89365	1.58016
C	-4.60553	0.81846	1.32854
C	-2.78149	0.32700	-0.72947
C	-5.06529	0.52502	0.04377
C	-4.16357	0.28464	-0.97844
H	-4.52668	0.03999	-1.97502
H	-5.32325	1.00326	2.12321
C	-1.92176	-0.08459	-1.81989
H	-2.42445	-0.18907	-2.79827
O	-0.72496	-0.38294	-1.77776
H	-2.86687	1.15197	2.56683
Cl	-6.76591	0.45770	-0.26832
H	-1.08247	-1.87037	5.35490
H	-1.25297	-2.79232	3.83883
Ir	1.41694	-0.21556	-0.32137
H	-1.49980	0.37953	0.32274
C	-2.97946	-0.72280	-0.83640
C	-3.99363	0.00621	-0.20013
C	-3.32706	-1.69968	-1.79362
C	-5.32310	-0.22802	-0.49568
H	-3.72011	0.76531	0.53161
C	-4.67627	-1.92142	-2.07765
C	-5.66829	-1.19566	-1.43610
H	-4.95046	-2.67602	-2.81397

346.4740	369.4098	372.3572
389.3448	394.5072	425.5712
435.7297	447.6052	455.9030
460.8268	464.6968	467.2919
533.6681	536.0130	541.7400
551.4521	576.0016	578.8191
583.4871	600.6510	624.4733
656.9223	708.8611	751.3461
785.4485	790.3029	802.9906
809.7570	813.3378	854.5397
869.5484	888.3371	917.4276
924.0418	943.9276	951.7217
951.9947	957.1268	966.7647
982.2243	1025.0764	1025.7218
1027.3214	1030.3617	1033.9125
1035.9937	1040.8683	1042.6649
1088.0916	1094.8999	1107.8656
1116.1910	1136.8030	1185.6930
1187.7489	1194.4262	1226.9356
1236.0270	1246.3903	1260.8047
1264.9499	1308.9325	1340.0877
1373.1227	1378.0229	1379.1114
1381.9001	1389.0920	1392.3540
1394.8497	1395.6138	1412.2311
1415.9155	1422.6738	1432.0908
1432.7399	1437.8027	1444.3951
1448.6794	1451.2635	1454.4229
1455.1942	1456.0962	1460.0167
1464.8226	1467.9286	1472.9656
1476.7920	1479.7411	1487.3866
1496.4850	1499.8958	1505.9818
1509.5973	1519.9994	1524.4393
1616.3050	1663.3716	1732.3042
1804.4939	3007.1800	3020.3474
3035.5914	3041.9791	3043.1762
3045.8025	3046.0018	3046.9102
3049.7758	3106.7139	3120.4800
3122.0391	3128.2376	3128.3995
3129.5864	3130.8403	3131.7888
3131.8819	3133.6800	3143.9764
3147.6508	3154.8156	3155.0709
3155.5904	3164.3564	3201.3661
3209.2656	3221.8495	3350.3710

H	-6.71538	-1.37713	-1.66349
O	-2.35238	-2.39011	-2.40731
H	-2.74769	-3.02473	-3.01655
Cl	-6.57374	0.68394	0.30640

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.465818 Electronic Energy = -1720.61753081
Internal Energy (E)= -1720.12024381 Enthalpy (H)= -1720.11929981
Gibbs Free Energy (G)=-1720.21384881 Gibbs Free Energy of Solvation=-1720.32064368

St.Pt.	General Structure	Ball & Stick model
TS_3-2		

Cartesian co-ordinate

Atoms	X	Y	Z
C	2.20169	-2.27474	-0.47658
C	2.94433	-1.04332	-0.50229
C	2.81620	-0.41508	0.80527
C	1.98054	-1.24727	1.61767
C	1.57038	-2.39477	0.82112
O	0.26561	1.46144	-0.72266
C	1.10240	2.54043	-0.79421
O	2.15880	2.43209	-1.36054
C	0.59907	3.77793	-0.06973
C	-2.22053	0.07813	0.59082
H	-0.40410	1.38977	0.10653
C	3.74178	-0.49930	-1.62957
H	3.57756	0.57772	-1.73807
H	4.81026	-0.67233	-1.44769
H	3.47923	-0.97871	-2.57616
C	3.50034	0.83801	1.21322
H	3.56570	1.54473	0.37973
H	2.98918	1.32966	2.04713
H	4.52247	0.60815	1.54020
C	0.73795	-3.53085	1.29563
H	0.22724	-4.02855	0.46607
H	1.36389	-4.27808	1.79916
H	-0.02369	-3.19864	2.00764
C	2.03436	-3.21988	-1.60824
H	1.03023	-3.65439	-1.61803
H	2.18970	-2.72250	-2.56974
H	2.75920	-4.03864	-1.52602
C	1.54993	-0.97408	3.01189
H	2.20390	-1.49847	3.71962

Frequencies

-307.5378	23.9177	40.2148
46.6621	53.9956	67.2808
79.5909	89.6812	98.8673
109.3536	120.3493	131.6429
135.2368	145.0888	148.6582
160.8859	168.5040	173.6413
182.6725	185.5278	190.4017
198.9658	211.1049	217.4944
234.7188	247.7240	258.4463
296.0243	303.8548	307.1446
309.6981	315.9183	323.5564
330.2157	337.0214	353.6508
357.1067	372.3126	380.2085
384.2591	410.9974	419.7369
444.2707	446.6119	452.9973
459.3472	466.0584	507.8979
519.9208	536.4138	537.2299
546.2875	546.7445	576.2901
584.4210	593.2646	601.2504
652.7933	716.0868	733.3010
754.7168	776.6342	793.0958
808.5015	810.1143	842.8354
849.6722	885.2822	922.0714
936.9648	945.4365	958.3532
960.6172	962.7021	965.0607
977.0322	1014.5437	1024.0523
1028.9397	1032.2011	1032.4531
1033.2342	1037.5553	1043.8409
1089.5851	1094.2531	1107.7519
1116.9878	1142.9769	1160.0637
1187.1946	1192.1895	1224.7332
1232.1841	1244.1700	1255.2766
1265.8195	1305.6754	1347.0143

H	1.59066	0.09448	3.24263	1379.9886	1384.9818	1387.2955
H	0.52444	-1.31418	3.18551	1394.2424	1395.0283	1396.7126
Ir	0.85726	-0.62555	-0.11815	1398.2875	1400.1353	1421.1633
C	-0.89263	4.01190	-0.32018	1421.6143	1430.8509	1431.7102
H	-1.53026	3.22700	0.10702	1433.3646	1436.4073	1438.9498
H	-1.18968	4.95528	0.15164	1445.9960	1452.9890	1453.6046
H	-1.11439	4.08976	-1.39044	1455.5402	1456.3200	1458.7206
C	0.85104	3.53059	1.42732	1464.2570	1465.6743	1475.1616
H	1.92456	3.42788	1.63033	1484.2959	1485.2935	1491.6742
H	0.48287	4.38735	2.00334	1493.2716	1499.0091	1500.9524
H	0.33391	2.63441	1.80031	1506.5915	1516.7739	1531.7265
C	1.40542	4.98518	-0.53428	1585.0143	1665.4857	1691.0991
H	2.47756	4.83145	-0.37931	1876.1043	2289.8550	3028.7692
H	1.24602	5.18213	-1.59988	3031.1397	3037.4793	3047.4066
H	1.09590	5.87308	0.02835	3049.8206	3049.9350	3050.2090
O	-0.95694	0.33518	0.87613	3052.8156	3054.8923	3115.5018
C	-3.20439	0.45964	1.52135	3121.9601	3131.8139	3134.6299
C	-4.54705	0.29326	1.25301	3135.0429	3135.2249	3137.6280
C	-2.65143	-0.51091	-0.63301	3138.9021	3140.0406	3140.8092
C	-4.96738	-0.27132	0.03762	3150.9690	3154.4980	3158.0722
C	-4.03580	-0.66622	-0.89038	3163.1009	3164.9350	3170.1805
H	-4.36022	-1.11012	-1.83004	3192.5222	3203.0506	3214.6308
H	-5.29448	0.60223	1.97965			
C	-1.77556	-1.02010	-1.63714			
H	-2.27145	-1.39450	-2.54806			
O	-0.53277	-1.14406	-1.62639			
H	-2.87128	0.90355	2.45565			
Cl	-6.66267	-0.46840	-0.27398			
H	-1.08247	-1.87037	5.35490			
H	-1.25297	-2.79232	3.83883			
Ir	1.41694	-0.21556	-0.32137			
H	-1.49980	0.37953	0.32274			
C	-2.97946	-0.72280	-0.83640			
C	-3.99363	0.00621	-0.20013			
C	-3.32706	-1.69968	-1.79362			
C	-5.32310	-0.22802	-0.49568			
H	-3.72011	0.76531	0.53161			
C	-4.67627	-1.92142	-2.07765			
C	-5.66829	-1.19566	-1.43610			
H	-4.95046	-2.67602	-2.81397			
H	-6.71538	-1.37713	-1.66349			
O	-2.35238	-2.39011	-2.40731			
H	-2.74769	-3.02473	-3.01655			
Cl	-6.57374	0.68394	0.30640			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.463396 Electronic Energy = -1720.61763543
Internal Energy (E)= -1720.12348743 Enthalpy (H)= -1720.12254343
Gibbs Free Energy (G)=-1720.21433743 Gibbs Free Energy of Solvation=-1720.31896223

St.Pt.	General Structure	Ball & Stick model

III-3

Cartesian co-ordinate

Atoms	X	Y	Z
C	2.99091	-1.30295	-0.68114
C	3.15612	0.10158	-0.49401
C	2.79748	0.42582	0.88441
C	2.43085	-0.78877	1.54541
C	2.50330	-1.86744	0.57082
O	-0.17496	1.39729	-1.15488
C	0.04872	2.68286	-0.71661
O	1.16792	3.11303	-0.77275
C	-1.13587	3.40410	-0.09689
C	-1.86810	-0.62432	0.69157
H	-1.12125	1.18382	-1.09813
C	3.61423	1.08883	-1.50252
H	2.98120	1.98195	-1.49052
H	4.64366	1.39457	-1.27563
H	3.60348	0.66890	-2.51151
C	2.89516	1.76803	1.51355
H	2.76976	2.56580	0.77784
H	2.13707	1.90126	2.29280
H	3.87961	1.88596	1.98441
C	2.24138	-3.30645	0.82614
H	1.85061	-3.80210	-0.06805
H	3.17061	-3.81570	1.11183
H	1.51858	-3.44751	1.63481
C	3.22125	-2.07240	-1.93088
H	2.46239	-2.84998	-2.06345
H	3.18803	-1.42544	-2.81174
H	4.20323	-2.56000	-1.90396
C	1.98774	-0.91998	2.95585
H	2.84550	-1.14667	3.60083
H	1.52869	0.00563	3.31558
H	1.25310	-1.72180	3.07501
Ir	1.07012	-0.47406	-0.09606
C	-2.48783	2.89749	-0.60213
H	-2.71656	1.86765	-0.28369
H	-3.28374	3.51711	-0.17531
H	-2.57506	2.96886	-1.69350
C	-0.99463	3.13471	1.41202
H	-0.07955	3.59977	1.79722
H	-1.84991	3.56956	1.94236
H	-0.95654	2.05778	1.63057
C	-1.00363	4.89850	-0.37807
H	-0.02974	5.27655	-0.05550
H	-1.11681	5.11629	-1.44617
H	-1.78527	5.44263	0.16367
O	-0.65339	-0.32254	1.03535
C	-2.89983	-0.35719	1.62937
C	-4.21793	-0.60167	1.33544
C	-2.25522	-1.19333	-0.56679
C	-4.59004	-1.14819	0.08781
C	-3.62854	-1.45159	-0.83584
H	-3.90898	-1.89204	-1.79115
H	-4.99324	-0.38020	2.06494

Frequencies

28.3660	30.9316	58.1587
63.7077	75.7670	79.4977
87.7207	90.9704	104.8494
106.3311	124.0986	126.5011
131.0015	151.7083	158.3667
159.2556	166.3868	187.9164
194.8950	196.1876	212.9119
214.7349	220.9253	237.5487
244.1375	262.0275	268.1900
294.9993	297.4275	312.5099
314.3264	321.5237	323.2414
329.0456	332.1709	342.6342
357.5022	373.6041	385.1865
391.3382	393.0145	422.6119
431.9777	441.9369	455.0891
459.4174	478.7764	509.0761
532.9789	535.7952	540.7924
543.5271	567.3188	575.0498
580.6389	589.7337	602.0823
615.6974	672.7257	743.3715
754.7389	763.6930	774.2845
804.1151	807.5816	812.5685
851.7624	874.1112	883.6966
927.6167	944.3710	955.3232
958.7084	962.2076	969.5518
984.4111	1010.0496	1020.4435
1029.1263	1034.8292	1036.2422
1037.1427	1039.9927	1042.7652
1090.4998	1097.2655	1107.1841
1108.3618	1115.1407	1149.6424
1187.5402	1189.5795	1220.8563
1226.4349	1241.8012	1250.4616
1262.7005	1321.8410	1353.9931
1378.1710	1381.9349	1385.4396
1390.7462	1395.2465	1395.7497
1402.0290	1404.3806	1418.2583
1428.3734	1428.8503	1431.9209
1437.2458	1438.9600	1441.5998
1450.4437	1455.4586	1458.8988
1460.1975	1462.1234	1465.9466
1469.6068	1472.9259	1477.2710
1482.7842	1484.8808	1489.5762
1493.1410	1495.7534	1498.1556
1514.8017	1522.4727	1540.9134
1573.7313	1665.7170	1686.1834
1901.8104	3015.4275	3028.9346
3039.3597	3044.8827	3046.5787
3048.3237	3049.0271	3049.8462
3050.4528	3101.2108	3118.5939
3124.1409	3130.1836	3132.7760
3134.3572	3135.3086	3136.6087
3136.7422	3138.0811	3150.0650
3153.9823	3155.6691	3160.7794
3165.1766	3169.5842	3195.3195
3200.5985	3213.1290	3758.8505

C	-1.32781	-1.59776	-1.56252
H	-1.74952	-2.13485	-2.42725
O	-0.08629	-1.42456	-1.59086
H	-2.60543	0.05680	2.59035
Cl	-6.26797	-1.44158	-0.24324
H	-1.08247	-1.87037	5.35490
H	-1.25297	-2.79232	3.83883
Ir	1.41694	-0.21556	-0.32137
H	-1.49980	0.37953	0.32274
C	-2.97946	-0.72280	-0.83640
C	-3.99363	0.00621	-0.20013
C	-3.32706	-1.69968	-1.79362
C	-5.32310	-0.22802	-0.49568
H	-3.72011	0.76531	0.53161
C	-4.67627	-1.92142	-2.07765
C	-5.66829	-1.19566	-1.43610
H	-4.95046	-2.67602	-2.81397
H	-6.71538	-1.37713	-1.66349
O	-2.35238	-2.39011	-2.40731
H	-2.74769	-3.02473	-3.01655
Cl	-6.57374	0.68394	0.30640

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.466839 Electronic Energy = -1720.63172579
Internal Energy (E)= -1720.13359779 Enthalpy (H)= -1720.13265479
Gibbs Free Energy (G)=-1720.22520579 Gibbs Free Energy of Solvation=-1720.32946379

St.Pt.	General Structure	Ball & Stick model
III'-3		

Cartesian co-ordinate

Atoms	X	Y	Z
C	1.29245	-2.38742	-1.00070
C	2.38592	-1.90200	-0.22033
C	1.94243	-1.82750	1.16454
C	0.58328	-2.35515	1.22279
C	0.17790	-2.68813	-0.10627
C	-2.30946	0.27813	-0.47742
Ir	0.69978	-0.55331	0.03324
C	-3.68240	0.27922	-0.78440
C	-4.57948	0.75007	0.14256
C	-1.83739	0.71314	0.79127
C	-4.13453	1.23779	1.38431
C	-2.79608	1.22463	1.70148
H	-2.44007	1.58673	2.66257
H	-4.86447	1.61932	2.09446

Frequencies

-67.4731	14.9227	31.4032
37.8431	47.0794	66.0333
73.0173	81.7746	90.6800
112.0070	123.2896	153.7593
159.1766	167.9272	175.6855
181.9620	183.4790	187.9798
198.4420	204.9845	213.0170
218.6907	222.2573	232.0124
237.3454	243.1820	259.3269
274.6334	287.6940	292.4271
296.4826	312.7315	316.9190
319.3205	323.8789	328.9831
337.5586	374.1989	392.1303
403.4710	417.8684	426.6998
430.8183	446.6593	457.1117
470.5812	526.9851	536.4959
538.4671	548.3045	572.0780
581.3796	587.3719	593.6065

H	-0.30143	0.36937	-1.36103
O	1.87748	1.13791	0.02172
C	1.45766	2.24613	-0.53303
C	2.29797	3.46698	-0.14300
O	0.46859	2.34837	-1.24550
H	-4.00379	-0.07883	-1.75979
C	-1.35786	-0.12513	-1.48791
O	-1.56963	-0.73668	-2.51732
O	-0.59031	0.63475	1.15731
C	2.13512	4.56061	-1.19178
H	1.08103	4.81896	-1.32796
H	2.68422	5.46035	-0.88475
H	2.52590	4.23782	-2.16454
C	1.72513	3.94316	1.19714
H	1.82083	3.16463	1.96363
H	2.25957	4.83916	1.53972
H	0.66156	4.19177	1.09532
C	3.77346	3.11281	0.02055
H	4.19296	2.71593	-0.91337
H	4.34547	4.01077	0.28952
H	3.92189	2.36296	0.80474
C	3.71425	-1.42986	-0.69776
H	3.84411	-0.36502	-0.46329
H	4.52307	-1.99215	-0.21560
H	3.81782	-1.54934	-1.77981
C	1.24221	-2.54792	-2.47833
H	2.11904	-2.10243	-2.95666
H	1.20576	-3.61084	-2.74889
H	0.34843	-2.06035	-2.89001
C	-1.11038	-3.30984	-0.51732
H	-1.41265	-2.98074	-1.51602
H	-1.01666	-4.40339	-0.53198
H	-1.92044	-3.05169	0.17281
C	-0.26000	-2.42711	2.44507
H	-1.32151	-2.32628	2.19621
H	-0.11637	-3.38118	2.96678
H	-0.01265	-1.61372	3.13432
C	2.78665	-1.38773	2.30653
H	2.17746	-1.11068	3.17190
H	3.47270	-2.18744	2.61532
H	3.38431	-0.51294	2.02768
Cl	-6.29582	0.76060	-0.20813
Cl	-6.26797	-1.44158	-0.24324
H	-1.08247	-1.87037	5.35490
H	-1.25297	-2.79232	3.83883
Ir	1.41694	-0.21556	-0.32137
H	-1.49980	0.37953	0.32274
C	-2.97946	-0.72280	-0.83640
C	-3.99363	0.00621	-0.20013
C	-3.32706	-1.69968	-1.79362
C	-5.32310	-0.22802	-0.49568
H	-3.72011	0.76531	0.53161
C	-4.67627	-1.92142	-2.07765
C	-5.66829	-1.19566	-1.43610
H	-4.95046	-2.67602	-2.81397
H	-6.71538	-1.37713	-1.66349
O	-2.35238	-2.39011	-2.40731
H	-2.74769	-3.02473	-3.01655
Cl	-6.57374	0.68394	0.30640

600.5114	607.8481	641.3163
645.0216	673.3942	736.3713
788.1039	806.9725	811.3998
817.7625	838.8629	853.1770
906.2131	914.4114	916.6203
946.7206	951.3539	953.7264
956.7067	964.9611	969.1551
1036.0328	1038.1724	1042.2601
1044.2633	1046.1434	1048.1184
1050.1062	1075.1728	1090.6540
1091.0059	1095.6345	1106.4719
1132.7686	1178.7184	1183.9128
1189.5093	1235.9658	1241.4368
1244.5634	1266.0307	1339.1908
1355.1361	1375.2189	1377.3694
1379.6706	1383.7066	1387.9526
1393.4765	1400.3529	1402.6096
1413.4780	1428.0466	1432.4893
1438.8216	1440.7719	1449.7887
1451.1125	1452.5212	1454.8843
1458.6656	1461.8183	1463.7934
1467.8411	1469.4732	1472.0748
1473.2122	1474.8256	1476.7378
1481.0518	1487.9817	1499.5365
1501.1671	1515.7221	1522.6734
1543.1230	1594.3118	1668.1367
1781.5798	1803.5129	2306.7591
3023.8867	3026.3365	3034.7790
3036.2024	3036.8391	3040.9518
3041.3402	3044.6941	3105.2279
3114.2948	3115.7777	3117.1668
3119.7584	3123.0754	3124.2443
3126.4837	3130.2716	3134.9045
3142.8328	3147.0304	3148.4127
3149.6370	3151.2587	3152.0481
3190.8828	3206.1111	3207.1632

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.452722 Electronic Energy = -1720.21484135
Internal Energy (E)= -1719.73185135 Enthalpy (H)= -1719.73090735
Gibbs Free Energy (G)=-1719.82242935 Gibbs Free Energy of Solvation=-1719.86984684

St.Pt.	General Structure	Ball & Stick model
TS_3-3		

Cartesian co-ordinate

Atoms	X	Y	Z
C	1.75033	-2.20391	-0.96907
C	2.69986	-1.36569	-0.30756
C	2.38866	-1.35625	1.11743
C	1.25760	-2.20788	1.32021
C	0.82668	-2.69950	0.03714
C	-2.24614	-0.19827	-0.32270
Ir	0.70566	-0.48401	-0.02403
C	-3.58940	-0.30994	-0.71483
C	-4.56121	0.20626	0.10984
C	-1.87624	0.40790	0.89648
C	-4.21811	0.84024	1.31682
C	-2.90134	0.94505	1.70837
H	-2.62512	1.43089	2.64047
H	-5.01011	1.24732	1.94108
H	-0.10972	0.30124	-1.28255
O	1.53013	1.42298	0.03788
C	0.91596	2.38668	-0.59027
C	1.41043	3.77984	-0.19193
O	-0.01973	2.23962	-1.36944
H	-3.83418	-0.79011	-1.65887
C	-1.17070	-0.69620	-1.16278
O	-1.27931	-1.35860	-2.17097
O	-0.62730	0.45244	1.26906
C	1.10713	4.77577	-1.30464
H	0.04232	4.77270	-1.55461
H	1.39474	5.78741	-0.99004
H	1.66413	4.53225	-2.21769
C	0.60561	4.13579	1.06446
H	0.78643	3.40542	1.86239
H	0.89091	5.13237	1.42601
H	-0.46923	4.14050	0.84463
C	2.90211	3.78447	0.12755
H	3.49737	3.48513	-0.74510
H	3.21739	4.79555	0.41671
H	3.13662	3.10112	0.95044
C	3.82086	-0.60124	-0.91627
H	3.77723	0.45002	-0.60578

Frequencies

-198.2276	23.5785	31.5928
32.9292	58.0770	67.6457
83.8881	94.5091	111.8183
123.4661	132.4889	143.0756
149.8510	155.8344	158.5344
170.9120	175.1471	182.0647
186.8156	194.8720	209.5628
211.2447	215.0188	218.2742
226.8256	229.4534	250.6609
259.3422	280.8372	283.7024
287.9490	299.2520	314.5810
316.6493	321.1041	345.4996
348.2390	357.8094	371.6648
391.9516	407.4578	414.9446
428.4544	432.8134	440.0660
471.4026	493.7762	535.3419
540.1219	542.2598	547.1980
569.2873	590.1828	596.4429
605.6739	631.3475	643.1342
652.2209	669.6107	714.2605
763.2110	793.0840	809.4732
812.9561	819.6964	829.7387
856.9504	891.0139	903.4917
921.5161	926.7986	939.6891
949.4760	951.3220	952.9128
958.4653	959.1598	1033.6583
1036.9502	1038.7523	1038.8622
1042.3850	1046.2067	1048.6753
1085.4560	1088.0608	1090.5333
1106.0755	1130.0416	1182.6369
1184.2704	1190.6474	1234.8130
1236.5761	1247.5918	1264.0188
1347.2327	1357.0633	1373.4124
1375.0210	1378.0112	1378.4852
1393.2069	1394.5222	1396.0955
1397.5354	1408.2484	1435.2244
1438.8543	1441.9841	1443.0450
1445.2414	1446.0932	1452.2170
1454.1475	1454.9482	1458.5358
1461.6481	1465.0388	1468.0227
1470.0046	1472.7122	1475.0167

H	4.78658	-1.01379	-0.59788	1481.9034	1485.7523	1504.4611
H	3.77853	-0.62839	-2.00869	1509.5731	1520.0576	1521.5086
C	1.69971	-2.54748	-2.41520	1543.6039	1608.8899	1661.5231
H	2.44939	-1.99025	-2.98382	1726.2927	1783.5510	1852.9548
H	1.89016	-3.61847	-2.55895	3025.8798	3029.2858	3035.2432
H	0.71324	-2.31480	-2.83013	3037.1297	3037.2400	3037.9548
C	-0.26702	-3.67989	-0.20518	3044.0099	3046.7784	3106.5726
H	-0.69787	-3.54998	-1.20218	3115.2408	3115.6964	3118.0944
H	0.11304	-4.70655	-0.12491	3119.3696	3120.6188	3127.5040
H	-1.07717	-3.56236	0.52270	3129.6282	3132.6495	3134.9973
C	0.55630	-2.44937	2.60830	3142.1511	3146.1073	3148.6167
H	-0.52557	-2.52760	2.45693	3149.0567	3149.5205	3160.3079
H	0.90237	-3.38303	3.06897	3199.5727	3213.6168	3214.5308
H	0.72729	-1.63265	3.31546			
C	3.15825	-0.60118	2.14381			
H	2.63416	-0.58168	3.10367			
H	4.14587	-1.05156	2.30680			
H	3.30537	0.43759	1.82727			
Cl	-6.25211	0.08693	-0.33553			
Cl	-6.26797	-1.44158	-0.24324			
H	-1.08247	-1.87037	5.35490			
H	-1.25297	-2.79232	3.83883			
Ir	1.41694	-0.21556	-0.32137			
H	-1.49980	0.37953	0.32274			
C	-2.97946	-0.72280	-0.83640			
C	-3.99363	0.00621	-0.20013			
C	-3.32706	-1.69968	-1.79362			
C	-5.32310	-0.22802	-0.49568			
H	-3.72011	0.76531	0.53161			
C	-4.67627	-1.92142	-2.07765			
C	-5.66829	-1.19566	-1.43610			
H	-4.95046	-2.67602	-2.81397			
H	-6.71538	-1.37713	-1.66349			
O	-2.35238	-2.39011	-2.40731			
H	-2.74769	-3.02473	-3.01655			
Cl	-6.57374	0.68394	0.30640			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.448860 Electronic Energy = -1720.20980032
Internal Energy (E)= -1719.73027632 Enthalpy (H)= -1719.72933232
Gibbs Free Energy (G)=-1719.82092532 Gibbs Free Energy of Solvation=-1719.86210786

St.Pt.	General Structure	Ball & Stick model
IV-3		

Cartesian co-ordinate

Atoms	X	Y	Z
C	0.99152	-2.37668	-1.02128

Frequencies

11.1822	19.7416	30.1100
48.2653	59.6344	71.5644
90.7160	103.0286	114.2643
140.5039	148.5290	153.3481
159.2250	168.6797	174.1535

C	2.22483	-1.68160	-0.70478	184.4109	189.4887	193.3048
C	2.42414	-1.72175	0.73670	196.3117	201.7892	214.6036
C	1.28791	-2.29711	1.31116	221.2944	228.5176	232.7815
C	0.34926	-2.64551	0.23329	234.3006	244.9539	268.2287
C	-2.33854	0.20117	-0.33243	276.6012	277.9965	290.4832
Ir	0.47606	-0.48500	-0.06914	298.3086	303.7381	320.5208
C	-3.61246	0.48599	-0.83740	330.5467	335.0293	347.7361
C	-4.62834	0.75028	0.05674	348.6980	369.0026	376.8014
C	-2.07845	0.17369	1.04829	390.4045	414.9166	422.5384
C	-4.39407	0.72840	1.43912	431.1063	436.2000	447.0282
C	-3.13707	0.44313	1.93741	474.5817	533.1396	535.2247
H	-2.94496	0.42814	3.00694	535.7834	552.9458	568.6833
H	-5.21707	0.94204	2.11729	594.8774	613.1819	618.2189
H	1.02428	0.17083	-1.41920	632.8271	646.5685	647.8677
O	1.04487	1.45140	0.42085	661.0255	679.9341	746.2236
C	1.77932	2.12449	-0.41665	788.2842	805.7080	811.0534
C	2.25894	3.46860	0.14265	813.9736	824.6514	833.5378
O	2.11819	1.73433	-1.53372	869.4661	908.4585	909.5578
H	-3.77493	0.49623	-1.91231	932.5788	942.5648	947.3552
C	-1.20362	-0.12279	-1.20662	948.7067	951.8933	953.7441
O	-1.26864	-0.23751	-2.40837	954.9258	967.8025	1027.4771
O	-0.86699	-0.10894	1.47103	1034.8891	1036.3012	1045.0119
C	-0.94543	-3.34730	0.45745	1046.2195	1048.8001	1054.2253
H	-1.57367	-3.32636	-0.43852	1083.9913	1087.6365	1088.8142
H	-0.78200	-4.39612	0.73683	1106.1421	1125.1800	1174.5655
H	-1.50805	-2.86444	1.26453	1183.0057	1189.9061	1236.9771
C	0.53456	-2.75488	-2.38611	1240.3870	1246.7225	1268.2796
H	1.22071	-3.48983	-2.82418	1338.5828	1360.1395	1364.0014
H	-0.46620	-3.19521	-2.36208	1373.3845	1374.5700	1380.0028
H	0.47799	-1.88084	-3.04410	1388.6818	1392.1849	1394.7685
C	3.26306	-1.24836	-1.68031	1397.9048	1414.6346	1429.3192
H	4.09029	-1.96984	-1.69799	1433.4400	1435.9764	1442.4289
H	2.84842	-1.17007	-2.68957	1447.6074	1448.8828	1449.7622
H	3.65859	-0.26072	-1.42124	1452.5871	1455.0171	1457.3664
C	3.58438	-1.09015	1.41996	1458.5488	1462.7558	1463.5990
H	4.53210	-1.51267	1.06408	1470.5863	1471.1772	1475.5513
H	3.60883	-0.01126	1.21382	1477.1320	1483.7120	1490.6074
H	3.53839	-1.21951	2.50469	1507.1418	1511.7422	1517.5942
C	0.94939	-2.42115	2.75020	1586.3056	1619.1718	1655.5225
H	1.79004	-2.14630	3.39289	1727.9408	1813.7606	2073.8590
H	0.10572	-1.75636	2.98425	3018.9710	3031.7112	3032.1271
H	0.64524	-3.44584	2.99604	3034.4779	3037.1248	3037.5015
C	3.32237	3.15329	1.19962	3042.2173	3043.8731	3101.4690
H	3.72261	4.08516	1.61962	3103.2258	3109.0057	3113.7416
H	2.89891	2.55850	2.01730	3119.5273	3123.1998	3130.0532
H	4.16166	2.59845	0.75669	3131.1688	3132.7140	3140.6448
C	2.87345	4.30224	-0.97482	3140.6662	3146.7052	3148.1428
H	2.13727	4.51710	-1.75752	3150.0032	3150.9114	3154.0909
H	3.23602	5.25626	-0.57068	3194.2026	3209.0765	3211.7259
H	3.71162	3.77983	-1.44715			
C	1.09830	4.22376	0.78696			
H	1.45503	5.18489	1.17972			
H	0.30848	4.43256	0.05507			
H	0.65682	3.65164	1.60813			
Cl	-6.23876	1.12282	-0.52719			
Cl	-6.26797	-1.44158	-0.24324			
H	-1.08247	-1.87037	5.35490			
H	-1.25297	-2.79232	3.83883			
Ir	1.41694	-0.21556	-0.32137			
H	-1.49980	0.37953	0.32274			
C	-2.97946	-0.72280	-0.83640			

C	-3.99363	0.00621	-0.20013
C	-3.32706	-1.69968	-1.79362
C	-5.32310	-0.22802	-0.49568
H	-3.72011	0.76531	0.53161
C	-4.67627	-1.92142	-2.07765
C	-5.66829	-1.19566	-1.43610
H	-4.95046	-2.67602	-2.81397
H	-6.71538	-1.37713	-1.66349
O	-2.35238	-2.39011	-2.40731
H	-2.74769	-3.02473	-3.01655
Cl	-6.57374	0.68394	0.30640

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.450933 Electronic Energy = -1720.21743674
Internal Energy (E)= -1719.73563074 Enthalpy (H)= -1719.73468774
Gibbs Free Energy (G)=-1719.82803874 Gibbs Free Energy of Solvation=-1719.87224651

St.Pt.	General Structure	Ball & Stick model
TS_3-4		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.17525	-2.21306	1.17458
C	-2.34565	-1.48280	0.74369
C	-2.51186	-1.67655	-0.69293
C	-1.40497	-2.38855	-1.16166
C	-0.51769	-2.66644	-0.02202
C	2.31531	0.13105	0.30512
Ir	-0.51276	-0.49389	0.01369
C	3.58459	0.41714	0.82025
C	4.62963	0.58479	-0.06395
C	2.08918	0.00380	-1.07646
C	4.42866	0.46655	-1.44669
C	3.17631	0.17947	-1.95513
H	3.01014	0.08891	-3.02534
H	5.27374	0.60613	-2.11688
H	-1.03927	0.43113	1.28556
O	-1.00795	1.45629	-0.60426
C	-1.51629	2.21588	0.30372
C	-2.00566	3.57432	-0.18913
O	-1.65752	1.87042	1.49068
H	3.72025	0.50412	1.89554
C	1.14298	-0.08130	1.16544
O	1.17209	-0.08562	2.37586

Frequencies

-319.8117	19.5398	31.6874
40.1012	54.6574	71.2226
82.5111	101.5312	106.2509
139.1360	144.5249	147.4426
150.7457	161.6117	166.5917
172.8620	185.1469	198.7793
203.3064	210.3522	213.4183
221.1985	230.0931	232.9039
234.9665	243.3101	246.6536
264.6994	280.3400	289.6293
299.0575	306.2800	314.1692
327.9555	331.4304	334.2948
347.8454	351.7407	373.2777
392.3633	414.1284	421.7338
430.5658	437.3487	444.5812
475.8478	502.2960	533.9825
535.9568	538.7581	552.1597
593.6165	612.6175	621.2761
622.1680	636.7664	646.4852
655.2173	660.5868	690.0968
748.7933	792.3421	810.1831
812.2346	833.1358	836.3994
863.7353	890.9269	910.1809
939.4432	946.3473	949.6750
953.6119	954.3368	955.8360
957.4973	961.1055	1034.0811

O	0.88200	-0.27863	-1.50851	1038.7530	1042.0058	1045.2866
C	0.72936	-3.47848	-0.10842	1047.4278	1052.3882	1058.0455
H	1.35799	-3.33490	0.77614	1083.9716	1087.0601	1088.2144
H	0.50124	-4.54876	-0.19574	1105.5904	1125.5968	1175.1611
H	1.32421	-3.18727	-0.98168	1181.7364	1189.1013	1236.3194
C	-0.77886	-2.45454	2.58825	1241.6851	1253.5616	1267.5097
H	-1.52121	-3.09157	3.08453	1340.2602	1367.2306	1372.9981
H	0.19353	-2.95072	2.65138	1377.8478	1380.0891	1380.2774
H	-0.68702	-1.51287	3.14064	1389.0019	1395.6719	1399.8920
C	-3.37783	-0.88528	1.63657	1400.5446	1424.1113	1428.1182
H	-4.18369	-1.60781	1.82212	1437.8715	1438.6692	1443.1655
H	-2.94938	-0.58912	2.59842	1448.5531	1451.0342	1453.4176
H	-3.82197	0.01125	1.19022	1455.6652	1456.3982	1459.5038
C	-3.60819	-1.04862	-1.47903	1459.7321	1464.0681	1465.6059
H	-4.59010	-1.41475	-1.15367	1466.9134	1469.2295	1474.1803
H	-3.60234	0.04176	-1.34235	1480.8576	1483.4351	1501.7202
H	-3.50809	-1.24724	-2.54959	1503.6574	1511.7993	1516.0956
C	-1.02967	-2.68371	-2.56831	1585.3149	1591.8249	1621.0729
H	-1.83464	-2.43996	-3.26704	1655.8470	1769.9451	1816.7794
H	-0.14602	-2.08916	-2.84330	3015.9542	3019.6772	3029.6247
H	-0.77343	-3.74259	-2.69412	3034.2431	3037.0529	3038.2179
C	-3.24196	3.30209	-1.05404	3040.2601	3045.1274	3098.4515
H	-3.66025	4.24951	-1.41674	3098.7441	3106.4835	3116.3150
H	-2.98714	2.68201	-1.92121	3117.2304	3119.5165	3125.4894
H	-4.02322	2.79166	-0.47354	3127.2661	3129.5626	3140.0199
C	-2.38246	4.46211	0.98964	3142.6849	3145.3470	3147.9027
H	-1.51892	4.64930	1.63732	3149.8743	3150.0435	3156.1601
H	-2.75306	5.42715	0.62142	3196.8017	3205.9782	3210.5312
H	-3.16197	3.99915	1.60347			
C	-0.92103	4.24259	-1.03297			
H	-1.28868	5.20578	-1.40949			
H	-0.01995	4.43627	-0.43853			
H	-0.63793	3.61775	-1.88522			
Cl	6.23700	0.95422	0.53318			
Cl	-6.26797	-1.44158	-0.24324			
H	-1.08247	-1.87037	5.35490			
H	-1.25297	-2.79232	3.83883			
Ir	1.41694	-0.21556	-0.32137			
H	-1.49980	0.37953	0.32274			
C	-2.97946	-0.72280	-0.83640			
C	-3.99363	0.00621	-0.20013			
C	-3.32706	-1.69968	-1.79362			
C	-5.32310	-0.22802	-0.49568			
H	-3.72011	0.76531	0.53161			
C	-4.67627	-1.92142	-2.07765			
C	-5.66829	-1.19566	-1.43610			
H	-4.95046	-2.67602	-2.81397			
H	-6.71538	-1.37713	-1.66349			
O	-2.35238	-2.39011	-2.40731			
H	-2.74769	-3.02473	-3.01655			
Cl	-6.57374	0.68394	0.30640			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.449259 Electronic Energy = -1720.21689034
Internal Energy (E)= -1719.73737434 Enthalpy (H)= -1719.73643034
Gibbs Free Energy (G)=-1719.82699334 Gibbs Free Energy of Solvation=-1719.86887276

St.Pt.	General Structure	Ball & Stick model
V-3		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.98114	-2.06537	1.41697
C	-2.15354	-1.31323	1.07432
C	-2.54684	-1.69089	-0.29088
C	-1.58451	-2.55865	-0.81002
C	-0.53462	-2.72826	0.20659
C	2.30353	0.23038	0.20969
Ir	-0.44407	-0.63284	-0.09998
C	3.51991	0.67643	0.74336
C	4.63065	0.68603	-0.07020
C	2.18319	-0.17368	-1.14217
C	4.54313	0.28055	-1.41262
C	3.34248	-0.13680	-1.95009
H	3.26759	-0.43943	-2.99150
H	5.43961	0.30531	-2.02821
H	-0.55231	1.61708	1.67828
O	-1.05058	1.40911	-0.69153
C	-1.42710	2.29773	0.08309
C	-2.24871	3.47257	-0.41307
O	-1.20855	2.31149	1.37060
H	3.56335	1.00244	1.77991
C	1.04039	0.23553	0.93255
O	0.87455	0.78360	2.03368
O	1.01982	-0.54074	-1.60490
C	0.63481	-3.63922	0.05731
H	1.41448	-3.40685	0.79055
H	0.34691	-4.69125	0.18509
H	1.08174	-3.52559	-0.93664
C	-0.33568	-2.10848	2.75686
H	-0.88479	-2.77927	3.42932
H	0.69712	-2.46522	2.68893
H	-0.30073	-1.11004	3.20598
C	-2.99049	-0.51518	2.01528
H	-3.80528	-1.11976	2.43716
H	-2.39111	-0.13478	2.84929
H	-3.44772	0.34966	1.51910
C	-3.72431	-1.10451	-0.98768
H	-4.66024	-1.38891	-0.48916
H	-3.67478	-0.00647	-0.98318
H	-3.78340	-1.42650	-2.03139

Frequencies

22.4986	41.5952	61.3718
65.7985	75.5771	81.0349
101.5729	120.8198	124.4874
135.0278	145.4749	154.4271
158.5175	161.9580	168.9678
175.7581	179.9019	190.5603
201.9352	206.7917	219.6653
230.6513	238.8125	249.5675
257.4923	277.3835	287.4748
289.2708	297.9627	307.5608
311.7111	316.7373	325.3800
328.4663	335.9091	340.6287
357.4154	370.2823	390.3778
397.6847	408.4007	413.1420
422.7748	431.8432	461.7291
486.7414	533.0041	534.0070
537.9104	546.2828	554.1676
593.8669	604.1980	611.2612
624.6509	639.8558	652.9445
670.6153	697.4792	753.6567
781.2911	787.1060	802.2076
809.8154	836.7902	868.6583
895.1665	909.0667	919.5898
950.5207	953.0473	953.5243
959.1468	960.2108	960.2966
964.4518	1029.4590	1041.1133
1043.4385	1044.6053	1047.6126
1048.1005	1051.0751	1077.9993
1085.9602	1090.8967	1104.2853
1127.9550	1176.7618	1184.1618
1190.6288	1229.2071	1238.7439
1248.1360	1260.8163	1333.4424
1348.6580	1368.5439	1376.0127
1381.9755	1386.3560	1391.1329
1391.2519	1403.1493	1403.8231
1417.9279	1428.1897	1434.2706
1445.6682	1449.7805	1451.4943
1452.8995	1455.2960	1455.4905
1458.7006	1459.2361	1461.8503
1467.4326	1468.1323	1470.2645
1473.4785	1477.6340	1482.7510
1484.7284	1491.2122	1506.5123
1511.0333	1516.1263	1519.5498

C	-1.48953	-3.12252	-2.18371	1594.6950	1604.8717	1657.8776
H	-2.32544	-2.80326	-2.81319	1665.1020	1742.3163	3022.8659
H	-0.56182	-2.79882	-2.67217	3029.2482	3030.5455	3033.1600
H	-1.48510	-4.21995	-2.15863	3033.3809	3038.7521	3042.4335
C	-3.63947	3.35405	0.22401	3048.4019	3089.8415	3103.1868
H	-4.26693	4.18601	-0.11775	3105.6816	3113.1721	3115.6473
H	-4.13482	2.41998	-0.07548	3123.8344	3126.8416	3135.2513
H	-3.58625	3.38729	1.31726	3136.9976	3138.9522	3140.3733
C	-1.58516	4.77915	0.02990	3141.9069	3143.0936	3145.7845
H	-0.58070	4.88013	-0.39825	3147.4121	3149.8270	3153.6652
H	-2.18556	5.62737	-0.32059	3186.9518	3202.3708	3204.9306
H	-1.50246	4.84072	1.11916			
C	-2.36834	3.42830	-1.93098			
H	-2.97186	4.27768	-2.27261			
H	-1.38634	3.48666	-2.41227			
H	-2.84888	2.50387	-2.26931			
Cl	6.18267	1.22054	0.55617			
Cl	-6.26797	-1.44158	-0.24324			
H	-1.08247	-1.87037	5.35490			
H	-1.25297	-2.79232	3.83883			
Ir	1.41694	-0.21556	-0.32137			
H	-1.49980	0.37953	0.32274			
C	-2.97946	-0.72280	-0.83640			
C	-3.99363	0.00621	-0.20013			
C	-3.32706	-1.69968	-1.79362			
C	-5.32310	-0.22802	-0.49568			
H	-3.72011	0.76531	0.53161			
C	-4.67627	-1.92142	-2.07765			
C	-5.66829	-1.19566	-1.43610			
H	-4.95046	-2.67602	-2.81397			
H	-6.71538	-1.37713	-1.66349			
O	-2.35238	-2.39011	-2.40731			
H	-2.74769	-3.02473	-3.01655			
Cl	-6.57374	0.68394	0.30640			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.455379 Electronic Energy = -1720.25157292
Internal Energy (E)= -1719.76589792 Enthalpy (H)= -1719.76495392
Gibbs Free Energy (G)=-1719.85480592 Gibbs Free Energy of Solvation=-1719.89468863

St.Pt.	General Structure	Ball & Stick model
V'-3		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.19155	-2.71278	0.57379

Frequencies

18.3677	25.7075	36.3789
50.9811	70.4543	79.3879
83.7297	90.7587	103.5241
109.2380	125.2950	131.2903
137.7850	144.8290	147.9051

C	-1.41852	-2.14034	1.05794	153.5822	161.1317	166.2820
C	-2.26695	-1.88057	-0.10297	182.5181	186.8564	194.0690
C	-1.53834	-2.15091	-1.27324	200.0559	202.6229	206.7200
C	-0.21069	-2.60809	-0.86124	214.8361	219.1434	219.6806
C	2.49381	0.19201	0.26122	229.2510	234.4247	239.0834
Ir	-0.28181	-0.59533	-0.03648	264.8658	267.1547	282.6697
C	2.18852	0.40985	-1.10136	297.5322	316.5093	329.2733
C	3.22698	0.84351	-1.95570	333.6255	340.0224	341.1833
C	3.77780	0.40986	0.77266	356.6352	361.2405	367.8811
C	4.49757	1.04071	-1.45009	382.6204	385.5241	406.1936
C	4.77011	0.82474	-0.09030	411.7231	433.4992	439.4790
H	3.96547	0.25371	1.83278	455.1461	481.3511	493.9596
H	5.30255	1.37178	-2.10270	503.6264	529.2655	534.0021
H	3.00277	1.02462	-3.00390	534.4096	538.8605	549.9038
C	-1.13527	1.42083	0.24844	587.3079	594.6237	599.1994
C	-2.55466	1.49417	-0.26883	610.2677	624.5894	636.1553
C	-0.23768	2.52058	-0.36922	655.6269	671.8064	688.0291
O	-0.54404	2.98267	-1.43626	752.6251	753.6898	778.5979
N	-1.09470	1.43170	1.63631	810.7679	814.1615	822.2714
N	-0.99335	1.40933	2.75649	833.4756	866.8526	876.6599
C	-3.68057	-1.42857	-0.00807	899.3151	935.2639	953.2108
H	-4.04150	-1.00812	-0.95123	956.2321	958.2685	969.8343
H	-4.32521	-2.27680	0.25739	983.0098	1017.0465	1037.1647
H	-3.81057	-0.67208	0.77629	1044.6708	1046.6634	1050.1696
C	-1.80557	-2.04247	2.49415	1051.1644	1055.9005	1080.8687
H	-2.65326	-1.36158	2.63506	1088.5909	1090.3420	1094.5444
H	-2.09280	-3.01666	2.91231	1110.3360	1120.7795	1124.9575
H	-0.96522	-1.65243	3.08383	1169.9593	1175.3589	1182.9615
C	0.88895	-3.28130	1.42429	1187.4818	1195.1504	1232.9888
H	0.98431	-2.72496	2.36245	1263.4334	1321.6837	1345.2418
H	0.67064	-4.32947	1.66633	1368.0213	1377.9138	1378.9324
H	1.86116	-3.24541	0.92122	1380.0682	1385.0719	1397.4978
C	0.86166	-3.03070	-1.80351	1404.8427	1405.4244	1412.6342
H	1.82129	-3.15308	-1.29069	1431.4268	1434.8136	1439.1324
H	0.60807	-3.98318	-2.28656	1446.4109	1448.2556	1452.0492
H	1.00212	-2.27701	-2.58650	1453.0169	1459.0599	1462.3986
C	-1.96522	-1.93796	-2.68419	1465.9393	1466.8144	1471.7487
H	-2.35863	-2.85803	-3.13729	1474.3822	1477.0539	1487.5765
H	-2.73180	-1.15950	-2.75342	1488.6686	1493.2090	1506.0857
H	-1.11884	-1.60182	-3.29391	1508.2693	1510.7946	1515.6262
C	1.33773	-0.16055	1.09588	1568.6720	1606.0952	1656.2654
O	0.96062	0.25661	-1.52481	1739.5246	1854.5008	1894.1991
O	1.35876	-0.21139	2.31974	2256.7245	3026.2216	3030.9720
O	-2.85712	1.26563	-1.40839	3034.5886	3037.8687	3038.4285
C	-4.76945	2.10759	0.28437	3053.8257	3054.3661	3076.5892
H	-5.35523	1.99692	1.20132	3101.9853	3105.5151	3110.9882
H	-5.06328	1.32754	-0.42618	3117.8242	3120.4168	3127.6001
O	-3.40618	1.87227	0.69871	3134.6920	3141.2891	3141.3554
C	-4.90486	3.48315	-0.31902	3144.2024	3144.7336	3146.9527
H	-4.30871	3.56012	-1.23344	3150.9319	3159.9553	3175.8617
H	-5.95082	3.68186	-0.57381	3190.1809	3201.3095	3206.0769
H	-4.57148	4.25107	0.38625			
C	0.94055	3.01649	0.42183			
H	1.79833	3.09172	-0.25432			
H	0.70321	4.02978	0.76731			
H	1.22135	2.40272	1.28030			
Cl	6.39997	1.09526	0.50572			
H	-1.25297	-2.79232	3.83883			
Ir	1.41694	-0.21556	-0.32137			
H	-1.49980	0.37953	0.32274			
C	-2.97946	-0.72280	-0.83640			

C	-3.99363	0.00621	-0.20013
C	-3.32706	-1.69968	-1.79362
C	-5.32310	-0.22802	-0.49568
H	-3.72011	0.76531	0.53161
C	-4.67627	-1.92142	-2.07765
C	-5.66829	-1.19566	-1.43610
H	-4.95046	-2.67602	-2.81397
H	-6.71538	-1.37713	-1.66349
O	-2.35238	-2.39011	-2.40731
H	-2.74769	-3.02473	-3.01655
Cl	-6.57374	0.68394	0.30640

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.451025 Electronic Energy = -1941.67714017
Internal Energy (E)= -1941.19203617 Enthalpy (H)= -1941.19109217
Gibbs Free Energy (G)=-1941.29008517 Gibbs Free Energy of Solvation=-1941.33205323

St.Pt.	General Structure	Ball & Stick model
TS_3-5		

Cartesian co-ordinate

Atoms	X	Y	Z
C	0.13305	-2.75099	0.42287
C	-1.04336	-2.29223	1.12098
C	-2.06570	-2.02474	0.12244
C	-1.51042	-2.23105	-1.16830
C	-0.12882	-2.63145	-0.97704
C	2.45114	0.32263	0.24262
Ir	-0.28872	-0.58029	-0.05521
C	2.13995	0.51521	-1.12191
C	3.17022	0.95056	-1.98467
C	3.73412	0.56184	0.74802
C	4.44055	1.16638	-1.48591
C	4.72025	0.97111	-0.12451
H	3.92755	0.42425	1.80954
H	5.23978	1.49640	-2.14601
H	2.94169	1.11418	-3.03473
C	-1.23103	1.21460	0.21117
C	-2.69090	1.31011	-0.19296
C	-0.53368	2.47562	-0.33470
O	-0.99435	2.97921	-1.33328
N	-1.24344	1.42394	1.83592
N	-0.92269	1.21706	2.88820
C	-3.47992	-1.68647	0.44734
H	-4.00316	-1.26317	-0.41382
H	-4.01694	-2.58796	0.76934
H	-3.54397	-0.96317	1.27113
C	-1.21769	-2.27563	2.60113

Frequencies

-400.5922	17.8949	32.1004
40.7618	56.4677	61.3532
71.9910	73.1581	87.1705
95.7648	115.9362	121.5605
134.8469	140.1917	144.7738
152.1346	156.7455	166.1937
180.3457	180.5206	184.9033
194.5456	199.0447	202.0493
214.8512	216.9323	218.7376
227.5989	231.7732	235.7155
254.3910	271.8009	278.5072
290.4042	297.8474	306.1924
317.5761	324.9140	330.0616
331.8576	341.3602	343.2703
357.1895	359.3687	402.9785
407.4907	411.1660	422.6476
433.6535	437.1789	459.0589
481.3860	518.4705	533.1152
534.3205	538.6381	543.6215
546.8359	590.1448	597.2253
603.8276	623.4850	638.5080
655.6523	668.2957	683.3787
703.5864	749.6658	756.0717
808.9768	811.5413	813.1437
831.6245	865.6320	890.1785
896.6961	902.2511	933.4224
952.9620	954.0014	956.2365
960.8570	1015.5705	1022.4654
1035.7081	1042.2334	1043.9960
1046.4395	1049.7991	1080.8088

H	-2.14189	-1.76064	2.88677	1083.2381	1087.0148	1088.4092
H	-1.26639	-3.29186	3.01383	1106.9980	1124.2753	1125.3255
H	-0.38399	-1.74798	3.08248	1175.5149	1179.7224	1186.2162
C	1.38287	-3.24048	1.06933	1188.2372	1198.7342	1232.2833
H	1.54233	-2.75524	2.03786	1281.3317	1316.0683	1344.0107
H	1.32934	-4.32350	1.24049	1371.6550	1378.1393	1380.1948
H	2.26679	-3.04264	0.45339	1380.7494	1384.3938	1396.4640
C	0.82661	-2.90434	-2.08573	1400.3886	1401.4715	1413.2199
H	1.85596	-2.97668	-1.72011	1433.0366	1433.9472	1441.5543
H	0.57841	-3.84447	-2.59466	1447.4505	1451.2895	1455.2212
H	0.79627	-2.09783	-2.82713	1458.2791	1463.7268	1465.6576
C	-2.17828	-2.07326	-2.48968	1466.1970	1468.7327	1473.7132
H	-2.53955	-3.03559	-2.87778	1476.8417	1478.6469	1479.9106
H	-3.02243	-1.38180	-2.42667	1487.5397	1494.8436	1496.2762
H	-1.48219	-1.65708	-3.22665	1501.2013	1510.6185	1521.5971
C	1.30150	-0.03304	1.08314	1548.2505	1605.6657	1654.8480
O	0.91397	0.33468	-1.54046	1730.7731	1832.1722	1871.8390
O	1.32343	-0.04782	2.30734	2253.4291	3025.5179	3029.7620
O	-3.09739	0.87537	-1.23942	3032.5579	3036.2060	3039.5645
C	-4.78847	2.26242	0.29362	3053.3343	3057.1381	3074.3336
H	-5.32377	2.43625	1.23140	3099.9225	3102.5320	3112.8534
H	-5.20366	1.37462	-0.19697	3114.7488	3119.7476	3125.6630
O	-3.43369	1.97525	0.69974	3134.4177	3137.3726	3140.3996
C	-4.81182	3.46818	-0.61219	3143.6305	3145.9028	3153.9773
H	-4.24669	3.27079	-1.52840	3158.9090	3159.7790	3184.2507
H	-5.84222	3.71622	-0.88688	3191.3389	3203.4543	3207.7419
H	-4.37040	4.33529	-0.11050			
C	0.66884	3.04754	0.36008			
H	1.48632	3.10775	-0.36722			
H	0.42412	4.07225	0.66056			
H	1.01624	2.48595	1.22878			
Cl	6.34981	1.26013	0.46070			
H	-1.25297	-2.79232	3.83883			
Ir	1.41694	-0.21556	-0.32137			
H	-1.49980	0.37953	0.32274			
C	-2.97946	-0.72280	-0.83640			
C	-3.99363	0.00621	-0.20013			
C	-3.32706	-1.69968	-1.79362			
C	-5.32310	-0.22802	-0.49568			
H	-3.72011	0.76531	0.53161			
C	-4.67627	-1.92142	-2.07765			
C	-5.66829	-1.19566	-1.43610			
H	-4.95046	-2.67602	-2.81397			
H	-6.71538	-1.37713	-1.66349			
O	-2.35238	-2.39011	-2.40731			
H	-2.74769	-3.02473	-3.01655			
Cl	-6.57374	0.68394	0.30640			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.448863 Electronic Energy = -1941.67108018
Internal Energy (E)= -1941.18818918 Enthalpy (H)= -1941.18724518
Gibbs Free Energy (G)=-1941.28606318 Gibbs Free Energy of Solvation=-1941.32426636

St.Pt.	General Structure	Ball & Stick model
VI-3		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.49897	2.39271	0.92702
C	0.70594	1.87049	1.53126
C	1.77620	1.99484	0.56400
C	1.21999	2.55027	-0.63768
C	-0.17774	2.78603	-0.40378
C	-2.44079	-0.58857	0.16436
Ir	0.25665	0.47028	-0.14186
C	-2.32466	-0.19141	-1.17957
C	-3.48085	-0.19389	-1.98412
C	-3.65977	-1.01049	0.70698
C	-4.68715	-0.60007	-1.44510
C	-4.77432	-1.00769	-0.10540
H	-3.70801	-1.32005	1.74813
H	-5.58530	-0.60910	-2.05805
H	-3.40178	0.11232	-3.02402
C	1.35663	-1.01505	-0.57662
C	2.84168	-0.82967	-0.65652
C	1.02926	-2.39786	-1.07609
O	1.93971	-3.04360	-1.57301
N	1.35022	-2.53311	2.14464
N	1.74530	-1.93347	2.98440
C	3.22419	1.81204	0.85731
H	3.79749	1.64197	-0.05896
H	3.61890	2.71091	1.34799
H	3.39597	0.96237	1.52795
C	0.85307	1.47341	2.95812
H	1.81388	0.98104	3.13675
H	0.79900	2.35756	3.60675
H	0.06585	0.77343	3.25723
C	-1.81352	2.53588	1.61709
H	-1.93742	1.77235	2.39258
H	-1.89393	3.51801	2.10071
H	-2.65435	2.43420	0.92236
C	-1.13122	3.27722	-1.43516
H	-2.15393	3.32364	-1.04948
H	-0.85194	4.27968	-1.78072
H	-1.13498	2.60340	-2.30165
C	1.96115	2.85493	-1.89227
H	2.44888	3.83756	-1.83415
H	2.72822	2.09761	-2.08405
H	1.28460	2.86804	-2.75293
C	-1.20100	-0.52109	0.94870
O	-1.14756	0.14912	-1.65411
O	-1.09581	-0.87121	2.10243
O	3.39177	-0.20924	-1.54110
C	4.91366	-1.45220	0.28509
H	5.24147	-1.59602	1.31921
H	5.28008	-0.48306	-0.07272
O	3.47598	-1.41189	0.36585
C	5.36061	-2.57735	-0.61490

Frequencies

24.4589	28.3216	36.9410
50.6980	64.0030	75.0848
81.6601	89.5123	93.3095
101.5125	120.5038	122.1033
129.9297	141.1312	146.7574
153.2183	156.0689	159.7813
171.4641	176.6668	180.6787
188.9794	190.4895	197.5785
203.3676	214.2976	219.8953
227.1598	233.2642	238.0933
242.9136	275.1694	284.4973
290.4777	295.4096	297.7635
309.3548	315.0011	320.8661
331.8487	334.9689	346.6905
352.1080	361.3249	372.6654
377.9673	401.7782	412.8177
429.5772	434.1950	441.2401
474.1250	480.7500	531.8837
538.0397	541.0057	550.0066
574.5719	588.5817	603.4218
604.1010	631.1273	651.7312
657.8178	673.1522	685.4405
730.3606	747.6950	757.6211
812.9417	815.5860	818.4047
838.5352	862.1436	885.0180
907.2451	921.0161	956.4189
960.6703	963.3911	967.3725
1009.4423	1033.0714	1037.9999
1042.5576	1047.0647	1048.4671
1050.5907	1051.3400	1082.7548
1088.1544	1095.4394	1107.2960
1112.2947	1125.5146	1127.0939
1177.9914	1180.3554	1187.2032
1188.8116	1230.8790	1244.2510
1295.3656	1326.2998	1335.3652
1378.8039	1380.8453	1382.9371
1384.0287	1387.1493	1394.0102
1402.9872	1406.2972	1419.2779
1439.7314	1440.2638	1446.1050
1449.0012	1453.5680	1454.5155
1462.6402	1463.0125	1465.9911
1471.5668	1472.0947	1473.6264
1478.4919	1482.0551	1485.4451
1492.6479	1496.9011	1501.7067
1504.9340	1507.3385	1518.3425
1536.0578	1615.7410	1652.8088
1779.2026	1801.9678	1819.2934
2469.7860	3034.4297	3036.0776
3038.0366	3039.1990	3042.2000
3054.5187	3060.1253	3066.8347
3114.0685	3117.8647	3120.1655
3121.5001	3123.0176	3128.2887
3136.9603	3144.0685	3145.0837
3147.9748	3149.2953	3153.1498

H	5.03256	-2.39908	-1.64298	3162.3574	3167.6814	3175.3746
H	6.45307	-2.65478	-0.60703	3191.9801	3205.9612	3208.4001
H	4.94048	-3.53053	-0.27967			
C	-0.35657	-2.94705	-0.98037			
H	-1.04137	-2.33475	-1.57651			
H	-0.35324	-3.97175	-1.35756			
H	-0.71599	-2.93671	0.05500			
Cl	-6.32861	-1.50480	0.53243			
H	-1.25297	-2.79232	3.83883			
Ir	1.41694	-0.21556	-0.32137			
H	-1.49980	0.37953	0.32274			
C	-2.97946	-0.72280	-0.83640			
C	-3.99363	0.00621	-0.20013			
C	-3.32706	-1.69968	-1.79362			
C	-5.32310	-0.22802	-0.49568			
H	-3.72011	0.76531	0.53161			
C	-4.67627	-1.92142	-2.07765			
C	-5.66829	-1.19566	-1.43610			
H	-4.95046	-2.67602	-2.81397			
H	-6.71538	-1.37713	-1.66349			
O	-2.35238	-2.39011	-2.40731			
H	-2.74769	-3.02473	-3.01655			
Cl	-6.57374	0.68394	0.30640			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.450296 Electronic Energy = -1941.72063755
Internal Energy (E)= -1941.23542455 Enthalpy (H)= -1941.23448055
Gibbs Free Energy (G)=-1941.33522455 Gibbs Free Energy of Solvation=-1941.36961584

St.Pt.	General Structure	Ball & Stick model
VI'-3		

Cartesian co-ordinate

Atoms	X	Y	Z
C	1.09649	-2.61164	-0.32074
C	2.13706	-1.85628	-0.99414
C	2.89764	-1.17420	0.01898
C	2.27121	-1.44258	1.29547
C	1.17540	-2.34439	1.07036
C	-2.08840	-0.49712	-0.27695
Ir	0.82363	-0.31044	-0.02919
C	-1.83216	0.03968	0.99982

Frequencies

29.8473	31.1268	37.1341
52.4440	59.2953	62.1180
74.4024	85.8627	99.5464
105.7965	109.3202	122.4073
130.1614	135.1096	140.8645
146.1898	157.1445	163.1781
168.1040	172.2304	176.5510
186.6622	194.3443	204.2613
211.3930	216.4347	223.0657
230.1131	234.5622	239.1473
239.8591	244.7162	254.2517
273.9324	282.6351	292.0139
294.2915	304.0594	314.0592

C	-2.92374	0.23406	1.87312
C	-3.38191	-0.83605	-0.69114
C	-4.19864	-0.11301	1.46947
C	-4.42490	-0.65038	0.19268
H	-3.53921	-1.23712	-1.68974
H	-5.04308	0.02534	2.14072
H	-2.73924	0.65623	2.85786
C	0.99390	1.45546	-0.70823
C	2.17837	1.91459	-1.49162
C	0.02001	2.50971	-0.30576
C	-2.21402	3.21559	-0.32125
H	-2.33503	3.04029	0.75675
H	-1.85991	4.24503	-0.45055
C	-3.47582	2.93280	-1.08993
H	-4.27382	3.60527	-0.75939
H	-3.32017	3.08436	-2.16291
H	-3.80925	1.90111	-0.93299
O	-1.19985	2.31302	-0.80120
O	0.32886	3.44036	0.40960
C	4.17302	-0.43537	-0.17705
H	4.29871	0.36049	0.56659
H	5.02229	-1.12308	-0.07379
H	4.22402	0.01618	-1.17077
C	2.43175	-1.95179	-2.45042
H	3.12877	-1.17487	-2.76924
H	2.85289	-2.93621	-2.69480
H	1.51320	-1.81562	-3.03215
C	0.17221	-3.56019	-0.99740
H	-0.04805	-3.23696	-2.01853
H	0.63572	-4.55408	-1.04937
H	-0.77976	-3.66109	-0.46483
C	0.24747	-2.82364	2.13211
H	-0.63355	-3.31309	1.70557
H	0.74344	-3.54041	2.79888
H	-0.10432	-1.98323	2.74329
C	2.72000	-0.99148	2.64141
H	3.25773	-1.79418	3.16420
H	3.38636	-0.12542	2.58213
H	1.85885	-0.71085	3.26025
C	-0.92305	-0.63940	-1.15276
O	-0.61002	0.35836	1.34538
O	-0.93519	-0.98242	-2.30697
N	2.30376	2.29145	2.37534
N	1.61006	2.49016	3.21215
C	2.79990	3.24034	-1.14466
H	2.98237	3.31979	-0.06797
H	3.72953	3.34481	-1.70903
H	2.12056	4.06297	-1.39345
O	2.64213	1.21319	-2.37688
Cl	-6.05900	-1.08536	-0.26997
H	-1.25297	-2.79232	3.83883
Ir	1.41694	-0.21556	-0.32137
H	-1.49980	0.37953	0.32274
C	-2.97946	-0.72280	-0.83640
C	-3.99363	0.00621	-0.20013
C	-3.32706	-1.69968	-1.79362
C	-5.32310	-0.22802	-0.49568
H	-3.72011	0.76531	0.53161
C	-4.67627	-1.92142	-2.07765
C	-5.66829	-1.19566	-1.43610
H	-4.95046	-2.67602	-2.81397

320.3494	326.3214	338.4687
340.8372	348.0952	361.7764
368.9436	401.1607	406.8228
415.3949	426.5163	432.9095
474.0490	517.3029	532.0842
533.1825	541.2941	551.6743
580.1886	587.3629	600.9604
608.9707	630.2883	644.6437
654.4050	659.4844	675.4052
742.2669	751.0731	799.3291
806.9013	811.2055	819.4351
833.9595	863.1447	888.8806
906.7480	920.6621	938.3602
954.9011	961.9661	968.6685
1015.7034	1022.1907	1031.2091
1034.7529	1037.5071	1040.1944
1051.9225	1069.4584	1090.8606
1092.1489	1094.0325	1107.8104
1109.5712	1129.0442	1139.9908
1169.3662	1180.3811	1183.9297
1187.3884	1239.7346	1244.4482
1288.5185	1312.0744	1342.5235
1375.2204	1377.6418	1379.5845
1381.2408	1383.7047	1394.0313
1398.7329	1402.6309	1419.5894
1436.4481	1439.4647	1444.6696
1445.7161	1449.2464	1454.8338
1455.2831	1460.5966	1461.0039
1461.6031	1462.9720	1468.2125
1472.2824	1472.7330	1481.0440
1485.2228	1495.1713	1496.5041
1508.2393	1512.4639	1518.1972
1548.9253	1612.8226	1653.2003
1779.3473	1815.5152	1832.5098
2466.5587	3028.4430	3038.3073
3039.9037	3040.7967	3043.8094
3045.5786	3055.7971	3061.1624
3101.9346	3103.5758	3114.4738
3118.2909	3118.6255	3130.2653
3142.6778	3145.7501	3146.7143
3148.1471	3156.0207	3156.8950
3175.9615	3178.0405	3183.9840
3192.8930	3203.8140	3206.4534

H	-6.71538	-1.37713	-1.66349
O	-2.35238	-2.39011	-2.40731
H	-2.74769	-3.02473	-3.01655
Cl	-6.57374	0.68394	0.30640

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.449576 Electronic Energy = -1941.72761241
Internal Energy (E)= -1941.24281441 Enthalpy (H)= -1941.24187041
Gibbs Free Energy (G)=-1941.34321441 Gibbs Free Energy of Solvation=-1941.37899713

St.Pt.	General Structure	Ball & Stick model
TS_3-6		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.33102	-2.50705	0.40490
C	-2.17578	-1.60550	1.18569
C	-3.02100	-0.90247	0.27804
C	-2.66724	-1.33632	-1.07004
C	-1.67161	-2.37244	-0.96453
C	1.98491	-0.44344	0.36222
Ir	-0.94193	-0.36358	-0.17332
C	1.79388	-0.38764	-1.04174
C	2.92001	-0.61673	-1.86472
C	3.23219	-0.75021	0.92405
C	4.14643	-0.91637	-1.30667
C	4.30023	-0.98870	0.08698
H	3.33813	-0.78270	2.00564
H	5.00822	-1.10465	-1.94290
H	2.79036	-0.55848	-2.94244
C	-0.36731	1.37514	0.49985
C	-1.00037	2.00775	1.69121
C	0.41879	2.30436	-0.37701
C	2.52958	3.12379	-1.00524
H	2.35365	2.74487	-2.02115
H	2.19255	4.16731	-0.98282
C	3.96267	2.96606	-0.57355
H	4.62170	3.54242	-1.23060
H	4.10226	3.32336	0.45195
H	4.26766	1.91396	-0.61428
O	1.72562	2.35358	-0.09715
O	-0.11295	3.00468	-1.20995
C	-4.09196	0.05651	0.66068
H	-4.45897	0.61769	-0.20419
H	-4.94579	-0.47585	1.09948
H	-3.71375	0.76985	1.40328

Frequencies

-260.7073	28.3380	32.6726
46.5217	55.4294	69.3184
78.0343	83.8080	88.3508
101.7496	110.3964	112.0196
116.1701	125.8345	133.4652
133.9158	148.6023	153.0383
160.3362	164.4004	176.3515
182.4264	189.0728	191.2959
194.2931	197.8808	208.9604
215.8907	223.4146	234.4709
241.5171	246.0491	268.2308
281.2919	283.1123	292.1522
300.5225	302.4750	312.5496
318.4858	327.5016	338.5382
349.3337	362.9566	383.9785
397.7656	401.2323	404.6527
410.3455	424.3079	445.9810
460.7486	473.3544	520.5657
536.9928	541.7716	554.4981
557.9445	575.4957	592.3672
600.9895	609.1383	620.5141
642.4824	661.5034	681.3979
725.3291	743.6127	811.4680
812.0581	818.9497	821.1968
835.8602	843.0855	891.2568
903.6162	908.0537	930.8824
957.4346	959.3185	972.0344
1019.2502	1027.6877	1032.8630
1042.8750	1044.2064	1046.6573
1048.7629	1054.5314	1089.4627
1090.2265	1097.7649	1108.0410
1115.5434	1125.5924	1140.2117
1169.3421	1179.8610	1183.1929
1190.8409	1235.9000	1244.7564
1279.5708	1308.8567	1339.9161

C	-2.22434	-1.56952	2.67252	1369.6595	1379.8637	1381.3460
H	-3.00820	-0.89648	3.02517	1383.0331	1389.6495	1400.1806
H	-2.42526	-2.57764	3.05834	1401.7642	1403.0153	1421.6880
H	-1.28105	-1.21230	3.09823	1433.5691	1434.2973	1440.2658
C	-0.31756	-3.42540	0.99431	1446.4205	1449.3839	1451.3864
H	0.07120	-3.02680	1.93676	1452.5090	1454.3587	1465.6183
H	-0.76338	-4.40631	1.20587	1467.7081	1471.4090	1471.8775
H	0.53309	-3.58094	0.32221	1473.1433	1476.4581	1481.4779
C	-1.00557	-3.03787	-2.11735	1488.8846	1501.5447	1513.8995
H	-0.05219	-3.48697	-1.82085	1524.5672	1530.0292	1531.4027
H	-1.63780	-3.83008	-2.53732	1555.8635	1598.5980	1655.3475
H	-0.79200	-2.31650	-2.91397	1775.7631	1831.4041	1841.6041
C	-3.30449	-0.88546	-2.33693	2468.5796	3035.0592	3037.0478
H	-4.12527	-1.55704	-2.62352	3038.2660	3040.9707	3043.8541
H	-3.71440	0.12511	-2.24461	3047.2529	3050.7352	3052.8552
H	-2.57970	-0.87019	-3.15763	3096.7485	3111.8661	3118.6605
C	0.86192	-0.10477	1.22884	3119.9213	3121.4734	3141.1940
O	0.62845	-0.11000	-1.56048	3141.3380	3142.8001	3145.0442
O	0.79910	-0.19879	2.42445	3147.4991	3149.9559	3155.9196
N	-3.09338	3.16457	-0.60534	3157.9802	3178.9970	3179.4036
N	-3.36061	2.75670	-1.59682	3193.9790	3206.6739	3208.1320
C	-0.73406	3.46924	1.93744			
H	-1.05246	4.06728	1.07585			
H	-1.27166	3.78909	2.83201			
H	0.34205	3.63905	2.07027			
O	-1.71065	1.35858	2.44237			
Cl	5.87301	-1.37956	0.75318			
H	-1.25297	-2.79232	3.83883			
Ir	1.41694	-0.21556	-0.32137			
H	-1.49980	0.37953	0.32274			
C	-2.97946	-0.72280	-0.83640			
C	-3.99363	0.00621	-0.20013			
C	-3.32706	-1.69968	-1.79362			
C	-5.32310	-0.22802	-0.49568			
H	-3.72011	0.76531	0.53161			
C	-4.67627	-1.92142	-2.07765			
C	-5.66829	-1.19566	-1.43610			
H	-4.95046	-2.67602	-2.81397			
H	-6.71538	-1.37713	-1.66349			
O	-2.35238	-2.39011	-2.40731			
H	-2.74769	-3.02473	-3.01655			
Cl	-6.57374	0.68394	0.30640			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.449051 Electronic Energy = -1941.70809433
Internal Energy (E)= -1941.22435333 Enthalpy (H)= -1941.22340933
Gibbs Free Energy (G)=-1941.32330433 Gibbs Free Energy of Solvation=-1941.36146074

St.Pt.	General Structure	Ball & Stick model
VII-3		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.09575	-2.38239	0.49141
C	-1.91669	-1.55532	1.35339
C	-2.96632	-0.99746	0.55014
C	-2.83404	-1.55101	-0.79370
C	-1.72015	-2.42749	-0.82643
C	2.28225	-0.01560	0.51080
Ir	-0.99844	-0.40769	-0.22925
C	1.99236	-0.53527	-0.77729
C	3.05558	-1.11109	-1.50782
C	3.57322	-0.12685	1.04000
C	4.33304	-1.18871	-0.98528
C	4.58669	-0.69643	0.29681
H	3.75380	0.25521	2.04178
H	5.13932	-1.64227	-1.55736
H	2.82940	-1.50860	-2.49520
C	0.03356	1.20049	0.72619
C	-0.75637	2.04492	1.73303
C	0.09728	1.84659	-0.60765
C	1.40590	2.76898	-2.34869
H	0.98667	1.93042	-2.91555
H	0.86172	3.67950	-2.62538
C	2.89522	2.89794	-2.52229
H	3.13795	3.07745	-3.57432
H	3.29149	3.72828	-1.92970
H	3.39502	1.97615	-2.20229
O	1.17537	2.51417	-0.94183
O	-0.86956	1.65386	-1.36750
C	-4.10084	-0.17187	1.04520
H	-4.63449	0.30327	0.21690
H	-4.82227	-0.79777	1.58731
H	-3.74267	0.61205	1.71922
C	-1.69170	-1.35783	2.81091
H	-2.32848	-0.56282	3.20297
H	-1.90859	-2.28870	3.35111
H	-0.65294	-1.07627	3.02474
C	0.09806	-3.16571	0.90971
H	0.58656	-2.70348	1.77407
H	-0.18465	-4.19064	1.18457
H	0.83657	-3.22096	0.10229
C	-1.14245	-3.14787	-1.99298
H	-0.10908	-2.81742	-2.16743
H	-1.13121	-4.23130	-1.82055
H	-1.71128	-2.95726	-2.90772
C	-3.70646	-1.16218	-1.93508
H	-4.69089	-1.64123	-1.85726
H	-3.86413	-0.07691	-1.94433
H	-3.26414	-1.44145	-2.89562
C	1.27013	0.65498	1.35606
O	0.79880	-0.52629	-1.32998
O	1.40181	0.72928	2.57678
N	-2.98502	3.29649	-0.13152
N	-3.78221	2.69397	-0.60287
C	-0.14741	3.38295	2.04707
H	-0.15347	4.01419	1.14844

Frequencies

25.9056	43.4439	45.7983
63.0768	65.6951	74.5869
84.9657	89.6204	96.8819
103.3794	110.7151	112.7451
117.9764	125.2360	134.5468
144.6628	149.2900	155.2397
164.6068	166.2908	168.0550
171.8753	180.6909	183.1439
196.0809	210.8484	216.3152
222.4827	226.4379	230.3966
243.2602	249.7458	257.4332
272.2763	282.1762	286.7917
303.8004	304.3251	308.6230
327.0072	339.8161	352.6662
356.2239	391.3927	397.1621
408.7387	412.0771	421.8705
425.5235	448.8475	474.0177
498.2800	522.0015	535.8265
540.4752	543.8650	548.2400
555.2071	586.0696	597.0527
608.8726	625.2200	654.4196
663.9080	695.4061	723.7651
748.2651	797.4797	806.2101
812.5265	815.7384	827.7466
840.5750	864.3925	890.3946
906.9280	925.2172	947.5882
954.8290	971.3711	989.9900
1015.2118	1035.7823	1039.1103
1044.4272	1045.8877	1048.4961
1053.2807	1081.4607	1090.9460
1094.4785	1106.7325	1109.6358
1126.3549	1131.0229	1159.4072
1177.1732	1181.1636	1189.2319
1206.1872	1241.3310	1267.8713
1287.1662	1339.6591	1354.1902
1368.8749	1370.7135	1376.2109
1382.5826	1393.2480	1396.8253
1400.4824	1402.2321	1425.4317
1436.4831	1437.8358	1441.7467
1443.5331	1447.0230	1447.6363
1452.6907	1457.4383	1459.8361
1461.7878	1462.8223	1468.7491
1472.3046	1474.9495	1475.0493
1487.6145	1496.4547	1500.0807
1506.9786	1516.8506	1536.5775
1551.5042	1605.1531	1657.5500
1676.8877	1737.9269	1848.4611
2467.0763	3029.4755	3034.5295
3036.0931	3041.5009	3042.8500
3045.4224	3046.2847	3065.0102
3105.9044	3110.1981	3115.7479
3121.3495	3125.2260	3133.6073
3133.7331	3138.1128	3139.7511
3142.7730	3150.3318	3152.1681
3175.1294	3176.1406	3182.9033
3186.9019	3201.7683	3209.7244

H	-0.71853	3.87548	2.83707
H	0.89567	3.25680	2.35515
O	-1.79862	1.68565	2.23374
Cl	6.20708	-0.80990	0.96052
H	-1.25297	-2.79232	3.83883
Ir	1.41694	-0.21556	-0.32137
H	-1.49980	0.37953	0.32274
C	-2.97946	-0.72280	-0.83640
C	-3.99363	0.00621	-0.20013
C	-3.32706	-1.69968	-1.79362
C	-5.32310	-0.22802	-0.49568
H	-3.72011	0.76531	0.53161
C	-4.67627	-1.92142	-2.07765
C	-5.66829	-1.19566	-1.43610
H	-4.95046	-2.67602	-2.81397
H	-6.71538	-1.37713	-1.66349
O	-2.35238	-2.39011	-2.40731
H	-2.74769	-3.02473	-3.01655
Cl	-6.57374	0.68394	0.30640

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.450524 Electronic Energy = -1941.74712506
Internal Energy (E)= -1941.26159006 Enthalpy (H)= -1941.26064606
Gibbs Free Energy (G)=-1941.36131406 Gibbs Free Energy of Solvation=-1941.40094985

St.Pt.	General Structure	Ball & Stick model
VII'-3		

Cartesian co-ordinate

Atoms	X	Y	Z
C	2.66893	-1.33340	-1.88578
C	2.54319	0.08842	-1.85531
C	2.95253	0.57205	-0.53914
C	3.26783	-0.56197	0.26465
C	3.03872	-1.74902	-0.55556
O	-0.91702	1.32734	-1.51315
C	-0.89414	2.65484	-1.29008
O	0.17064	3.22909	-1.28265
C	-2.22300	3.39209	-1.12716
C	-1.61491	-1.83536	-0.63998
H	-1.81182	0.96584	-1.42063
C	2.11327	0.97669	-2.96466
H	1.58799	1.85471	-2.57230
H	2.98996	1.32117	-3.53017
H	1.44069	0.45963	-3.65626
C	3.09500	2.01050	-0.19688

Frequencies

27.2175	37.3969	42.7862
57.8166	60.9563	68.0893
72.6512	78.8888	86.1301
89.3833	94.1185	98.8943
109.4684	115.2622	118.3602
120.6806	127.9444	135.9739
140.5444	145.5359	150.9743
156.4113	159.3738	168.7626
183.3495	185.1132	191.1845
207.6482	211.8038	218.1814
224.2393	233.6679	239.6447
250.5455	262.0943	269.5798
277.1301	281.2784	287.1329
290.9953	298.2429	302.5598
307.0470	316.6434	320.4336
330.6808	331.7725	339.2497
345.7562	357.0039	369.5675
373.6461	392.8437	396.7140
399.7269	415.3575	428.1075
431.8696	442.7390	450.5332

H	3.87240	2.46541	-0.82502
H	2.15537	2.54906	-0.37024
H	3.38919	2.14463	0.84817
C	3.23202	-3.15040	-0.10784
H	2.65519	-3.84233	-0.72969
H	4.29271	-3.42767	-0.17596
H	2.90218	-3.27198	0.92732
C	2.31861	-2.25184	-3.00422
H	1.99294	-1.69447	-3.88713
H	3.17842	-2.86786	-3.29405
H	1.49813	-2.92047	-2.71544
C	3.79244	-0.58324	1.65506
H	4.87592	-0.76009	1.65001
H	3.59382	0.35463	2.18207
H	3.31353	-1.37615	2.23852
Ir	1.18965	-0.71671	-0.34307
C	-2.31503	4.37502	-2.29938
H	-2.38099	3.84974	-3.26088
H	-3.21420	4.99380	-2.19095
H	-1.43891	5.03075	-2.32337
C	-3.44046	2.47226	-1.12421
H	-3.42408	1.78864	-0.26610
H	-4.35082	3.07669	-1.03809
H	-3.53560	1.90029	-2.05876
C	-2.15389	4.16275	0.19200
H	-2.00539	3.47542	1.03388
H	-1.32648	4.87992	0.16915
H	-3.09024	4.71316	0.34644
O	-0.36537	-1.80214	-1.04740
C	-2.18709	-0.94744	0.30396
C	-3.56585	-1.00435	0.56954
C	-2.46532	-2.78433	-1.25204
C	-4.36412	-1.94052	-0.05146
C	-3.81267	-2.84392	-0.96448
C	-1.40831	0.05502	1.07945
O	-1.96914	1.05939	1.50384
H	-2.01763	-3.46170	-1.97488
H	-4.45066	-3.58175	-1.44468
H	-3.98102	-0.30384	1.29131
C	0.01766	-0.28790	1.41333
C	0.03797	-1.58000	2.27197
C	0.71442	0.74966	2.23188
C	1.30639	2.98239	2.54784
H	2.37751	2.74389	2.61814
H	0.90723	2.91661	3.56694
C	1.06910	4.33289	1.93008
H	1.64055	5.09591	2.46887
H	1.36924	4.34452	0.87666
H	0.00984	4.60070	1.98028
O	0.66341	1.99391	1.73027
O	1.32138	0.48706	3.25585
O	0.82552	-2.48296	2.07611
C	-0.96686	-1.64851	3.38984
H	-0.70978	-2.46922	4.06264
H	-1.00466	-0.70212	3.93875
H	-1.96643	-1.82964	2.97364
Cl	-6.07711	-2.01513	0.30862

459.4069	486.9312	498.1654
527.7674	532.9917	533.5476
542.6233	545.9201	547.9595
554.7174	576.6525	585.6682
591.1064	607.1621	631.8033
645.5314	678.6514	706.1885
724.8977	771.0603	772.1933
783.7621	798.4654	807.5557
813.1168	815.5065	839.9428
872.4758	881.1000	885.9466
900.7521	932.1997	941.8281
949.3728	956.1623	963.9755
966.5803	968.8440	971.5234
999.0369	1010.2226	1032.2371
1037.2651	1038.8882	1045.6723
1048.4147	1048.4885	1049.6342
1063.9415	1094.4509	1098.5047
1102.3413	1107.2500	1110.3090
1121.8519	1138.4251	1151.3566
1166.9332	1184.5109	1187.2143
1192.5580	1194.5097	1228.5679
1242.7548	1251.8172	1260.2944
1268.6988	1277.0285	1296.8686
1330.9986	1369.7213	1375.6544
1378.3835	1380.5726	1381.3987
1384.5350	1385.1817	1386.2942
1397.6052	1404.6527	1410.8804
1414.7430	1418.6014	1430.8798
1432.4445	1435.7755	1441.5919
1448.5386	1450.6377	1452.6375
1456.3545	1457.5564	1459.7179
1462.3589	1465.6195	1470.1651
1471.5672	1476.0499	1476.9365
1477.1429	1479.4191	1479.8826
1490.1453	1491.7579	1494.7685
1497.2865	1501.8600	1505.0539
1511.9389	1525.5776	1552.0782
1602.4289	1658.5201	1754.6441
1792.7588	1823.1495	1862.7278
3021.5907	3032.0968	3036.4813
3037.4768	3038.8954	3039.0733
3040.7300	3042.2917	3045.5561
3047.4483	3056.4572	3094.8989
3108.1572	3116.3150	3117.0717
3126.0872	3128.4133	3130.1274
3131.2543	3134.0484	3135.2377
3136.2218	3144.2977	3145.2852
3146.4764	3149.9268	3161.4884
3162.8288	3164.9563	3168.6167
3173.9110	3174.5409	3195.5338
3198.9928	3210.4507	3791.0028

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.592873 Electronic Energy = -2179.11747833
Internal Energy (E)= -2178.48370633 Enthalpy (H)= -2178.48276333
Gibbs Free Energy (G)=-2178.59485233 Gibbs Free Energy of Solvation=-2178.65307825

St.Pt.	General Structure	Ball & Stick model
TS_3-7		

Cartesian co-ordinate

Atoms	X	Y	Z
C	1.88011	-2.05795	-1.86354
C	2.82362	-1.17718	-1.27971
C	2.81786	-1.38473	0.16580
C	1.91102	-2.47215	0.45302
C	1.26506	-2.82872	-0.78711
O	0.53681	1.34185	-1.03480
C	1.08340	2.55889	-1.04709
O	2.25332	2.71641	-0.77382
C	0.14253	3.71771	-1.37040
C	-2.19100	-0.33375	-1.12516
H	-0.35905	0.89202	-1.49642
C	3.63490	-0.13256	-1.95819
H	3.48880	0.84287	-1.47710
H	4.70154	-0.38659	-1.90435
H	3.36311	-0.03134	-3.01307
C	3.74016	-0.71342	1.12058
H	4.74067	-1.16466	1.07840
H	3.83742	0.35104	0.87297
H	3.37136	-0.79371	2.14860
C	0.23788	-3.88198	-0.99635
H	-0.44875	-3.59394	-1.80107
H	0.71372	-4.82964	-1.28229
H	-0.35837	-4.03400	-0.09542
C	1.47985	-2.15056	-3.29348
H	1.93108	-1.35182	-3.88939
H	1.78612	-3.11187	-3.72528
H	0.39159	-2.06617	-3.39590
C	1.74914	-3.13365	1.77425
H	2.61645	-3.78049	1.96106
H	1.69171	-2.39513	2.58212
H	0.84462	-3.74515	1.80934
Ir	0.83789	-0.77662	-0.36792
C	0.81381	4.58960	-2.43140
H	0.89544	4.06263	-3.39081
H	0.21977	5.49697	-2.59597
H	1.81936	4.88270	-2.11416
C	-1.23570	3.27025	-1.84634
H	-1.78382	2.74132	-1.05636
H	-1.82823	4.15335	-2.11364

Frequencies

-886.8923	-82.8894	-19.2444
13.3790	25.9366	31.4025
52.3488	59.8864	73.3765
75.5702	88.0795	92.8310
102.3175	109.3346	113.4088
120.5302	122.8476	127.3460
136.3723	138.9427	144.8546
147.0558	151.8958	161.6222
171.1023	177.9199	183.3442
185.7386	190.5720	201.6103
212.5701	217.1999	227.4983
231.5922	235.5984	251.8782
257.4789	263.3457	264.2401
272.3018	278.5507	289.4273
294.3691	305.9901	308.7886
324.1922	331.1057	334.4978
348.1335	358.6134	370.6962
372.6138	383.6406	389.8624
395.1513	403.9970	407.8343
417.3079	429.5204	436.1274
446.9553	457.5969	496.8328
526.8883	535.2485	536.1864
546.2751	554.9388	561.2907
578.5437	585.5925	588.4843
601.8948	605.7325	624.7839
650.8300	672.2943	702.6717
722.8605	769.3431	775.0148
799.5072	803.6558	805.9680
812.4078	829.2373	835.0065
866.5837	878.3506	891.9038
894.2986	928.0918	939.8088
945.7337	946.9787	952.9056
955.7620	956.0741	971.2982
997.7402	1014.6526	1031.1470
1032.6888	1035.4462	1036.7604
1039.0893	1044.2219	1046.7495
1051.3347	1089.1431	1089.7674
1096.0819	1100.0711	1108.6517
1115.8560	1135.7687	1148.8266
1173.2865	1175.5113	1184.3113
1185.4041	1194.8280	1219.7368
1233.8976	1238.7351	1255.9645
1263.1001	1293.2393	1312.1351

H	-1.18385	2.63113	-2.73830	1319.3741	1344.5372	1352.4489
C	-0.00949	4.50655	-0.06335	1373.3825	1373.9827	1374.7861
H	-0.43251	3.87516	0.72964	1374.9083	1382.6494	1383.8883
H	0.96140	4.88794	0.27181	1387.7740	1398.7928	1400.0814
H	-0.68360	5.35668	-0.22760	1411.8546	1422.7698	1433.2210
O	-0.94145	-0.29951	-1.62062	1437.3750	1439.9042	1442.0371
C	-2.50182	0.27229	0.10402	1442.8641	1443.0292	1445.2161
C	-3.83113	0.36824	0.51977	1446.0458	1450.8220	1455.5570
C	-3.21887	-0.89676	-1.88665	1456.3413	1457.3696	1460.1698
C	-4.83292	-0.19699	-0.25157	1463.7972	1464.9357	1467.5691
C	-4.53386	-0.84083	-1.44991	1471.5566	1477.8614	1479.2991
C	-1.45252	0.79255	1.02732	1483.0145	1484.2151	1490.6953
O	-1.60135	1.87111	1.57707	1499.8511	1505.3917	1507.0670
H	-2.96181	-1.36095	-2.83606	1515.8885	1521.4394	1554.8504
H	-5.33426	-1.28236	-2.03785	1621.8621	1656.7018	1774.1206
H	-4.06132	0.87127	1.45654	1783.7779	1828.9148	1829.9453
C	-0.33880	-0.18230	1.36661	2026.2936	3019.8416	3023.8639
C	-1.07395	-1.38455	1.99502	3029.1863	3032.7601	3036.7900
C	0.68631	0.34943	2.31513	3036.9621	3039.0813	3039.7542
C	2.09456	2.11867	2.92998	3051.3533	3052.9250	3054.1374
H	2.99508	1.49183	2.89485	3099.8996	3100.9339	3108.8225
H	1.70169	2.05770	3.95225	3108.8482	3110.3247	3114.7526
C	2.37925	3.53309	2.50614	3116.8998	3118.5617	3120.3237
H	3.14083	3.97399	3.15771	3126.8729	3133.5072	3139.4132
H	2.73883	3.55568	1.47227	3142.1065	3142.5027	3143.5767
H	1.47302	4.14464	2.57042	3146.9346	3147.9346	3161.1596
O	1.11537	1.58204	2.02813	3162.0278	3168.7270	3194.2019
O	1.15163	-0.30104	3.23976	3206.4050	3208.6152	3211.7406
O	-1.22417	-2.44186	1.41798			
C	-1.67977	-1.16181	3.35678			
H	-2.51066	-1.85634	3.50186			
H	-0.91017	-1.35667	4.11110			
H	-2.00962	-0.12599	3.49814			
Cl	-6.49615	-0.10816	0.28690			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.585908 Electronic Energy = -2179.10664954
Internal Energy (E)= -2178.48131654 Enthalpy (H)= -2178.48037254
Gibbs Free Energy (G)=-2178.59031954 Gibbs Free Energy of Solvation=-2178.63887952

St.Pt.	General Structure	Ball & Stick model
VIII-3		

Cartesian co-ordinate

Atoms	X	Y	Z
C	1.90196	-2.19687	-1.63843

Frequencies

30.7069	55.8270	60.2408
69.4488	75.3417	79.6877
84.7054	89.4116	96.7855
108.9986	114.0726	120.5139
128.3737	129.7622	133.3001

C	2.84001	-1.30673	-1.06142	141.7183	146.4183	155.0680
C	2.71203	-1.40579	0.39159	164.0954	167.7612	175.0270
C	1.77121	-2.48022	0.68481	184.4877	192.5049	196.9907
C	1.21774	-2.90507	-0.55979	198.6622	199.1576	208.8824
O	0.56231	1.15338	-1.10622	216.9780	227.4754	229.3009
C	1.38978	2.16156	-1.02027	240.1617	245.0966	257.9179
O	2.51277	2.10595	-0.53801	266.3292	272.2958	274.1394
C	0.82739	3.48238	-1.56205	282.9867	293.5362	295.5757
C	-2.39412	-0.36510	-1.22951	306.0499	309.7594	314.7201
H	-0.72202	0.31200	-1.91195	323.6815	330.9533	337.6656
C	3.75594	-0.39736	-1.79892	354.5469	357.6257	367.5132
H	4.02299	0.47256	-1.19546	370.8992	378.5170	380.8137
H	4.66639	-0.93719	-2.09075	393.6802	397.4893	403.4966
H	3.28000	-0.01481	-2.70879	404.8440	408.1348	423.6928
C	3.55293	-0.68303	1.38034	426.0819	429.1483	459.2705
H	4.53331	-1.16639	1.48624	467.3722	475.8462	507.2949
H	3.70295	0.35411	1.05685	533.6992	536.8106	544.1897
H	3.06444	-0.67436	2.36177	549.9730	565.4267	581.8213
C	0.16745	-3.93407	-0.78158	585.9456	591.9035	592.4075
H	-0.60923	-3.54915	-1.45309	602.7652	632.3418	643.1050
H	0.60292	-4.83097	-1.24180	658.6113	692.2589	708.3125
H	-0.32472	-4.21269	0.15182	762.8005	790.2546	796.9586
C	1.62536	-2.40101	-3.08575	807.7908	808.9476	810.6880
H	1.99155	-1.56455	-3.68888	814.0795	827.1475	839.3299
H	2.11404	-3.31493	-3.44878	857.2923	876.7234	883.6652
H	0.55083	-2.50575	-3.27025	895.0774	927.1567	928.2938
C	1.49821	-3.05315	2.02904	951.3239	953.3345	955.5677
H	2.33540	-3.69830	2.32656	960.8399	961.7925	978.7641
H	1.38391	-2.26947	2.78579	993.4410	1014.4353	1019.9786
H	0.58551	-3.65527	2.02723	1037.8293	1038.8820	1039.7583
Ir	0.82009	-0.78341	-0.31403	1048.9749	1055.5476	1058.3325
C	1.83108	4.05341	-2.56257	1058.7996	1090.2221	1095.4476
H	1.91753	3.41348	-3.45123	1098.7510	1101.0397	1112.1554
H	1.50743	5.04784	-2.89638	1113.6658	1138.5918	1154.0698
H	2.82267	4.14169	-2.10713	1174.4466	1187.0041	1190.3835
C	-0.53887	3.32165	-2.21949	1201.4141	1225.9872	1237.1908
H	-1.28302	2.95428	-1.50215	1245.1402	1250.3206	1262.2666
H	-0.88445	4.29452	-2.59283	1269.6975	1283.6470	1322.2326
H	-0.50139	2.63401	-3.07496	1341.9574	1363.2135	1364.1281
C	0.69845	4.42295	-0.35988	1378.2510	1379.1651	1380.4692
H	0.06026	3.97865	0.41641	1384.3010	1384.9254	1389.7338
H	1.68314	4.62739	0.07395	1396.4232	1404.2936	1404.7609
H	0.25342	5.37510	-0.67775	1416.5341	1426.7314	1434.3706
O	-1.13086	-0.57132	-1.74485	1441.7397	1442.0869	1444.6766
C	-2.58542	0.43785	-0.10336	1446.5506	1451.6635	1453.8278
C	-3.88956	0.71515	0.30876	1455.8724	1456.3589	1458.9078
C	-3.47081	-0.94235	-1.88753	1463.9768	1464.9922	1466.1835
C	-4.96247	0.13884	-0.35532	1469.5763	1470.7134	1477.0942
C	-4.76519	-0.70486	-1.44275	1483.8167	1490.5958	1493.3271
C	-1.47694	0.97808	0.76229	1496.2011	1499.8123	1503.6006
O	-1.51912	2.14370	1.10640	1508.7482	1510.9431	1522.1376
H	-3.27991	-1.55989	-2.76123	1529.1205	1531.2413	1558.3177
H	-5.61842	-1.15240	-1.94455	1633.7955	1667.7616	1767.7065
H	-4.04825	1.37001	1.16248	1776.5334	1791.6572	1827.8203
C	-0.49912	-0.05310	1.28450	3022.9895	3027.3984	3033.3073
C	-1.35617	-1.20839	1.83108	3037.8181	3038.3492	3038.9985
C	0.43488	0.44162	2.34236	3040.2194	3040.4520	3044.6239
C	1.88273	2.12158	3.09625	3048.8222	3053.0475	3095.1700
H	2.67037	1.36815	3.21878	3103.5871	3106.8197	3113.1422
H	1.37667	2.21433	4.06580	3117.8999	3118.4440	3119.4163
C	2.43697	3.42965	2.60259	3128.0567	3128.5422	3129.9147

H	3.20700	3.79343	3.29115	3139.3244	3140.7100	3141.2661
H	2.87663	3.29704	1.60747	3145.1678	3149.7111	3157.6252
H	1.65050	4.18843	2.53336	3159.5442	3162.7977	3166.3777
O	0.93432	1.65561	2.12550	3176.3594	3186.6245	3201.3099
O	0.76317	-0.23519	3.30769	3207.1976	3216.4650	3453.8951
O	-1.51516	-2.25083	1.22740			
C	-2.08060	-0.96173	3.13047			
H	-2.99327	-1.56271	3.15390			
H	-1.42726	-1.26536	3.95498			
H	-2.31345	0.09903	3.28176			
Cl	-6.58881	0.47501	0.18622			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.594975 Electronic Energy = -2179.11961790
Internal Energy (E)= -2178.4852439 Enthalpy (H)= -2178.4842999
Gibbs Free Energy (G)=-2178.5910479 Gibbs Free Energy of Solvation=-2178.60495575

St.Pt.	General Structure	Ball & Stick model
VIII'-3		

Cartesian co-ordinate

Atoms	X	Y	Z
H	0.79429	1.32672	0.56003
C	-2.12557	-2.22131	-1.87626
C	-1.62743	-2.85409	-0.69793
C	-2.50853	-2.51794	0.41464
C	-3.56773	-1.68746	-0.09520
C	-3.30747	-1.44938	-1.50647
C	-2.81504	1.86556	0.59724
O	-1.87257	0.99622	0.81384
O	-3.76063	1.72222	-0.17243
C	-2.61054	3.18760	1.35425
O	0.12747	-0.81963	1.18825
C	0.60788	0.03846	1.92887
O	0.95112	1.23959	1.53182
C	0.85999	-0.24571	3.39800
C	-4.71867	-1.14767	0.67217
H	-5.58929	-1.80612	0.55414
H	-4.48538	-1.08067	1.73991
H	-4.97182	-0.14307	0.32251
C	-4.15621	-0.62804	-2.40788
H	-5.06385	-1.17632	-2.69253
H	-4.43531	0.30224	-1.90141
H	-3.61568	-0.36252	-3.32101
C	-2.36380	-3.02669	1.80383
H	-1.31880	-2.97210	2.12906

Frequencies

6.7977	30.9764	34.3262
42.3937	48.1557	53.1796
57.7765	63.2363	70.5002
76.1286	80.2591	87.9160
92.2436	98.0214	102.8716
109.0209	111.5860	121.0785
124.9946	131.8856	136.3048
142.7389	148.0441	153.7563
162.4303	167.9033	173.7349
180.1801	181.2480	187.7825
191.3380	196.1583	200.3868
206.5399	208.0367	213.8988
222.4451	225.5948	227.5218
234.7290	235.9882	246.2688
258.7195	263.2389	268.9030
271.7148	276.4133	288.2496
292.8997	297.1623	300.9030
303.2221	316.4387	318.6146
321.9882	323.2108	328.7435
339.7234	343.1074	348.0539
352.2939	352.6036	358.1472
373.3719	374.2236	382.0130
389.2705	390.5371	398.9397
399.8876	405.5867	414.0450
426.8894	432.3020	441.1059
453.3803	465.4517	480.7965
503.5517	535.0153	538.1386
540.3698	541.8726	547.4232

H	-2.96240	-2.43669	2.50563	570.7152	581.7980	583.3397
H	-2.68951	-4.07247	1.87564	595.1479	597.9340	602.4199
C	-0.39542	-3.67926	-0.59301	616.9273	622.6357	631.3040
H	-0.03041	-3.70415	0.43865	647.5572	656.8953	694.5745
H	-0.59620	-4.71105	-0.90850	722.4109	770.3952	777.8885
H	0.40334	-3.26037	-1.21165	787.2048	788.1194	792.9433
C	-1.51731	-2.27343	-3.23059	800.1116	806.7852	811.0254
H	-0.43886	-2.43590	-3.16736	817.0488	819.9679	834.4936
H	-1.96901	-3.07966	-3.82247	861.5192	896.3244	902.3846
H	-1.67207	-1.32969	-3.76276	906.8531	910.5192	916.2404
C	-0.51664	-0.43356	4.04508	946.7639	947.9805	952.8861
H	-0.39305	-0.69935	5.10216	958.2713	958.7954	960.4908
H	-1.11057	0.48636	3.98625	965.4740	971.1116	986.7956
H	-1.07715	-1.23055	3.54471	1008.4484	1031.1766	1031.8381
C	1.61221	0.88608	4.08782	1037.3938	1037.7599	1042.9049
H	1.76622	0.62864	5.14296	1045.0544	1047.4865	1047.7286
H	2.59349	1.05200	3.62954	1049.7471	1052.6676	1053.8516
H	1.05483	1.82796	4.04265	1093.2801	1099.0835	1100.2931
C	1.66716	-1.54302	3.49036	1111.3510	1121.4998	1133.0165
H	1.14860	-2.37254	2.99574	1144.4373	1162.7687	1167.2221
H	2.65440	-1.43374	3.02194	1184.9496	1190.3581	1191.3974
H	1.82163	-1.80778	4.54329	1233.5596	1239.4181	1242.3027
C	-3.94573	3.90655	1.50443	1250.3935	1251.5903	1269.4873
H	-4.63554	3.32834	2.13190	1272.5054	1282.1885	1289.3826
H	-3.79788	4.88725	1.97553	1291.7788	1314.5967	1319.1153
H	-4.42429	4.04776	0.53080	1363.1426	1365.6234	1369.2069
C	-1.66689	4.02597	0.48505	1372.6079	1374.1216	1374.6876
H	-1.47749	4.99929	0.95681	1375.3884	1383.1932	1386.5257
H	-0.70009	3.51890	0.35214	1387.9026	1391.2238	1394.8961
H	-2.10669	4.20497	-0.50441	1403.0568	1406.5466	1408.7760
C	-1.97253	2.97146	2.72321	1412.0884	1417.7812	1429.2691
H	-1.85370	3.93551	3.23599	1433.6684	1436.6509	1437.5326
H	-2.59925	2.33025	3.35784	1439.6199	1447.5562	1449.3781
H	-0.98477	2.50725	2.62528	1449.6209	1452.5189	1454.3646
Ir	-1.68722	-0.71041	-0.39017	1456.6317	1457.2190	1459.3249
C	1.18594	1.30903	-1.50849	1459.7932	1465.6176	1467.0963
C	1.61686	-0.07281	-1.42633	1469.4089	1472.5213	1472.8889
O	0.86370	-1.03607	-1.61801	1474.1112	1475.3973	1476.0941
C	3.04490	-0.44576	-1.10779	1479.6499	1482.7484	1483.9807
C	4.16069	-0.00098	-1.82752	1489.0949	1492.4100	1493.9585
C	3.22965	-1.38753	-0.09996	1494.5645	1500.9809	1509.2939
C	5.43417	-0.46494	-1.50834	1515.1838	1519.2987	1529.2031
C	4.50605	-1.82905	0.22362	1537.5912	1578.8894	1651.2760
H	2.35659	-1.76791	0.42867	1662.5924	1705.3970	1760.7277
C	5.61665	-1.37689	-0.47361	1764.9186	1834.5388	3020.8801
H	6.29388	-0.11437	-2.07950	3024.4951	3027.2314	3031.8664
H	6.60889	-1.73999	-0.22060	3033.7920	3040.8558	3041.2614
O	3.94700	0.88274	-2.83424	3041.5607	3042.3046	3042.9704
H	4.78403	1.11741	-3.24858	3045.3897	3046.1647	3046.9512
C	-0.13883	1.59681	-1.96882	3059.3031	3087.6027	3100.5545
C	2.14675	2.42123	-1.38909	3110.3259	3111.8994	3115.5487
C	4.10301	3.09197	-0.24370	3120.3173	3123.6396	3125.8301
H	3.71879	4.11040	-0.10683	3127.6668	3128.4980	3129.4742
H	4.68233	3.09134	-1.17955	3133.1301	3133.2115	3133.8777
C	4.91745	2.61900	0.93258	3134.8496	3136.8827	3142.4744
H	5.78869	3.26338	1.08786	3147.7438	3147.9134	3149.0454
H	4.31083	2.62952	1.84442	3153.6853	3157.2475	3157.8774
H	5.26570	1.59181	0.77045	3163.9410	3168.8672	3171.4674
O	3.01368	2.18424	-0.37476	3172.3737	3175.0483	3207.4404
O	2.17554	3.45614	-2.02232	3215.0757	3475.8370	3900.5362
C	-0.46184	2.87925	-2.68158			

H	-1.53097	2.88340	-2.90914
H	-0.20506	3.74875	-2.06949
H	0.13751	2.97647	-3.59202
O	-1.12343	0.82046	-1.82749
Cl	4.71368	-3.00029	1.51293

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.741483 Electronic Energy = -2525.94478986
Internal Energy (E)= -2525.15342386 Enthalpy (H)= -2525.15247986
Gibbs Free Energy (G)=-2525.28395086 Gibbs Free Energy of Solvation=-2525.35266912

St.Pt.	General Structure	Ball & Stick model
TS_3-8		

Cartesian co-ordinate

Atoms	X	Y	Z
H	0.97705	1.31239	0.14999
C	-1.98488	-2.29108	-1.81584
C	-1.49528	-2.90347	-0.62469
C	-2.43462	-2.60438	0.45173
C	-3.52007	-1.83093	-0.10533
C	-3.22174	-1.58420	-1.49995
C	-3.03991	1.77940	0.39545
O	-2.10461	0.97344	0.79836
O	-3.90873	1.51659	-0.43246
C	-2.92577	3.19574	0.98178
O	0.03301	-0.73299	1.14584
C	0.43818	0.25522	1.81081
O	0.78646	1.37357	1.32225
C	0.55727	0.09020	3.32122
C	-4.70605	-1.33134	0.63635
H	-5.54494	-2.02956	0.52077
H	-4.48624	-1.23468	1.70488
H	-4.99624	-0.34434	0.26641
C	-4.06395	-0.83991	-2.47183
H	-4.73332	-1.52267	-3.01164
H	-4.64791	-0.06985	-1.96409
H	-3.43198	-0.32460	-3.20243
C	-2.31584	-3.10521	1.84598
H	-1.28931	-2.98781	2.21107
H	-2.97654	-2.55650	2.52452
H	-2.57832	-4.16957	1.90156
C	-0.23495	-3.67842	-0.47191
H	0.13086	-3.62439	0.55877

Frequencies

-313.3372	-167.9220	-132.7116
-58.5965	-28.1614	12.8041
32.1508	36.6499	44.5373
46.4505	58.5831	61.6260
67.5709	76.8195	81.0299
89.5879	95.9224	97.5214
105.5163	108.8407	117.3577
121.2490	134.9706	137.5634
141.9531	146.5473	150.6814
152.4956	155.9706	164.5466
167.6985	175.3658	179.2488
190.1402	191.6765	196.6796
198.1789	201.3759	206.1664
217.8558	221.6564	222.5324
225.4073	228.8161	231.3845
234.3903	246.9781	262.4838
266.7880	277.5293	289.8165
293.4134	297.3646	304.6030
306.7391	309.9591	310.8575
326.9960	331.6654	333.4361
336.8064	341.4318	349.0751
352.5975	365.3907	374.5790
379.8391	392.8753	395.2758
399.9379	406.8275	421.9964
428.7355	433.5573	444.4181
453.4808	462.4023	468.0403
473.1434	514.7727	533.3591
537.0108	538.0467	546.4339
559.4054	568.5465	585.4681
587.3336	597.7879	602.7040
609.3284	622.9798	630.0364
648.2286	682.6021	691.3890

H	-0.39701	-4.73569	-0.71796
H	0.55080	-3.27540	-1.11768
C	-1.34727	-2.32844	-3.15719
H	-0.27351	-2.51051	-3.08362
H	-1.80479	-3.11984	-3.76509
H	-1.48411	-1.37815	-3.68233
C	-0.85596	-0.11982	3.87210
H	-0.81763	-0.22791	4.96350
H	-1.50913	0.72563	3.62223
H	-1.30887	-1.02303	3.44867
C	1.20004	1.31278	3.96572
H	1.29599	1.15195	5.04713
H	2.19782	1.50220	3.55249
H	0.60087	2.21549	3.80555
C	1.41834	-1.14660	3.59318
H	0.99093	-2.04247	3.12876
H	2.43453	-1.01024	3.19967
H	1.49592	-1.31765	4.67415
C	-4.28745	3.87915	0.95281
H	-5.00058	3.36384	1.60852
H	-4.19666	4.91688	1.30014
H	-4.70542	3.87830	-0.05789
C	-1.95078	3.93617	0.05887
H	-1.82936	4.97683	0.38778
H	-0.96156	3.45657	0.08006
H	-2.32189	3.94253	-0.97441
C	-2.36478	3.19930	2.39913
H	-2.31645	4.22909	2.77813
H	-2.99973	2.62168	3.08423
H	-1.35374	2.77905	2.41811
Ir	-1.66919	-0.76962	-0.29536
C	1.25181	1.29283	-1.24006
C	1.75447	-0.09706	-1.36347
O	1.04415	-1.03528	-1.70054
C	3.17351	-0.44608	-1.00800
C	4.27244	0.00077	-1.74673
C	3.36598	-1.35335	0.02685
C	5.55279	-0.44326	-1.43257
C	4.65215	-1.77126	0.35029
H	2.50014	-1.71734	0.58139
C	5.74877	-1.32713	-0.37454
H	6.40484	-0.09917	-2.01858
H	6.74727	-1.67255	-0.12118
O	4.02111	0.86214	-2.76613
H	4.84649	1.11915	-3.19064
C	-0.02856	1.53725	-1.91517
C	2.23141	2.41159	-1.16183
C	4.24076	3.05621	-0.10541
H	3.85072	4.03437	0.20227
H	4.70209	3.19284	-1.09484
C	5.20198	2.46646	0.89462
H	6.07540	3.11493	1.01778
H	4.71946	2.34544	1.87030
H	5.54505	1.47828	0.56084
O	3.15632	2.13662	-0.22361
O	2.20891	3.46517	-1.76115
C	-0.23050	2.68653	-2.85025
H	-1.24407	2.63440	-3.25506
H	-0.07402	3.63476	-2.32739
H	0.51996	2.66827	-3.64719
O	-1.00713	0.79077	-1.74203

737.0791	771.5786	792.0596
794.7089	800.6008	803.2670
806.4626	807.8635	809.3770
816.7948	824.4081	849.6835
892.2578	897.9786	907.5070
911.7134	913.4795	923.2692
935.1315	937.5206	943.5543
945.9349	949.2976	957.7206
964.2484	971.7478	973.1266
1006.5272	1028.6158	1030.8104
1032.4640	1033.3104	1035.5834
1036.9163	1037.4119	1037.7521
1042.8113	1044.7107	1054.6513
1093.3364	1093.6328	1095.0299
1108.2791	1114.7432	1131.6630
1146.2049	1164.7873	1175.3699
1181.7756	1185.3458	1189.5033
1234.5766	1236.1691	1247.0435
1248.3954	1256.0049	1261.4185
1263.2512	1268.6390	1279.9757
1283.3150	1308.8460	1319.4221
1360.2203	1367.3056	1368.1298
1368.4640	1369.2472	1375.8034
1377.2187	1380.8770	1382.0048
1383.4604	1384.8131	1392.4004
1394.1876	1398.5188	1401.8381
1407.0591	1415.5850	1423.0079
1424.5098	1430.9038	1431.9688
1434.7414	1435.5066	1437.6597
1442.2839	1445.9019	1446.5230
1446.7481	1448.6184	1451.9929
1453.4079	1457.4707	1460.9976
1463.4617	1464.5733	1465.8750
1467.6875	1471.6157	1473.3288
1474.9511	1475.3178	1480.9176
1482.4138	1487.2273	1488.6184
1489.0411	1500.9517	1501.7839
1510.6506	1528.2745	1530.7245
1539.8925	1546.6495	1654.5031
1665.0732	1674.9939	1726.1504
1758.6941	1780.5771	1847.6278
3016.3132	3017.1783	3023.0676
3026.2687	3029.0859	3032.7753
3037.0549	3037.4715	3041.3252
3042.6560	3043.2827	3045.0374
3050.6597	3058.3617	3084.7120
3100.3591	3101.7115	3110.8897
3112.3794	3112.6017	3113.5274
3123.1044	3123.5698	3124.2351
3124.6915	3125.1148	3131.1358
3132.7644	3134.7078	3143.6192
3143.9583	3144.9330	3145.8383
3147.4022	3148.9702	3152.0283
3153.4006	3161.6315	3166.0197
3174.4345	3177.2347	3193.4584
3196.8982	3214.5920	3899.9676

Cl	4.88706	-2.89570	1.67105

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.732978 Electronic Energy = -2525.93066911
Internal Energy (E)= -2525.15005811 Enthalpy (H)= -2525.14911411
Gibbs Free Energy (G)=-2525.27543411 Gibbs Free Energy of Solvation=-2525.34210567

St.Pt.	General Structure	Ball & Stick model
IX-3		

Cartesian co-ordinate

Atoms	X	Y	Z
H	1.07024	1.24830	-0.12154
C	-1.97693	-1.73329	-2.20542
C	-1.47505	-2.61795	-1.20727
C	-2.41571	-2.60012	-0.09624
C	-3.52186	-1.72362	-0.45508
C	-3.23137	-1.15603	-1.74224
C	-3.06150	1.74701	0.74702
O	-2.15753	0.85092	1.02207
O	-3.94646	1.63895	-0.09647
C	-2.85609	3.05417	1.52475
O	0.07136	-0.76616	0.88352
C	0.38310	0.07383	1.83569
O	0.68235	1.25281	1.65559
C	0.39518	-0.52473	3.24817
C	-4.70410	-1.42925	0.39561
H	-5.53320	-2.10534	0.15111
H	-4.46095	-1.55459	1.45663
H	-5.01877	-0.39198	0.25242
C	-4.07513	-0.23019	-2.54263
H	-4.57292	-0.77352	-3.35738
H	-4.82300	0.26202	-1.91980
H	-3.46178	0.56385	-2.98269
C	-2.30742	-3.45974	1.11125
H	-1.28702	-3.44200	1.50901
H	-2.98603	-3.13391	1.90504
H	-2.55446	-4.49970	0.85953
C	-0.20200	-3.38786	-1.22106
H	0.27504	-3.33906	-0.23442
H	-0.38242	-4.44437	-1.45787

Frequencies

23.1263	33.7342	40.3935
46.1555	49.0061	59.0877
64.4298	67.2785	71.8282
72.8419	80.2864	84.6936
87.1198	96.1440	101.3768
103.8491	110.5123	111.3296
114.9406	121.2896	129.9342
133.7129	139.0297	141.5364
144.8319	156.9111	157.4286
163.2423	170.5240	177.3730
179.7001	186.8733	192.0660
197.4591	206.4579	216.5766
223.6322	236.3060	237.6136
239.8572	255.3898	259.6920
263.7928	265.9986	273.9743
278.4883	287.1204	289.8438
300.2409	306.1723	314.1889
315.5726	319.3446	323.7970
334.6703	336.3445	337.5321
338.9313	340.0410	343.2727
345.9650	350.7643	354.2456
379.9889	381.3171	385.4411
386.7902	389.4868	397.7331
407.5406	415.5080	423.1195
430.2078	438.7683	443.8961
448.5154	456.6917	466.0724
510.7702	518.8832	536.0226
536.3979	545.5572	554.2530
566.8623	574.0991	580.6224
586.2106	600.3463	603.9069
605.8049	631.2313	642.2884
661.4636	671.0798	705.9751
752.0109	788.9321	789.3257

H	0.50803	-2.97601	-1.94495	799.9006	802.5710	808.5598
C	-1.37449	-1.42582	-3.52845	809.7056	813.5956	814.1292
H	-0.38015	-1.86059	-3.64100	816.5257	854.8380	861.1277
H	-2.02673	-1.81453	-4.32146	886.9705	901.5084	909.0119
H	-1.27988	-0.34460	-3.67322	913.7929	922.9795	940.5387
C	-1.05033	-0.85783	3.62915	943.8984	949.7173	955.3622
H	-1.08111	-1.28269	4.64159	958.2459	962.2493	965.2773
H	-1.68244	0.03772	3.60427	967.3070	971.0670	1003.6456
H	-1.48071	-1.58615	2.93252	1009.7429	1032.2149	1033.1678
C	0.96857	0.47851	4.24111	1038.0361	1041.7758	1043.3614
H	0.97687	0.04474	5.24996	1044.3266	1045.0692	1045.5241
H	1.99507	0.75619	3.97516	1050.6961	1051.3888	1070.4816
H	0.37398	1.39815	4.26349	1093.1581	1097.5624	1108.1503
C	1.24059	-1.79764	3.25863	1109.0580	1114.8591	1130.7238
H	0.85028	-2.54689	2.55909	1139.6458	1169.5256	1173.2320
H	2.28170	-1.58557	2.97898	1184.3990	1188.5315	1230.3047
H	1.24980	-2.23696	4.26489	1233.1723	1239.6849	1245.0804
C	-4.16209	3.83600	1.58032	1250.0330	1261.7704	1262.5053
H	-4.92190	3.29604	2.15943	1272.7021	1274.9765	1280.0204
H	-3.99958	4.81077	2.05902	1282.8966	1290.6416	1321.0342
H	-4.56474	3.99644	0.57541	1356.7399	1362.2962	1366.6853
C	-1.80875	3.83667	0.71964	1371.4945	1372.1643	1375.0125
H	-1.61790	4.80809	1.19531	1375.9024	1379.8348	1385.0771
H	-0.86367	3.27895	0.67833	1386.2701	1387.7505	1390.3570
H	-2.16112	4.01776	-0.30430	1393.1746	1395.2001	1399.1988
C	-2.31782	2.80880	2.93146	1412.4368	1417.7108	1424.1133
H	-2.20177	3.76707	3.45593	1426.8429	1427.9580	1429.2373
H	-3.00454	2.18649	3.52134	1437.9255	1440.4626	1443.7228
H	-1.34119	2.31330	2.89164	1450.3142	1451.5341	1452.8358
Ir	-1.68522	-0.64235	-0.32342	1453.4958	1453.7713	1457.1916
C	1.40468	1.40292	-1.17879	1457.6146	1461.9358	1465.3700
C	1.94664	0.04159	-1.57929	1468.8563	1470.6195	1471.8284
O	1.30343	-0.68354	-2.31220	1472.6749	1473.5932	1475.3110
C	3.22617	-0.45205	-0.97937	1480.9546	1481.9817	1482.6343
C	4.45804	0.01701	-1.44041	1485.1963	1489.7468	1493.8056
C	3.17632	-1.45896	-0.02294	1496.6175	1499.6243	1508.1118
C	5.63955	-0.50581	-0.92756	1516.9267	1526.5957	1532.9806
C	4.36516	-1.97494	0.48152	1545.2636	1657.1523	1673.1571
H	2.20692	-1.81089	0.32943	1732.2160	1760.4830	1771.4577
C	5.59474	-1.50532	0.03957	1812.5071	1865.2475	2781.3852
H	6.59945	-0.13886	-1.28986	3017.8197	3023.1538	3024.2082
H	6.51218	-1.92482	0.44284	3030.5247	3031.1490	3035.5652
O	4.42130	0.98181	-2.39648	3036.4665	3038.1863	3038.5582
H	5.31482	1.22763	-2.65882	3038.8867	3039.0121	3042.2063
C	0.15418	1.67374	-1.98183	3045.3405	3051.6385	3097.9051
C	2.42083	2.52007	-1.08838	3098.4781	3106.6998	3107.5012
C	4.31998	3.18761	0.13330	3110.2028	3112.5282	3118.4659
H	3.92480	4.20224	0.26232	3119.0097	3120.2662	3123.4297
H	4.93154	3.18812	-0.78065	3124.6806	3125.0464	3126.2925
C	5.08256	2.70272	1.33777	3126.5020	3128.2596	3137.4303
H	5.94370	3.34955	1.53298	3142.8238	3143.5576	3144.7496
H	4.43966	2.70198	2.22341	3148.0670	3152.5367	3153.2662
H	5.44243	1.67884	1.18039	3159.6626	3167.6855	3169.3456
O	3.22797	2.28134	-0.05392	3173.4967	3181.9685	3205.9581
O	2.49314	3.49736	-1.79561	3208.0389	3212.0735	3897.7099
C	0.24950	2.36838	-3.29491			
H	-0.73729	2.42825	-3.75973			
H	0.70229	3.35721	-3.17318			
H	0.93875	1.79484	-3.93057			
O	-0.92513	1.25581	-1.57657			
Cl	4.31619	-3.25778	1.66855			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.740942 Electronic Energy = -2525.93844601
Internal Energy (E)= -2525.14767801 Enthalpy (H)= -2525.14673401
Gibbs Free Energy (G)=-2525.27712301 Gibbs Free Energy of Solvation=-2525.34786111

St.Pt.	General Structure	Ball & Stick model
X-3		

Cartesian co-ordinate

Atoms	X	Y	Z
C	1.36249	1.25626	0.10723
C	1.17535	-0.10614	-0.09170
C	-0.18017	-0.65807	-0.29467
C	-0.95529	1.66996	-0.03289
O	0.30574	2.12113	0.12575
C	2.28939	-0.94912	-0.10763
C	2.62991	1.80264	0.29174
C	3.54647	-0.41145	0.07874
C	3.72724	0.96169	0.27791
H	2.12833	-2.01182	-0.26972
H	4.72916	1.35705	0.41899
H	2.73272	2.87347	0.44118
O	-0.34936	-1.83987	-0.54463
C	-1.24852	0.34847	-0.20550
C	-1.91307	2.80662	0.01086
H	-2.15962	3.12585	-1.00753
H	-2.85666	2.52251	0.47829
H	-1.45582	3.64411	0.54316
C	-2.67531	-0.03437	-0.37530
C	-4.27740	-1.71582	0.00717
H	-4.17514	-2.80298	0.06771
H	-4.63783	-1.44581	-0.99091
C	-5.18822	-1.17759	1.08322
H	-6.18027	-1.63398	1.00225
H	-4.78802	-1.40208	2.07723
H	-5.30190	-0.09413	0.98375
O	-3.50659	0.66400	-0.91901
O	-2.93880	-1.22184	0.16923

Frequencies

36.1097	41.9415	68.5190
83.0060	102.8029	133.7843
138.0399	151.7872	180.0934
189.0060	235.7565	250.6920
278.5045	310.9833	353.3898
359.2878	362.6424	393.3119
402.3150	439.5135	478.9014
520.4291	544.8407	559.8704
590.5372	593.6383	668.7026
685.4624	701.8716	760.9837
772.8551	813.4604	832.9692
837.8626	878.6661	897.3228
927.1524	943.9291	963.7081
1011.3149	1043.6801	1049.4769
1086.9422	1114.3562	1126.9601
1131.7552	1166.1057	1195.4814
1230.4367	1244.9315	1274.9484
1313.5087	1339.8010	1380.2651
1390.0347	1391.9913	1407.0744
1422.5899	1447.3646	1450.3399
1466.6711	1472.5608	1482.6747
1488.8931	1503.2727	1629.9504
1668.6954	1678.0022	1803.9944
1828.3541	3048.9908	3063.9380
3074.5395	3131.3368	3139.7081
3147.5441	3154.9489	3186.8133
3203.4419	3212.8313	3215.8210

Cl	4.94823	-1.45165	0.06528	

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.217125 Electronic Energy = -1262.60023117
Internal Energy (E)= -1262.36680717 Enthalpy (H)= -1262.36586317
Gibbs Free Energy (G)=-1262.42801817 Gibbs Free Energy of Solvation=-1262.44838145

Energetic Span Model

The Energetic Span Model plays a crucial role. It provides us the simple way to calculate the catalytic efficiency in terms of TOF (Turn Over Frequency). Instead of Rate-determining-step (RDS), the energetic span model offers us TOF Determining Intermediate (TDI) and TOF Determining Transition State (TDTS) to calculate the energetic span (∂E) of the catalytic cycle. According to the Energetic Span Model,

$\partial E = T_{TDTS} - I_{TDI}$ **(if TDTS appears after TDI)**

$= T_{TDTS} - I_{TDI} + \Delta G_r$ **(if TDTS appears before TDI)**

Where, ΔG_r is reaction energy and ∂E is Energetic Span of the catalytic cycle.

The TOF is formulated as

$$TOF = K_B T/h \frac{e^{\frac{-\Delta Gr}{RT}} - 1}{\sum_{i,j=1}^{N} e^{\frac{Ti - Ij - \partial Gi,j'}{RT}}} = \Delta/M$$

Where, $\partial G_{i,j}' = \Delta G_r$ if i > j

0 if i ≤ j

Here the TOF is represented as the forward chemical current of the reaction and it is determined by potential divided by resistance. Δ is the potential of the process, which is a function of the energy of the reaction (ΔG_r). **The term "-1" represents thermodynamic consistency for the case where $\Delta G_r = 0$. For this case TOF is 0. While in case of an endothermic reaction, the current flows in the backward direction and the TOF is negative. M represents the resistance to the chemical flow, corresponding to the sum of the exponentials of Gibbs energy differences between all the combinations of intermediates (I_j) and transition states (T_i).**

For the kinetic analysis, we have also performed Energetic Span Model, for substrate-1. According to this model, we see that, the TDTS and TDI are TS-2A and VII-1A respectively, for Path-A.

For catalytic path-A,

$\partial E = T_{TDTS} - I_{TDI} + \Delta G_r$ (As TDTS appears before TDI)

$=22.46 – (-31.06) – 57.87$ $[\Delta G_r = -57.87]$

$= -4.35$ kcal/mol

For catalytic path-A', the TDTS and TDI are TS-3A' and VII-1A respectively. Therefore,

$\partial E = T_{TDTS} - I_{TDI} + \Delta G_r$ (As TDTS appears before TDI)

$=41.68 – (-31.06) – 57.87$ $[\Delta G_r = -57.87]$

$=14.87$ kcal/mol

For catalytic path-B, the TDTS and TDI are TS-2B and VI'-1B respectively. Therefore,

$\partial E = T_{TDTS} - I_{TDI} + \Delta G_r$ (As TDTS appears before TDI)

$=38.39 – (-27.52) – 57.87$ $[\Delta G_r = -57.87]$

$=8.04$ kcal/mol

As catalytic path-A is the lowest energy requiring path and an exothermal one so, for this reaction TOF is calculated based on this path

$TOF = (K_BT/h)\, e^{-\partial E/RT}$

For this path, $\partial E = -4.35$ kcal/mol

$R = 1.987\times10^{-3}$ kcal/^{0}/mol

$T = 298.15K$

$K_BT/h = 6.21\times 10^{12}\ s^{-1}$

$RT = 0.59242405KIL9$ kcal/mol

Therefore, $TOF = 6.21\times 10^{12}\ s^{-1} \times e^{-(-4.35/\mathbf{0.59242405})}$

$=9.59 \times 10^{15}\ S^{-1}$

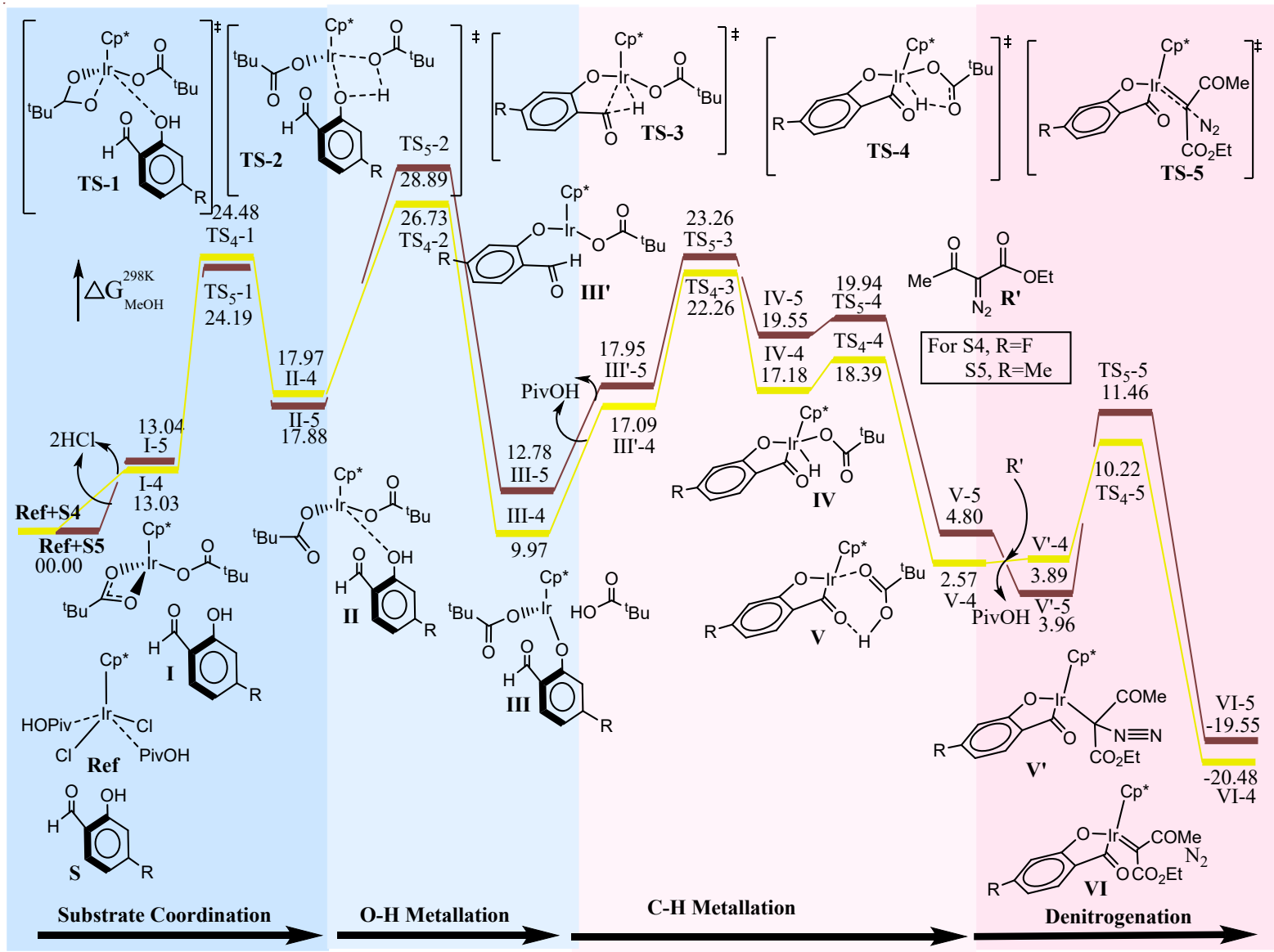


Fig-25: PES with Gibbs free energy (kcal/mol) and the structures of the stationary points of first part of path using M06 functional & 6-31G(d,p) basis set (Yellow colour for S4 and Brown colour for S5)

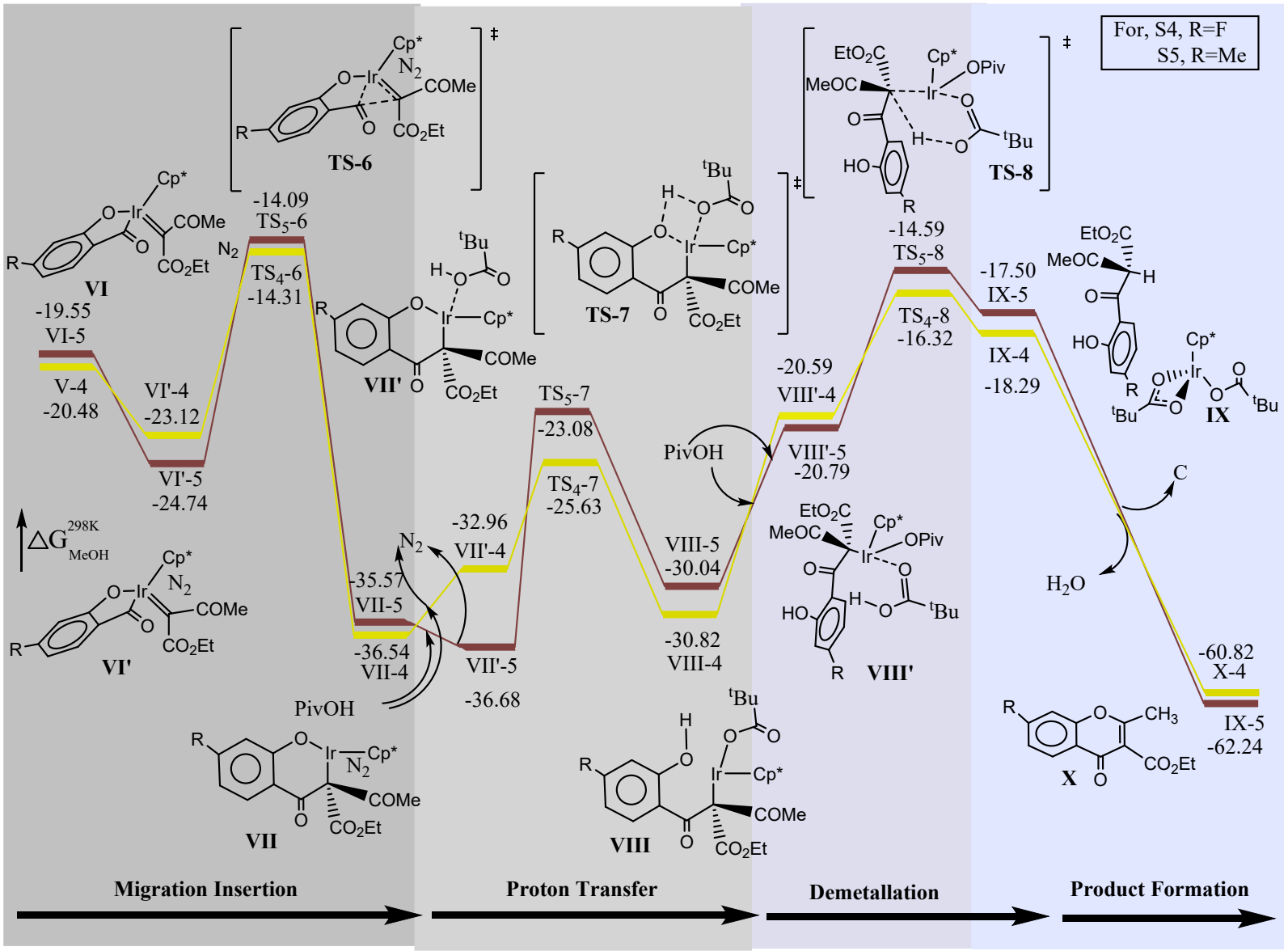


Fig-26: PES with Gibbs free energy (kcal/mol) and the structures of the stationary points of first part of path using M06 functional & 6-31G(d,p) basis set (Yellow colour for S4 and Brown colour for S5) (As the details of coordinates associated to these paths have already been given so we only provide here the PES .)

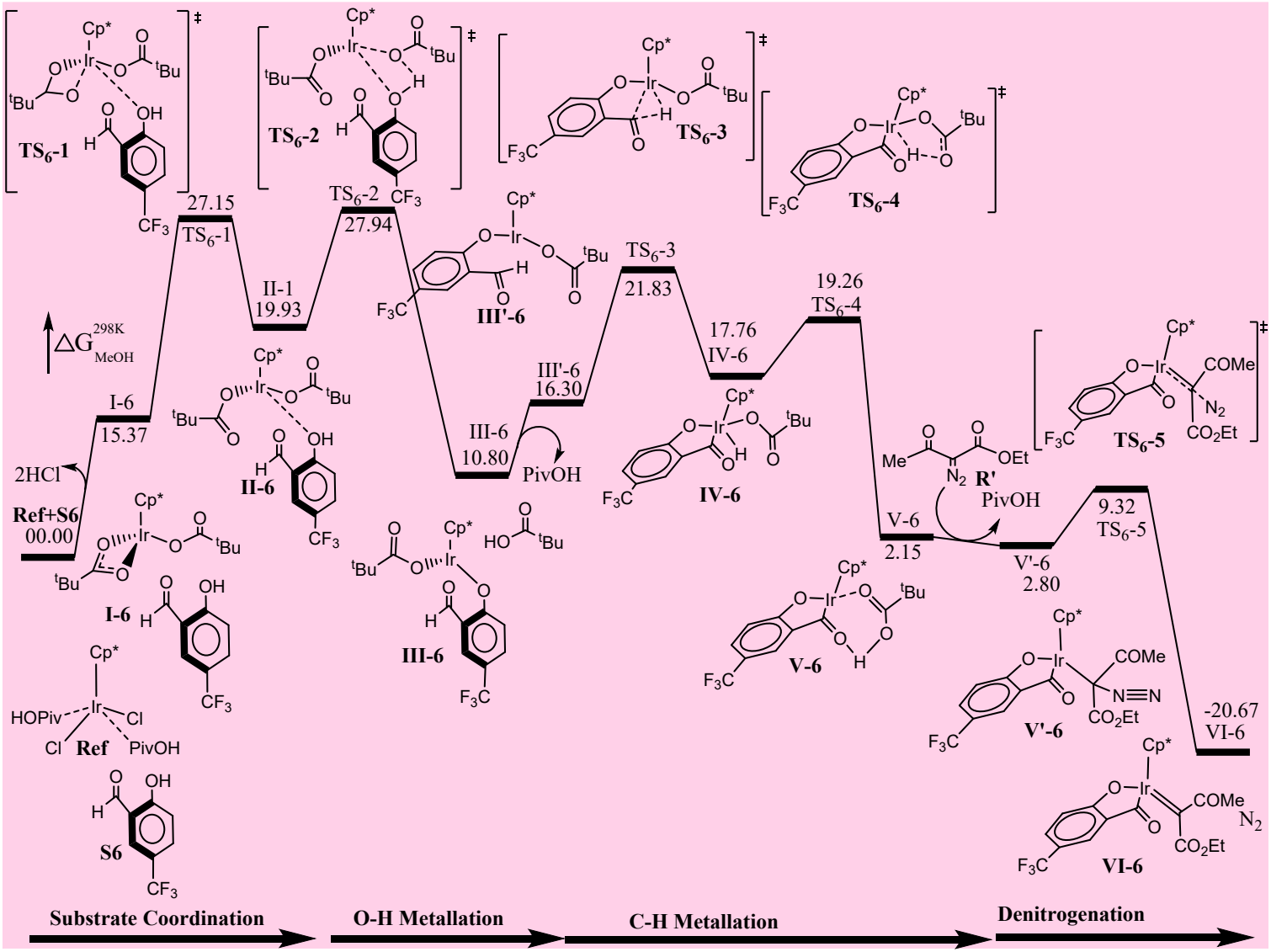


Fig-27: PES with Gibbs free energy (kcal/mol) and the structures of the stationary points of first part of path using M06 functional & 6-31G(d,p) basis set for non-metals and LANL2DZ for metals for S6

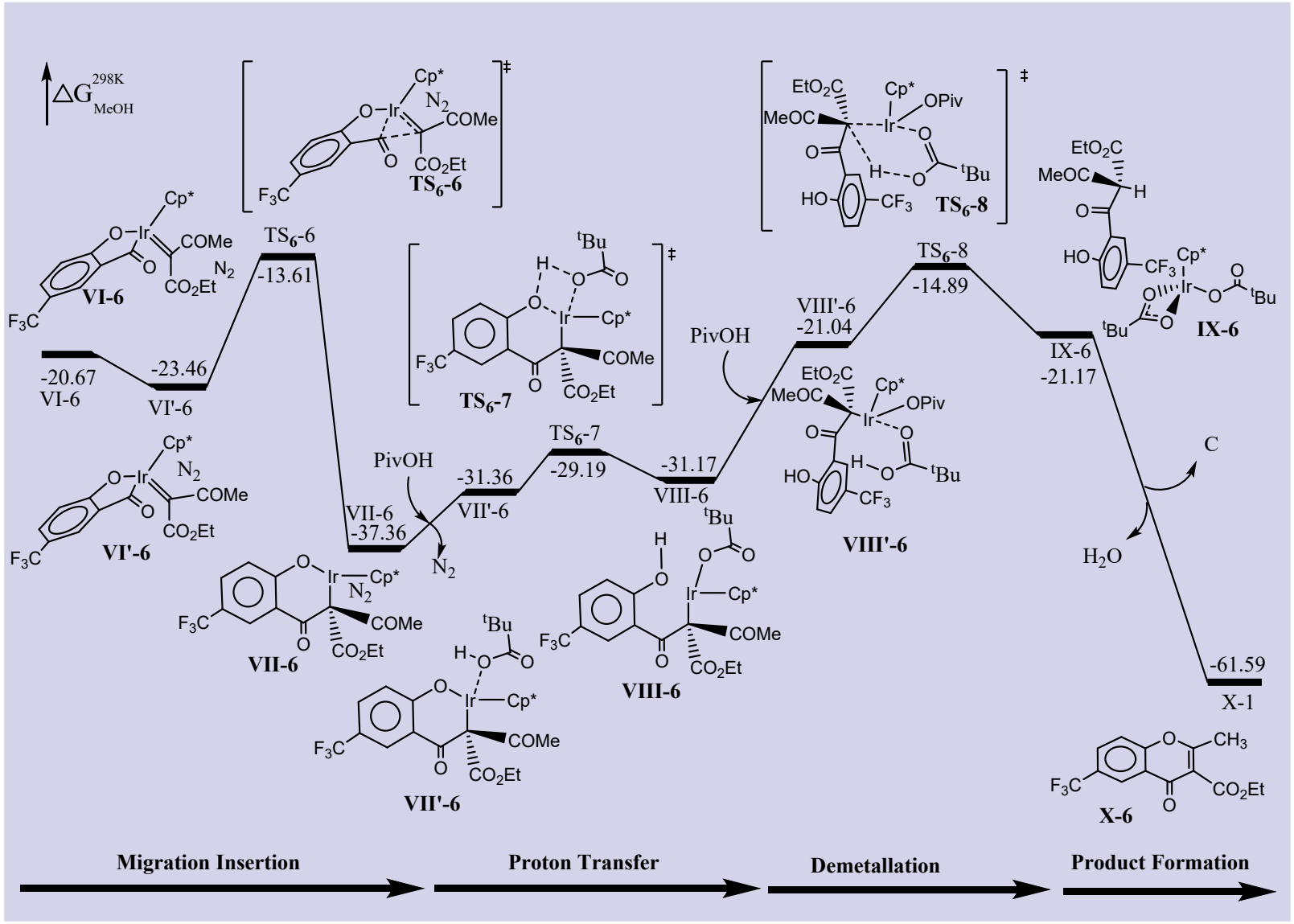
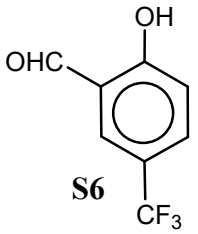
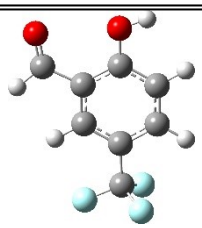


Fig-28: PES with Gibbs free energy (kcal/mol) and the structures of the stationary points of first part of path using M06 functional & 6-31G(d,p) basis set for non-metals and LANL2DZ for metals for S6

St.Pt.	General Structure	Ball & Stick model
S6		

Cartesian co-ordinate

Atoms	X	Y	Z
C	1.80828	0.89985	-0.00027
O	3.10269	1.24361	-0.00019
C	0.79391	1.86468	-0.00043
C	-0.53567	1.48755	-0.00052
C	1.46517	-0.46684	-0.00021
C	-0.88522	0.13642	-0.00062
C	0.11468	-0.81990	-0.00041
H	-0.14809	-1.87669	-0.00039
C	2.45130	-1.56420	0.00020
H	1.96012	-2.57000	-0.00046
O	3.65373	-1.45912	-0.00001
H	1.06479	2.91996	-0.00049
H	3.18045	2.20531	-0.00026
H	-1.31604	2.24515	-0.00061
C	-2.33439	-0.22787	0.00019
F	-2.96169	0.26685	1.07684
F	-2.96540	0.27621	-1.06993
F	-2.52412	-1.54949	-0.00511

Frequencies

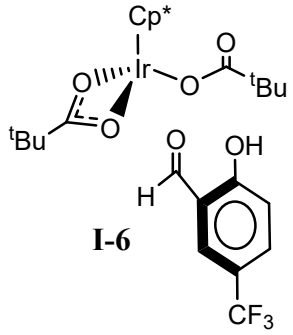
-10.9705	69.8322	94.1336
151.2465	190.8876	221.0783
262.3018	303.0824	361.7171
406.5714	419.6907	420.3404
460.6496	463.2838	532.6855
589.9927	634.5574	637.4412
710.0884	738.0533	778.0200
799.1440	824.2016	928.0727
930.1759	943.7770	1018.3822
1126.7282	1144.9724	1186.7627
1234.6752	1236.1840	1260.6224
1332.2256	1351.5264	1374.3996
1415.1828	1420.4108	1482.6239
1566.4592	1655.6157	1696.7621
1858.4479	2837.0423	3163.4458
3189.4274	3201.3450	3867.7081

Statistical Thermodynamic Analysis

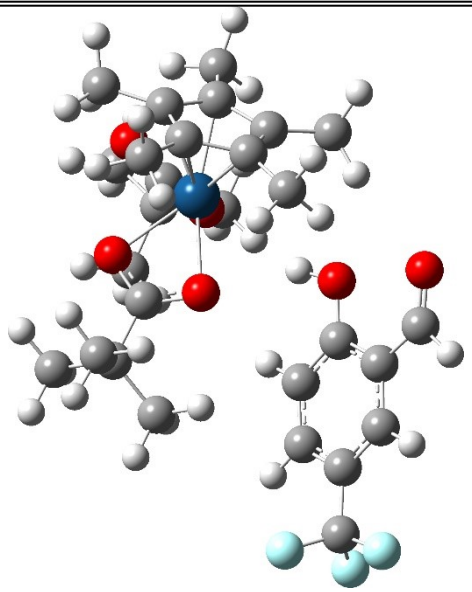
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.119586 Electronic Energy = -757.465965609
Internal Energy (E)= -757.336219609 Enthalpy (H)= -757.335275609
Gibbs Free Energy (G)=-757.382663609 Gibbs Free Energy of Solvation=-757.402377146

St.Pt.	General Structure	Ball & Stick model

I-6



I-6



Cartesian co-ordinate

Atoms	X	Y	Z
C	3.47668	-0.96241	-0.86111
C	3.73870	-0.86996	0.54747
C	2.87408	-1.81847	1.23917
C	2.07682	-2.47973	0.23742
C	2.42658	-1.94081	-1.06150
C	-2.01142	-0.56643	-1.55234
C	-0.98573	1.15208	2.90142
C	-0.00885	0.65802	1.85541
O	1.17306	1.11078	1.78936
O	-0.32050	-0.30702	1.08688
C	2.81553	-2.03856	2.71065
H	2.98324	-1.10146	3.25303
H	1.83097	-2.41413	3.00994
H	3.56960	-2.76366	3.04167
C	0.99957	-3.47528	0.47173
H	0.18603	-3.33752	-0.25020
H	1.38765	-4.49468	0.35158
H	0.58173	-3.38334	1.47915
C	1.87861	-2.37988	-2.37230
H	0.82070	-2.65453	-2.30462
H	1.95803	-1.57769	-3.11387
H	2.44317	-3.24262	-2.75008
C	4.16679	-0.20275	-1.93598
H	3.47695	0.04025	-2.75076
H	4.56958	0.74034	-1.56115
H	4.98383	-0.80453	-2.35506
C	4.67248	0.10048	1.17867
H	4.47491	0.20261	2.24987
H	5.71466	-0.21842	1.05148
H	4.54439	1.08814	0.72057
C	1.62978	2.24036	-1.10688
O	0.89343	1.15494	-1.02882
O	2.79061	2.31567	-0.73130
C	0.87199	3.46108	-1.63656
O	-0.78100	-0.70497	-2.03188

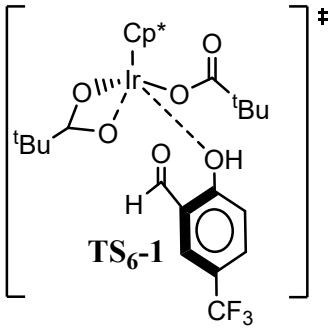
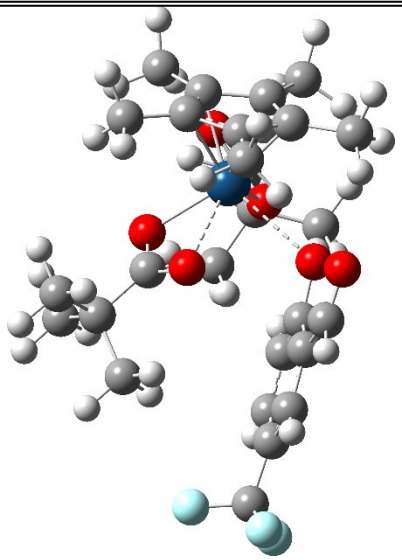
Frequencies

20.9081	40.5289	42.2768
52.5876	56.3889	61.9616
68.4055	70.7180	81.0591
82.6423	87.9662	96.5397
100.3583	109.6154	127.5246
128.2190	132.7093	148.3912
152.3716	158.5051	163.1522
165.6326	173.1674	175.0382
178.1546	190.3352	193.6191
195.5734	209.8333	214.0034
216.8633	220.6920	226.6013
231.7069	236.5741	242.6296
251.7058	268.0337	278.9895
282.7992	291.1329	298.6952
304.9361	309.3306	316.6820
318.9128	321.2732	327.0193
330.1447	342.9931	353.2193
366.9586	368.5450	390.9240
393.9201	410.6925	416.4265
429.1171	433.6636	438.0678
440.2856	452.8212	456.0476
461.8169	470.2692	478.7608
533.0820	536.0543	538.9241
546.0949	550.6191	567.6644
585.4915	589.9135	592.7383
603.6048	628.0748	632.6529
639.1011	639.5010	708.9370
746.8406	780.8291	786.8801
795.7611	800.0654	806.3783
813.0178	813.2195	834.9848
844.0432	873.3870	909.2137
918.0961	934.0791	936.7218
943.9623	948.1429	953.9884
956.6982	959.6969	966.5306
971.0581	972.6438	987.7035
1032.4019	1034.9150	1035.5355
1037.6643	1038.8068	1039.4552
1044.8646	1045.9678	1053.0607
1074.9296	1090.9965	1097.5795

C	0.11843	3.13233	-2.92429	1108.0513	1117.6375	1154.8453
H	-0.61793	2.33281	-2.79266	1185.5306	1186.9233	1202.5799
H	-0.41446	4.02254	-3.28290	1228.0997	1232.1062	1237.3286
H	0.81116	2.81953	-3.71600	1239.8780	1241.8188	1259.5459
C	1.84584	4.60273	-1.90014	1265.1738	1267.8933	1273.8158
H	1.29784	5.49503	-2.22994	1346.4993	1359.2064	1360.3831
H	2.41486	4.85147	-0.99934	1374.0437	1375.0650	1377.8355
H	2.56646	4.33386	-2.68116	1381.4162	1382.1897	1389.5342
C	-0.10139	3.86905	-0.52307	1393.4665	1396.1393	1398.3994
H	0.45525	4.15738	0.37870	1405.4369	1415.4670	1418.4818
H	-0.71008	4.72642	-0.83909	1433.5291	1436.8552	1439.0859
H	-0.77036	3.04278	-0.24724	1440.8073	1441.3829	1442.5500
C	-2.41881	1.06677	2.38655	1444.1617	1448.5116	1451.8897
H	-2.65259	0.06340	2.01328	1453.6575	1455.6395	1460.7297
H	-3.12128	1.31650	3.19158	1461.0256	1463.4756	1472.3945
H	-2.58365	1.77490	1.56459	1474.8706	1475.8093	1477.8878
C	-0.64897	2.57730	3.32435	1479.8508	1482.1488	1485.6740
H	-1.34434	2.90316	4.10821	1486.8937	1490.3997	1493.0398
H	0.37228	2.64930	3.71140	1496.0662	1499.8595	1504.7935
H	-0.73847	3.27342	2.48146	1515.1928	1524.2464	1530.5429
C	-0.80397	0.19890	4.09254	1549.5842	1567.9713	1604.4473
H	0.23342	0.21542	4.45086	1649.5247	1694.3696	1780.4952
H	-1.45758	0.50599	4.91847	1831.2920	2848.5661	3021.0801
H	-1.06159	-0.83002	3.81311	3021.8866	3032.8506	3034.1768
Ir	1.68752	-0.37307	0.20431	3035.1285	3037.4031	3037.8352
C	-2.51979	0.69856	-1.21533	3038.1926	3039.4944	3040.7096
C	-3.79938	0.83806	-0.72510	3041.9870	3109.2739	3112.0137
C	-4.62001	-0.28122	-0.54544	3112.4991	3113.1786	3117.9020
C	-2.84049	-1.70030	-1.39344	3118.2493	3120.3286	3120.6448
C	-4.13540	-1.52842	-0.88711	3121.7671	3122.6471	3122.7688
H	-4.17406	1.82538	-0.45885	3124.4814	3125.2614	3137.5209
H	-4.76208	-2.40873	-0.75238	3139.5302	3140.6477	3143.2248
H	-0.25150	0.10725	-1.85251	3144.8227	3146.2741	3148.4618
H	-1.87067	1.56384	-1.32601	3154.4723	3164.4826	3190.6095
C	-2.43106	-3.07841	-1.67764	3191.4878	3219.0948	3484.8663
H	-3.26796	-3.80399	-1.52009			
O	-1.34197	-3.48316	-2.03015			
C	-5.96323	-0.08391	0.07113			
F	-6.70087	0.79916	-0.61713			
F	-6.66324	-1.21976	0.14966			
F	-5.85214	0.40784	1.31645			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.619254 Electronic Energy = -1944.45124533
Internal Energy (E)= -1943.78986633 Enthalpy (H)= -1943.78892233
Gibbs Free Energy (G)=-1943.90366533 Gibbs Free Energy of Solvation=-1943.95563413

St.Pt.	General Structure	Ball & Stick model
TS_6-1		

Cartesian co-ordinate

Atoms	X	Y	Z
C	3.45887	-0.81236	-0.87397
C	3.58652	-0.67488	0.56460
C	2.77141	-1.71418	1.18566
C	2.13625	-2.45649	0.14371
C	2.54486	-1.89583	-1.13666
C	-1.74693	-0.82367	-1.40933
C	-1.28954	0.57220	2.94458
C	-0.33455	0.15721	1.82911
O	0.73701	0.82434	1.65958
O	-0.57345	-0.87520	1.16318
C	2.59403	-1.88828	2.65282
H	2.41384	-0.91829	3.13138
H	1.73654	-2.53110	2.87304

Frequencies

-80.9200	-36.4446	-29.4715
32.9970	36.8142	41.0235
51.1011	53.2965	69.0162
74.3517	75.7660	80.9359
90.5977	107.8192	109.2764
114.9581	117.9822	125.9885
136.4934	146.5268	149.9629
154.9514	160.8667	168.3738
183.2526	192.6770	199.6486
206.1473	206.4017	212.9867
217.2787	221.2042	231.9138
235.6768	237.7164	243.0575
267.6157	275.4342	280.8669
287.3912	290.8811	302.2530
307.6744	312.5458	318.2000
319.7113	332.5059	341.8173
343.3462	355.7808	365.8542

H	3.48545	-2.33612	3.10926	367.3410	374.2555	386.1579
C	1.16968	-3.56953	0.31271	389.2409	407.8746	416.0334
H	0.36715	-3.50875	-0.42910	420.4316	425.1347	432.7885
H	1.67812	-4.53440	0.18755	441.4405	447.3880	454.3836
H	0.70842	-3.54580	1.30370	456.7686	466.0517	469.2922
C	2.16353	-2.44029	-2.46852	532.9840	533.9544	539.0204
H	1.14177	-2.83370	-2.46248	546.9002	548.2892	569.7436
H	2.22200	-1.66987	-3.24530	579.4283	587.6241	589.8229
H	2.84422	-3.25200	-2.75682	593.5556	604.7111	620.5030
C	4.14375	0.02679	-1.89115	627.7001	634.8677	646.0426
H	3.54874	0.08777	-2.80850	707.5664	747.5638	782.9633
H	4.27847	1.04462	-1.51554	783.9100	793.0872	801.0027
H	5.12081	-0.40196	-2.14770	809.3984	810.1408	811.1498
C	4.43344	0.30390	1.28899	829.2496	860.1094	909.1831
H	4.04336	0.48112	2.29658	927.8776	929.7377	933.6565
H	5.45976	-0.07577	1.37987	940.0679	949.9657	951.9201
H	4.43841	1.26284	0.76514	954.2797	963.3982	974.3549
C	1.77571	2.49290	-0.77847	975.1674	980.2785	981.0470
O	1.07637	1.41375	-1.00367	1024.0458	1033.4669	1037.3589
O	2.90220	2.52089	-0.29992	1038.3178	1039.9015	1041.6203
C	1.01518	3.78074	-1.12288	1045.9330	1046.5623	1047.6252
O	-0.47757	-1.17294	-1.68511	1063.2857	1097.1341	1102.8797
C	0.40706	3.70075	-2.52241	1110.9292	1125.9585	1152.2656
H	-0.30252	2.87236	-2.61777	1186.8498	1191.0281	1199.1257
H	-0.12633	4.63288	-2.75100	1231.0549	1235.7573	1243.8023
H	1.18508	3.56797	-3.28516	1244.2939	1244.9463	1257.1494
C	1.95781	4.97512	-1.04496	1260.6281	1263.3558	1273.6535
H	1.40952	5.90146	-1.26115	1332.0999	1340.7369	1357.8380
H	2.40937	5.05697	-0.05153	1370.3853	1373.2765	1375.1773
H	2.77403	4.88052	-1.77058	1377.2423	1380.4544	1388.9509
C	-0.09156	3.93289	-0.07234	1392.6428	1393.7576	1400.0724
H	0.33919	4.00704	0.93458	1407.2241	1409.9959	1413.2567
H	-0.67374	4.84369	-0.26574	1418.5912	1423.9795	1428.2384
H	-0.77472	3.07293	-0.07566	1433.3088	1439.2683	1445.4997
C	-2.72638	0.52662	2.43080	1448.9457	1451.7232	1454.4817
H	-2.95482	-0.44837	1.98648	1459.7975	1460.4748	1461.5750
H	-3.42980	0.71293	3.25248	1463.4360	1468.5994	1471.5063
H	-2.90011	1.29469	1.66580	1473.4239	1474.4288	1477.2167
C	-0.96210	1.96130	3.47720	1480.5573	1481.0635	1484.8034
H	-1.65590	2.22123	4.28724	1485.7398	1488.3954	1490.9329
H	0.06073	2.01066	3.86506	1500.0452	1504.4821	1509.3299
H	-1.05595	2.71987	2.69122	1511.3692	1524.8454	1526.5558
C	-1.11273	-0.46620	4.05910	1538.8317	1559.3196	1653.9061
H	-0.08258	-0.46355	4.44005	1667.1551	1694.1535	1775.0465
H	-1.78174	-0.23388	4.89749	1835.4751	2850.2194	3020.3944
H	-1.34635	-1.47333	3.69535	3024.8261	3028.1327	3035.9992
Ir	1.56168	-0.36606	0.02550	3037.2426	3039.5732	3040.5078
C	-2.09350	0.52430	-1.27632	3041.4826	3042.1859	3043.4068
C	-3.38780	0.87877	-0.95796	3045.2705	3107.2262	3108.1243
C	-4.36375	-0.10351	-0.76099	3108.5549	3113.2734	3116.7022
C	-2.72196	-1.82318	-1.24407	3119.5589	3122.9027	3123.7593
C	-4.02457	-1.43581	-0.90811	3124.6431	3126.4262	3128.8127
H	-3.64986	1.92898	-0.83913	3132.0729	3132.5393	3135.2187
H	-4.78109	-2.20668	-0.76655	3139.8738	3141.5591	3143.4903
H	0.01361	-0.36880	-1.93103	3148.0865	3158.6600	3168.7985
H	-1.30523	1.27045	-1.37593	3169.4934	3174.0352	3177.4128
C	-2.46591	-3.25554	-1.42801	3185.1561	3193.8363	3708.7072
H	-3.38029	-3.87654	-1.25847			
O	-1.41937	-3.78275	-1.74261			
C	-5.71929	0.32154	-0.30579			
F	-6.18569	1.34489	-1.03374			

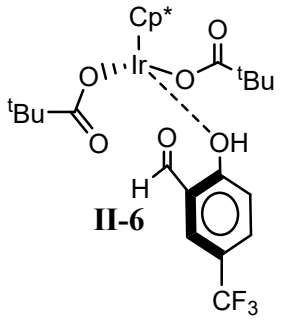
F	-6.61469	-0.66870	-0.37451	
F	-5.68780	0.74581	0.96753	

Statistical Thermodynamic Analysis

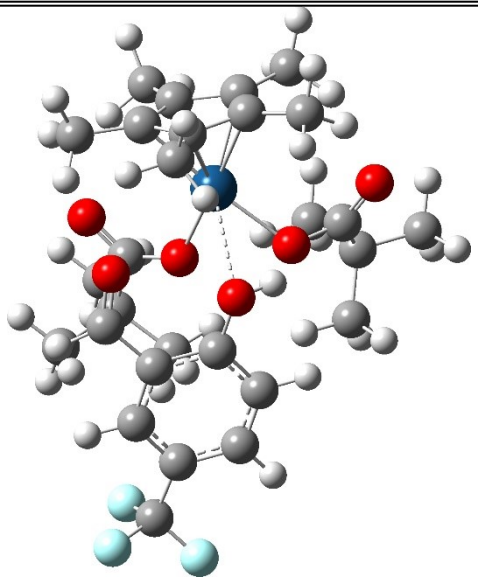
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.618483 Electronic Energy = -1944.42730487
Internal Energy (E)= -1943.76875287 Enthalpy (H)= -1943.76780887
Gibbs Free Energy (G)=-1943.87764987 Gibbs Free Energy of Solvation=-1943.93685968

St.Pt.	General Structure	Ball & Stick model

II-6



II-6



Cartesian co-ordinate

Atoms	X	Y	Z
C	3.46342	-0.51998	-1.18939
C	3.69374	-0.14898	0.17500
C	3.14272	-1.20022	1.03441
C	2.58155	-2.21427	0.19174
C	2.74914	-1.76898	-1.17760
Ir	1.57255	-0.30022	-0.10934
O	-0.19092	-0.17860	0.88769
O	0.77783	1.54344	-0.76089
O	-0.55070	-2.85330	-1.48102
C	-1.71282	-2.56812	-1.28501
H	-2.42542	-3.33547	-0.89255
C	-2.35057	-1.25924	-1.47202
C	-1.67150	-0.10138	-1.90723
C	-3.68433	-1.14630	-1.07524
C	-2.33819	1.12839	-1.90204
C	-4.33998	0.07400	-1.07229
H	-4.20781	-2.03991	-0.73235
C	-3.65324	1.21778	-1.48089
H	-1.79600	2.01652	-2.21990
H	-4.15363	2.18238	-1.46536
O	-0.40151	-0.19053	-2.32123
H	0.04382	0.66770	-2.14273
C	-0.52478	-0.92821	1.91018
C	-1.79304	-0.47185	2.64874
C	1.46872	2.66036	-0.64628
C	0.84728	3.65952	0.33559
O	2.52930	2.88867	-1.21027
O	0.09409	-1.90877	2.30006
C	2.30589	-2.49706	-2.39468
H	1.72667	-3.38733	-2.14461
H	1.66429	-1.86600	-3.01872
H	3.18438	-2.78847	-2.98507
C	3.86629	0.24252	-2.40094
H	3.75622	1.31838	-2.23369
H	4.90751	0.01853	-2.66767

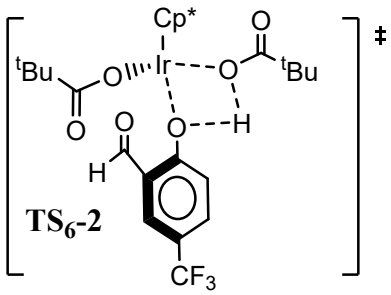
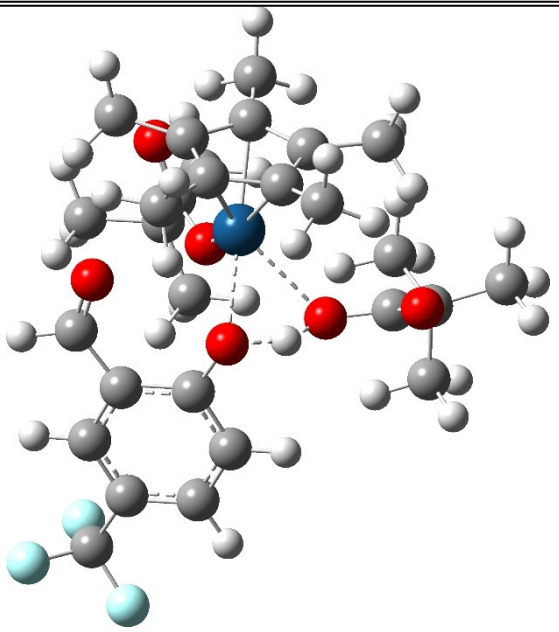
Frequencies

25.7533	36.1375	37.9520
45.3259	52.6635	61.0895
66.1945	76.6310	85.1547
90.1384	95.3675	96.3613
101.2419	106.1485	120.3432
126.8057	128.7336	130.7933
136.0815	147.0164	162.6064
169.5561	181.6022	183.1507
189.4884	196.0677	209.3099
212.4850	219.0409	223.5852
230.1694	234.0954	238.9936
245.8214	259.3318	274.8485
279.1170	282.4657	288.6996
294.6823	300.1500	302.9456
314.8190	319.0983	323.2937
329.7527	335.4896	344.9385
350.7836	362.9360	366.3238
377.2166	388.1224	391.4265
394.7425	414.6480	417.9813
432.4637	433.3615	439.4733
448.4771	454.2860	461.3386
467.9647	470.9360	476.3790
534.8123	535.3412	540.7899
551.8523	562.4946	575.5315
576.9853	585.3272	589.4592
599.2664	603.3852	633.1241
640.2352	641.3194	701.7904
732.5510	746.2239	779.6252
792.5071	794.5896	803.0898
811.0613	812.4773	819.4284
822.0869	843.8732	906.0872
923.1240	925.8803	932.9466
949.1229	952.0811	953.1165
957.6273	958.8106	960.6309
962.1878	967.7837	982.9922
1033.4499	1034.8276	1037.3815
1041.2150	1043.2534	1045.6537
1048.3009	1049.5561	1050.7521
1061.1980	1099.4685	1101.0566

H	3.23602	-0.02877	-3.25482	1118.0605	1118.4649	1145.9961
C	4.40895	1.07012	0.62823	1189.9619	1193.6435	1200.8559
H	4.22730	1.27073	1.68898	1223.7260	1229.0375	1235.3679
H	5.49050	0.93957	0.49184	1240.1661	1242.7299	1247.7531
H	4.09376	1.94493	0.04676	1264.5425	1265.8856	1271.9995
C	3.18743	-1.21382	2.51823	1334.5590	1343.4136	1350.5560
H	2.29286	-1.69961	2.91844	1356.5426	1375.0391	1375.4917
H	4.07937	-1.74771	2.87101	1376.8212	1378.1608	1381.1226
H	3.22318	-0.19431	2.91872	1385.9131	1388.9010	1395.8323
C	2.01307	-3.52536	0.59672	1397.0602	1409.0420	1411.8520
H	2.72515	-4.32467	0.35088	1414.7530	1417.5541	1420.3095
H	1.79535	-3.55158	1.66433	1428.8170	1433.2635	1434.5269
H	1.07650	-3.72072	0.06620	1442.2036	1444.1704	1453.7224
C	-2.37766	0.82047	2.09416	1456.7317	1461.6750	1464.3053
H	-2.61149	0.72650	1.02828	1466.5464	1467.0207	1467.9496
H	-3.30518	1.06689	2.62817	1471.5009	1473.6942	1477.4727
H	-1.68161	1.66181	2.20741	1478.4048	1479.3220	1482.5614
C	-1.40381	-0.27632	4.11640	1489.5960	1490.4851	1495.5378
H	-2.28265	0.02332	4.70187	1501.5404	1507.0836	1508.8213
H	-0.99738	-1.20141	4.53756	1515.4250	1523.9483	1540.7319
H	-0.64518	0.51145	4.22217	1545.6705	1561.5848	1650.6520
C	-2.82760	-1.59503	2.54612	1686.4174	1769.7253	1775.4523
H	-2.40378	-2.54787	2.88073	1836.5098	2862.7955	3016.2423
H	-3.70090	-1.35875	3.16807	3020.3013	3023.7638	3033.1565
H	-3.18504	-1.70916	1.51363	3033.5023	3034.3365	3037.8756
C	1.54591	5.00806	0.22630	3039.0523	3043.3042	3045.8793
H	1.42363	5.43920	-0.77425	3047.5910	3098.3386	3099.5423
H	1.12540	5.71017	0.95780	3105.8827	3116.1483	3118.3178
H	2.62090	4.91137	0.41150	3119.6282	3120.1136	3123.2827
C	-0.65186	3.81263	0.08556	3125.1212	3128.7061	3132.8949
H	-1.16723	2.84940	0.17388	3137.0309	3141.7218	3141.7911
H	-1.08238	4.50720	0.81913	3142.5533	3143.7529	3155.9758
H	-0.84772	4.22512	-0.91402	3161.8934	3168.7952	3169.4143
C	1.06817	3.07147	1.73687	3171.2552	3181.0801	3188.4448
H	2.14073	2.93753	1.94069	3207.9159	3215.9674	3527.2986
H	0.66611	3.75495	2.49664			
H	0.56793	2.10002	1.83903			
C	-5.71575	0.15117	-0.49857			
F	-6.33129	1.29631	-0.80775			
F	-6.48738	-0.85620	-0.92694			
F	-5.68219	0.06430	0.84073			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.620192 Electronic Energy = -1944.43634466
Internal Energy (E)= -1943.77447066 Enthalpy (H)= -1943.77352766
Gibbs Free Energy (G)=-1943.88725866 Gibbs Free Energy of Solvation=-1943.94836339

St.Pt.	General Structure	Ball & Stick model
TS_6-2		

Cartesian co-ordinate

Atoms	X	Y	Z
C	3.15987	-0.64981	-1.46067
C	3.50689	-0.20337	-0.13751
C	3.09667	-1.21059	0.82084
C	2.50116	-2.30016	0.07184
C	2.55478	-1.94231	-1.33601
Ir	1.36838	-0.51557	-0.21171
O	-0.23458	-0.31693	1.00607
O	0.65006	1.80989	-0.54756
O	-0.51585	-2.73575	-1.17550
C	-1.68020	-2.41486	-1.03572

Frequencies

-156.3937	26.1171	33.7985
40.4337	50.1541	59.2200
63.8890	71.0863	75.7416
86.5532	88.7122	91.9741
94.4449	101.1250	106.2972
112.8984	115.7159	125.6207
127.3067	136.8038	158.2539
161.8127	165.2153	174.4723
181.6735	182.9804	190.8736
195.4808	204.3995	213.1114
214.9148	221.9653	234.6101
244.8062	246.7523	253.1383
261.8519	270.7676	286.8876
293.4708	297.5445	307.6710
310.8517	316.0694	319.9483

H	-2.43559	-3.17916	-0.72889	320.9633	324.6819	329.9584
C	-2.26289	-1.08899	-1.21923	340.7558	345.5680	348.9486
C	-1.52624	0.07663	-1.55197	357.6803	375.8403	379.1809
C	-3.63954	-0.98824	-0.99667	385.4429	392.1002	403.0981
C	-2.22300	1.29406	-1.65423	406.1059	436.6575	444.8031
C	-4.30771	0.21931	-1.09594	448.8746	454.1414	456.4721
H	-4.19163	-1.88981	-0.72852	471.0937	475.2851	505.0628
C	-3.58401	1.36636	-1.42907	532.9820	537.1216	540.0750
H	-1.66269	2.18983	-1.91213	553.2567	578.9313	584.3047
H	-4.09641	2.32147	-1.51012	586.4047	589.9741	593.7568
O	-0.21476	0.06357	-1.78711	603.5792	614.0360	640.5813
H	0.23765	1.12716	-1.42521	644.6878	649.8110	717.4493
C	-0.44574	-0.95583	2.12655	723.2118	758.1686	780.3864
C	-1.68282	-0.47932	2.90064	792.4618	794.6427	805.9139
C	1.47949	2.82852	-0.66944	812.9767	816.1461	817.6488
C	1.39915	3.78157	0.52209	819.1272	862.6771	908.1173
O	2.19970	3.01745	-1.63631	922.3575	924.5904	938.6466
O	0.25381	-1.85758	2.56969	947.2646	949.9451	952.3788
C	2.08400	-2.75752	-2.48552	955.4580	958.8283	963.7786
H	1.62868	-3.69386	-2.16055	971.7338	976.8905	983.6821
H	1.33609	-2.21268	-3.07065	1017.6481	1026.7131	1037.0681
H	2.93582	-2.98478	-3.13918	1040.8456	1041.9896	1042.8804
C	3.35315	0.11529	-2.72253	1043.9508	1045.5997	1047.0302
H	3.09166	1.17258	-2.58390	1050.4816	1099.8046	1105.2337
H	4.39480	0.05364	-3.06344	1113.4498	1126.6883	1167.2504
H	2.71316	-0.28483	-3.51525	1188.2786	1195.1498	1215.7612
C	4.21323	1.06625	0.16357	1230.0616	1232.9866	1234.7252
H	4.07131	1.37621	1.20352	1240.2195	1245.1515	1262.5571
H	5.29036	0.92143	0.00517	1266.9551	1269.4429	1275.5399
H	3.88614	1.87797	-0.49680	1344.9487	1356.1966	1364.8805
C	3.33123	-1.17312	2.28746	1373.6849	1374.4795	1378.8342
H	2.51852	-1.68223	2.81212	1380.7944	1385.9078	1387.9463
H	4.28609	-1.65307	2.53852	1393.8389	1395.9392	1399.7959
H	3.36448	-0.14045	2.65240	1404.1540	1407.6865	1416.0941
C	2.02872	-3.59257	0.62674	1417.6790	1422.4602	1423.5549
H	2.85425	-4.31706	0.63580	1434.3904	1436.6241	1438.7683
H	1.65173	-3.45579	1.64254	1441.4787	1451.2023	1452.8189
H	1.21042	-3.99653	0.02449	1455.3510	1460.6233	1461.5634
C	-2.44702	0.62983	2.18789	1463.1626	1464.9742	1465.5029
H	-2.88784	0.27563	1.24862	1467.6816	1472.5931	1476.2197
H	-3.26755	0.98233	2.82712	1478.7701	1482.4986	1485.3126
H	-1.79693	1.48145	1.95049	1486.4487	1490.1980	1497.7868
C	-1.18702	0.02124	4.26010	1501.2666	1503.4500	1506.4324
H	-2.03936	0.31038	4.88841	1508.5081	1510.9363	1514.8138
H	-0.61719	-0.75822	4.77654	1526.8880	1554.6267	1624.2427
H	-0.54178	0.90270	4.14532	1632.8669	1690.7828	1771.6273
C	-2.59447	-1.69054	3.10363	1811.0118	1822.6848	2856.0760
H	-2.06203	-2.49883	3.61530	3018.8668	3024.2711	3025.6839
H	-3.47079	-1.40851	3.70147	3029.0507	3032.1179	3035.3076
H	-2.95807	-2.07483	2.14036	3037.1223	3037.6459	3038.9969
C	2.53294	4.79500	0.46074	3043.8117	3046.3286	3098.6581
H	2.50359	5.36720	-0.47219	3104.1867	3106.1002	3112.6562
H	2.46002	5.49383	1.30364	3113.9479	3115.2045	3116.9656
H	3.51103	4.30010	0.51155	3119.3843	3121.1148	3128.0930
C	0.04555	4.49565	0.40289	3130.9540	3137.1104	3138.4346
H	-0.78134	3.77803	0.46626	3139.0559	3141.7594	3144.3107
H	-0.06512	5.22648	1.21402	3145.4086	3150.7153	3153.4817
H	-0.03266	5.03521	-0.54994	3157.1234	3168.8764	3179.3625
C	1.43941	3.00554	1.84068	3192.3434	3193.6061	3211.9569
H	2.42373	2.54531	2.00551			
H	1.25634	3.69053	2.67867			

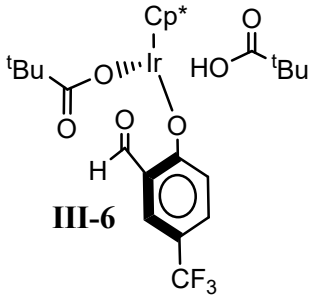
H	0.68257	2.21208	1.85978
C	-5.75246	0.28782	-0.72928
F	-6.33570	1.40433	-1.17803
F	-6.43937	-0.75408	-1.21711
F	-5.91740	0.26393	0.60241

Statistical Thermodynamic Analysis

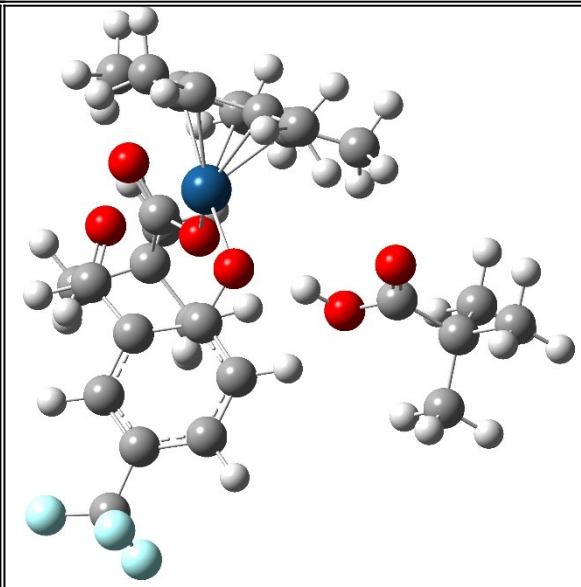
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.614893 Electronic Energy = -1944.42520962
Internal Energy (E)= -1943.76881662 Enthalpy (H)= -1943.76787262
Gibbs Free Energy (G)=-1943.88140162 Gibbs Free Energy of Solvation=-1943.93560078

St.Pt.	General Structure	Ball & Stick model

III-6



III-6



Cartesian co-ordinate

Atoms	X	Y	Z
C	2.94644	0.07655	-1.73035
C	3.14143	0.51247	-0.35770
C	3.41380	-0.66585	0.44395
C	3.31211	-1.81565	-0.40395
C	3.03489	-1.35334	-1.76301
Ir	1.43988	-0.77191	-0.41982
O	0.25853	-0.44142	1.26440
O	-0.09816	2.50219	0.49104
O	0.14716	-2.51842	-0.59220
C	-1.09245	-2.47958	-0.65511
H	-1.61009	-3.45603	-0.60603
C	-1.94894	-1.34724	-0.80852
C	-1.46677	-0.03249	-1.10392
C	-3.33789	-1.59043	-0.73864
C	-2.44071	0.97620	-1.34349
C	-4.24923	-0.58308	-0.93050
H	-3.68076	-2.60042	-0.51823
C	-3.78123	0.71180	-1.24295
H	-2.07466	1.96700	-1.60228
H	-4.50522	1.50780	-1.40995
O	-0.22073	0.30121	-1.20013
H	-0.00324	1.68811	-0.05699
C	0.27136	-1.27019	2.26434
C	-0.86644	-1.03191	3.26964
C	0.20663	3.55956	-0.25683
C	-0.00966	4.86980	0.48526
O	0.62756	3.47299	-1.39534
O	1.06317	-2.19534	2.42346
C	2.86686	-2.23815	-2.94752
H	2.26018	-3.11469	-2.69458
H	2.36591	-1.71401	-3.76704
H	3.83751	-2.59377	-3.31566
C	2.59224	0.98605	-2.85209
H	1.87421	1.74744	-2.52071
H	3.48737	1.49883	-3.22602

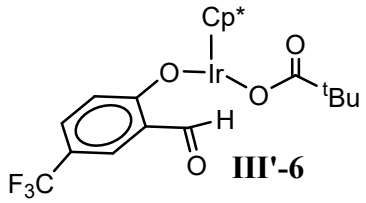
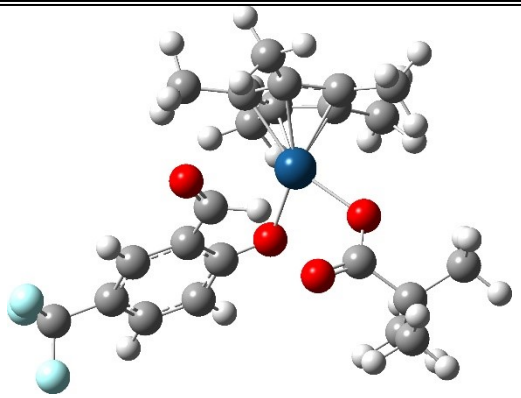
Frequencies

23.4540	26.7098	33.7679
37.0927	44.0459	45.5880
53.8890	60.8818	75.7882
79.6385	85.2042	87.8952
94.5753	100.2534	105.9597
115.5658	123.4687	133.0322
139.7708	150.2417	160.7734
165.5703	179.2569	190.4794
194.7125	199.1921	202.7399
204.5464	210.5448	215.8161
220.0403	223.2673	236.3300
242.6957	247.5367	250.8611
272.0503	284.2524	288.3980
300.3979	305.0761	308.5599
320.0259	325.6204	327.4067
329.0852	331.1036	341.9268
348.7535	354.0346	362.0073
379.3073	381.4286	385.4497
391.5352	393.9136	401.3951
403.7475	423.6733	440.4737
443.9482	457.1524	461.9912
468.0991	469.4150	528.0626
531.8975	537.0603	543.1315
551.0296	553.8140	570.6507
585.5870	586.9084	593.1204
593.4556	606.9735	635.4792
643.0028	652.5296	716.6659
755.3622	761.8154	785.6580
789.3609	792.2386	811.4033
815.3445	818.2520	818.5079
850.0559	887.4004	911.4404
920.2811	941.7092	946.4810
946.6690	955.0157	958.0422
958.7762	963.7671	969.7703
969.8822	992.0776	995.8396
1004.9963	1033.8671	1038.9448
1040.3798	1043.2454	1045.7706
1047.8765	1049.8337	1052.3305
1055.1158	1098.9418	1105.6426

H	2.14019	0.43752	-3.68396	1112.9712	1120.4629	1171.4866
C	3.20260	1.91703	0.13095	1188.8223	1191.8229	1216.9888
H	2.70201	2.01139	1.10211	1222.6364	1229.4110	1241.7094
H	4.24551	2.23774	0.25472	1243.0639	1249.0041	1251.1016
H	2.71150	2.60414	-0.56603	1257.6815	1266.8923	1269.5237
C	3.73016	-0.65658	1.89536	1305.6456	1365.0177	1373.7817
H	3.40346	-1.57916	2.37984	1376.6540	1379.3884	1380.1078
H	4.81129	-0.52818	2.03837	1380.9400	1384.3923	1385.8609
H	3.22274	0.17299	2.39927	1391.0512	1397.9476	1403.0891
C	3.43899	-3.22807	0.04639	1405.2756	1407.5030	1409.6431
H	4.48817	-3.49262	0.22797	1424.8707	1427.1074	1435.8948
H	2.86967	-3.36835	0.97220	1438.3531	1439.8344	1447.1589
H	3.03755	-3.92060	-0.69974	1453.0466	1456.4448	1456.6010
C	-1.67672	0.22028	2.95128	1458.1879	1459.9161	1461.0940
H	-2.15031	0.15163	1.96306	1464.7852	1466.2638	1468.2729
H	-2.46679	0.35198	3.70321	1470.9980	1473.1197	1475.9544
H	-1.04765	1.11852	2.94596	1480.2711	1483.5212	1484.3679
C	-0.25782	-0.93004	4.66693	1484.7404	1488.3580	1491.2831
H	-1.04978	-0.84321	5.42248	1499.3092	1500.9807	1507.2895
H	0.34683	-1.81500	4.88997	1510.8810	1518.7727	1524.6598
H	0.38559	-0.04442	4.75335	1531.1607	1535.7150	1595.8791
C	-1.77091	-2.26525	3.19453	1701.0651	1720.7426	1761.8112
H	-1.20334	-3.17578	3.41468	1831.6932	2985.4366	3012.8287
H	-2.59453	-2.17713	3.91514	3022.9556	3024.8096	3026.7748
H	-2.21361	-2.36558	2.19244	3031.3869	3033.8368	3035.6542
C	0.25625	6.03410	-0.45916	3037.4838	3039.0901	3039.8057
H	-0.42291	6.01154	-1.31860	3040.8650	3092.8433	3103.3392
H	0.11414	6.98408	0.07070	3107.7682	3108.0978	3112.2839
H	1.27908	6.00174	-0.84948	3114.5892	3115.6633	3117.2587
C	-1.44736	4.92650	1.00708	3120.7943	3121.7447	3123.5412
H	-1.65206	4.11353	1.71111	3128.2062	3131.7435	3135.0029
H	-1.61538	5.88171	1.52049	3139.5350	3140.1190	3142.3715
H	-2.17110	4.85704	0.18478	3144.1309	3144.2496	3145.4537
C	0.96973	4.91672	1.66265	3147.1570	3176.9239	3181.0341
H	2.00942	4.86508	1.31297	3186.6919	3200.3543	3526.5663
H	0.84670	5.86169	2.20675			
H	0.79603	4.09098	2.36141			
C	-5.72069	-0.80581	-0.84573			
F	-6.33133	-0.47590	-1.99464			
F	-6.03091	-2.07831	-0.57695			
F	-6.27821	-0.04430	0.10662			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.619825 Electronic Energy = -1944.45785451
Internal Energy (E)= -1943.79594751 Enthalpy (H)= -1943.79500451
Gibbs Free Energy (G)=-1943.91141951 Gibbs Free Energy of Solvation=-1943.96291127

St.Pt.	General Structure	Ball & Stick model
III'-6	 **III'-6**	

Cartesian co-ordinate

Atoms	X	Y	Z
C	1.79897	-2.32605	-0.99266
C	2.87527	-1.74222	-0.25510
C	2.47017	-1.68277	1.14187
C	1.15943	-2.31418	1.25105
C	0.73967	-2.69827	-0.05984
C	-1.97922	0.08244	-0.45496
Ir	1.10109	-0.52592	0.03126
C	-3.35158	-0.00777	-0.73845
C	-4.27879	0.42521	0.18089
C	-1.52242	0.57425	0.79939
C	-3.83756	0.96863	1.40678
C	-2.50200	1.04942	1.71106
H	-2.15546	1.45401	2.65842
H	-4.57716	1.32326	2.12324
H	0.00697	0.28012	-1.37335
O	2.14025	1.25004	0.00001
C	1.63170	2.31713	-0.56177
C	2.35122	3.60603	-0.15300
O	0.64961	2.33000	-1.29020

Frequencies

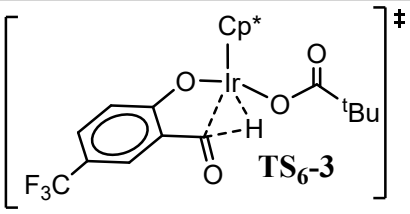
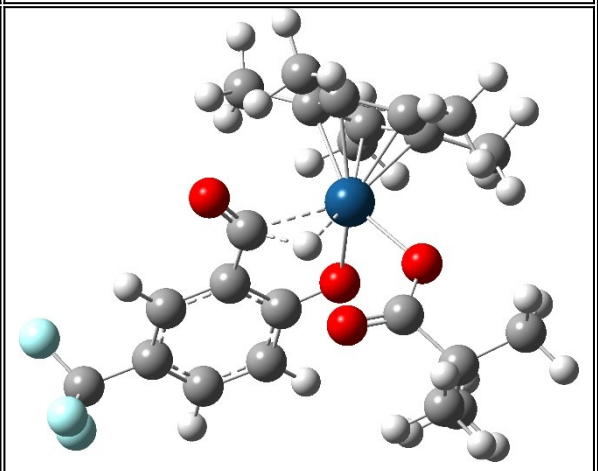
17.6091	29.4070	40.1568
41.0955	47.7044	55.2852
60.8828	70.0958	81.5216
96.2686	110.8982	124.3148
136.0718	144.2415	155.2243
163.4305	168.5625	174.6559
181.4957	191.6149	192.6205
195.4380	201.5833	211.1722
225.6588	228.5127	239.0829
244.1437	255.3851	267.2178
281.2305	285.5201	288.8460
302.3379	310.5909	313.1662
317.3516	327.4973	343.9776
367.3395	387.8672	396.9329
414.4444	420.9704	426.1587
428.9839	446.1647	455.2128
466.5592	523.4809	535.7803
536.7021	545.1650	562.9099
573.9737	577.3647	579.1989
592.5804	596.8111	603.8801
638.9173	643.8092	649.8437
659.5729	752.4813	767.0249
789.2648	805.0024	810.1411
817.0066	845.6755	858.7587

H	-3.65587	-0.40865	-1.70236
C	-1.01864	-0.27789	-1.47218
O	-1.20533	-0.92683	-2.48309
O	-0.27271	0.57998	1.15327
C	2.09581	4.69004	-1.19258
H	1.02265	4.83616	-1.34659
H	2.54201	5.63824	-0.86531
H	2.53588	4.42163	-2.16082
C	1.72230	4.00987	1.18626
H	1.87946	3.23168	1.94292
H	2.16822	4.94579	1.54839
H	0.64143	4.16230	1.07499
C	3.85125	3.38722	0.02393
H	4.31567	3.04262	-0.90943
H	4.33491	4.33037	0.31083
H	4.05810	2.64338	0.80080
C	4.15029	-1.18164	-0.77970
H	4.22706	-0.11522	-0.53025
H	5.01120	-1.70294	-0.34379
H	4.21255	-1.27512	-1.86740
C	1.71694	-2.52437	-2.46388
H	2.53896	-2.02321	-2.98240
H	1.75825	-3.59373	-2.70704
H	0.77356	-2.12362	-2.85755
C	-0.51357	-3.41367	-0.42481
H	-0.86307	-3.11898	-1.41890
H	-0.34913	-4.49877	-0.42665
H	-1.32004	-3.19581	0.28318
C	0.37106	-2.43740	2.50463
H	-0.70057	-2.50000	2.29158
H	0.66398	-3.33324	3.06578
H	0.52372	-1.56260	3.14459
C	3.31173	-1.16117	2.25095
H	2.71289	-0.94084	3.13954
H	4.08097	-1.89239	2.53240
H	3.81384	-0.23516	1.94999
C	-5.74526	0.34579	-0.07219
F	-6.32667	1.55303	0.00024
F	-6.03079	-0.16658	-1.27307
F	-6.36028	-0.41879	0.84662
H	-2.21361	-2.36558	2.19244
C	0.25625	6.03410	-0.45916
H	-0.42291	6.01154	-1.31860
H	0.11414	6.98408	0.07070
H	1.27908	6.00174	-0.84948
C	-1.44736	4.92650	1.00708
H	-1.65206	4.11353	1.71111
H	-1.61538	5.88171	1.52049
H	-2.17110	4.85704	0.18478
C	0.96973	4.91672	1.66265
H	2.00942	4.86508	1.31297
H	0.84670	5.86169	2.20675
H	0.79603	4.09098	2.36141
C	-5.72069	-0.80581	-0.84573
F	-6.33133	-0.47590	-1.99464
F	-6.03091	-2.07831	-0.57695
F	-6.27821	-0.04430	0.10662

915.4243	936.6970	940.3309
942.0291	949.2434	950.6890
953.0938	959.3177	972.2654
1030.2675	1036.7113	1037.2606
1040.3737	1042.7684	1046.3752
1048.9400	1070.2126	1087.8874
1093.7533	1099.9845	1106.2500
1147.2365	1177.9364	1183.5330
1187.7314	1223.1982	1236.6609
1244.3253	1257.0196	1265.6059
1267.7669	1353.4587	1356.1868
1366.5134	1374.9043	1375.7418
1377.3777	1383.5683	1390.6722
1395.9216	1400.6825	1402.3328
1411.9073	1432.1871	1437.2702
1439.6164	1442.9883	1447.1847
1447.8861	1449.5252	1450.9638
1455.9947	1458.8036	1461.5768
1467.1225	1467.6552	1471.1328
1473.8206	1477.5728	1481.1270
1481.6588	1488.1083	1493.3168
1505.4097	1519.1395	1539.4164
1554.7606	1605.2929	1691.9857
1780.7247	1807.5577	2310.5384
3023.4721	3026.7680	3035.1449
3036.3928	3037.9823	3041.1950
3044.6213	3044.7342	3106.8801
3114.1123	3115.4211	3116.2654
3121.8540	3123.1917	3125.6666
3128.9465	3130.3846	3134.3654
3147.0766	3148.9299	3149.3252
3150.3476	3150.9604	3155.3641
3179.3410	3204.6472	3213.6522

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.467447 Electronic Energy = -1597.58896653
Internal Energy (E)= -1597.08796853 Enthalpy (H)= -1597.08702453
Gibbs Free Energy (G)=-1597.18635553 Gibbs Free Energy of Solvation=-1597.23341499

St.Pt.	General Structure	Ball & Stick model
TS_6-3		

Cartesian co-ordinate

Atoms	X	Y	Z
C	2.09522	-2.19054	-0.99106
C	3.05336	-1.33947	-0.35850
C	2.78190	-1.32933	1.07471
C	1.66600	-2.19211	1.31110
C	1.20489	-2.69223	0.04160
C	-1.90281	-0.21573	-0.24518
Ir	1.05918	-0.47914	-0.02342
C	-3.25093	-0.33594	-0.59212
C	-4.22116	0.16637	0.25400
C	-1.50721	0.39476	0.96730
C	-3.83904	0.80265	1.44910
C	-2.51415	0.92179	1.80686
H	-2.21512	1.40661	2.73232
H	-4.61093	1.20049	2.10313
H	0.20685	0.29456	-1.26449
O	1.86195	1.43778	0.01784
C	1.21738	2.39288	-0.59272
C	1.69695	3.79383	-0.20434
O	0.26484	2.23180	-1.34860
H	-3.51573	-0.82100	-1.53005
C	-0.84440	-0.70878	-1.11252
O	-0.97671	-1.37552	-2.11415
O	-0.25128	0.44592	1.30501
C	1.36967	4.77985	-1.31915
H	0.30397	4.75369	-1.56392

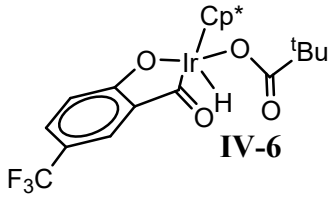
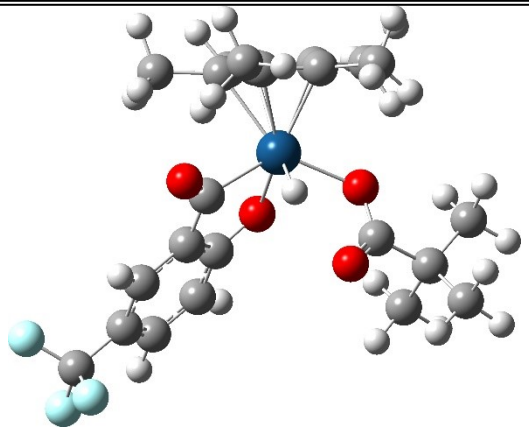
Frequencies

-195.0511	10.6465	14.6112
27.1607	34.9877	53.1214
65.1181	76.5178	77.1476
87.5935	110.7031	115.6440
120.8993	146.6302	148.4131
158.2186	161.1836	166.8782
177.2559	180.8937	189.8316
197.0023	205.9650	212.1674
217.5444	223.8392	230.0333
237.3852	257.3256	260.8204
274.9996	280.4125	286.8409
294.5304	300.3339	308.6950
321.5605	348.2791	352.5198
362.4843	369.4849	390.4781
409.9786	412.8815	416.4918
426.4210	433.1128	438.6812
469.3833	498.0813	526.7028
540.4008	540.7820	547.8665
569.1609	582.8976	590.3762
597.3367	606.5585	618.8275
633.2482	642.4565	650.9479
661.4142	735.8512	765.7049
781.7569	794.1948	810.6245
813.9954	819.0575	841.7646
855.9286	886.7420	914.1804
921.7422	936.2123	943.3117
949.2340	950.0581	950.8430
963.0356	975.8819	1031.4429
1037.1024	1039.2484	1040.9297
1042.2021	1044.1787	1047.2747

H	1.63840	5.79817	-1.00973	1086.7561	1089.8013	1091.6703
H	1.92750	4.54410	-2.23380	1106.8677	1148.9796	1182.7683
C	0.89683	4.14410	1.05689	1183.2524	1190.0171	1230.7724
H	1.09072	3.41824	1.85608	1234.8072	1243.0266	1247.2911
H	1.17437	5.14446	1.41395	1259.3676	1263.1304	1355.3935
H	-0.17941	4.13750	0.84449	1360.5436	1371.6859	1374.3951
C	3.19073	3.82123	0.10344	1375.1770	1377.7843	1380.6015
H	3.78342	3.52095	-0.77060	1394.0098	1396.5080	1400.5003
H	3.49434	4.83941	0.37981	1406.6108	1417.2885	1436.7424
H	3.44099	3.15006	0.93169	1438.0298	1441.0302	1443.8277
C	4.14876	-0.56514	-1.00052	1444.2655	1444.8780	1454.2449
H	4.10631	0.48519	-0.68672	1455.3501	1457.0649	1461.4437
H	5.12706	-0.97062	-0.71317	1465.6339	1465.8504	1466.7920
H	4.07294	-0.59093	-2.09117	1470.1598	1472.4296	1476.8299
C	2.00844	-2.53881	-2.43418	1483.0733	1486.1818	1504.6608
H	2.72399	-1.96280	-3.02744	1509.8648	1520.5612	1543.1452
H	2.22290	-3.60461	-2.58247	1557.8222	1617.0382	1676.9216
H	1.00390	-2.33298	-2.81843	1721.5053	1782.9538	1850.7478
C	0.11523	-3.68508	-0.16571	3025.9238	3029.6179	3035.2129
H	-0.33905	-3.57002	-1.15390	3037.6351	3038.5217	3040.2014
H	0.50653	-4.70728	-0.08324	3041.2718	3043.7673	3106.7000
H	-0.67922	-3.56724	0.57926	3115.2460	3115.7921	3119.9310
C	1.00151	-2.43675	2.61798	3120.8150	3121.4772	3124.2404
H	-0.08392	-2.51814	2.49627	3127.1486	3129.1143	3134.0902
H	1.36286	-3.37005	3.06748	3146.5336	3148.8402	3148.9021
H	1.19023	-1.62047	3.32113	3149.3650	3150.2365	3154.1463
C	3.56986	-0.56107	2.07676	3200.9592	3203.6373	3214.7735
H	3.05988	-0.52295	3.04368			
H	4.55817	-1.01239	2.23262			
H	3.71555	0.47166	1.74064			
C	-5.65322	0.04907	-0.14791			
F	-5.93376	0.79557	-1.22624			
F	-5.97149	-1.21360	-0.47432			
F	-6.48780	0.43215	0.82658			
H	-2.21361	-2.36558	2.19244			
C	0.25625	6.03410	-0.45916			
H	-0.42291	6.01154	-1.31860			
H	0.11414	6.98408	0.07070			
H	1.27908	6.00174	-0.84948			
C	-1.44736	4.92650	1.00708			
H	-1.65206	4.11353	1.71111			
H	-1.61538	5.88171	1.52049			
H	-2.17110	4.85704	0.18478			
C	0.96973	4.91672	1.66265			
H	2.00942	4.86508	1.31297			
H	0.84670	5.86169	2.20675			
H	0.79603	4.09098	2.36141			
C	-5.72069	-0.80581	-0.84573			
F	-6.33133	-0.47590	-1.99464			
F	-6.03091	-2.07831	-0.57695			
F	-6.27821	-0.04430	0.10662			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.463618 Electronic Energy = -1597.58328352
Internal Energy (E)= -1597.08649252 Enthalpy (H)= -1597.08554852
Gibbs Free Energy (G)=-1597.18501852 Gibbs Free Energy of Solvation=-1597.22458817

St.Pt.	General Structure	Ball & Stick model
IV-6	 **IV-6**	

Cartesian co-ordinate

Atoms	X	Y	Z
C	1.58016	-2.29411	-1.05162
C	2.73325	-1.47225	-0.73777
C	2.95571	-1.51318	0.70066
C	1.89403	-2.21491	1.27868
C	0.98494	-2.64637	0.20534
C	-1.99572	-0.07494	-0.25984
Ir	0.87903	-0.48013	-0.06196
C	-3.30014	0.09793	-0.72942
C	-4.32426	0.27809	0.18059
C	-1.70390	-0.07706	1.11643
C	-4.04265	0.27881	1.55934
C	-2.76113	0.10210	2.03343
H	-2.54018	0.10343	3.09732
H	-4.86307	0.42119	2.26091
H	1.30598	0.25168	-1.41632
O	1.25956	1.49846	0.44117
C	1.86609	2.26325	-0.41978
C	2.21471	3.64698	0.13862
O	2.19333	1.92671	-1.55765
H	-3.48421	0.08987	-1.80086
C	-0.85542	-0.29798	-1.15848
O	-0.93839	-0.43165	-2.35704
O	-0.46772	-0.25545	1.51073
C	-0.23179	-3.47552	0.43239
H	-0.87461	-3.49161	-0.45338
H	0.03319	-4.51045	0.68405
H	-0.82359	-3.06516	1.25877
C	1.15433	-2.70236	-2.41828
H	1.93433	-3.31368	-2.88791
H	0.23364	-3.29169	-2.38868
H	0.95166	-1.83199	-3.05244
C	3.70020	-0.91292	-1.72248

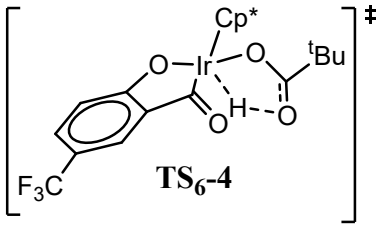
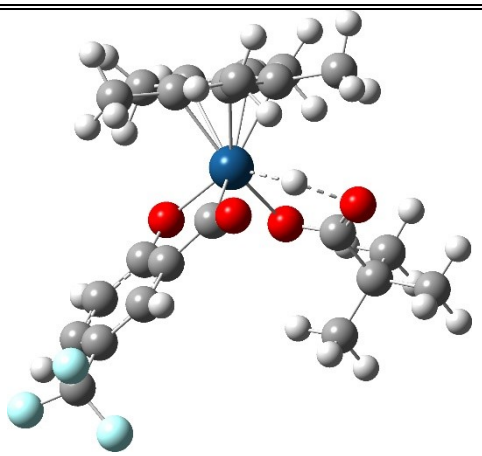
Frequencies

14.6314	31.6766	34.8710
39.4858	52.3602	60.1338
64.1955	84.0600	99.9873
118.9990	125.7998	133.4870
143.2006	148.5350	151.8984
170.1681	176.9337	182.2253
195.3676	199.0941	203.9297
207.5322	215.6634	216.3004
227.9904	234.0469	239.4770
258.9803	272.0144	279.0131
281.8991	285.7945	298.7886
302.9203	307.7356	323.1636
329.9184	347.1336	359.8949
374.0105	381.9275	390.0225
405.7690	418.8161	427.1787
434.3373	439.9666	451.5951
475.1578	526.5536	534.9754
536.5135	555.2345	568.9070
584.6279	596.9534	606.5949
615.2340	621.0455	631.6299
641.9362	651.4674	668.3013
680.0201	761.0346	772.4452
790.6528	811.1367	814.5914
818.0198	825.3814	844.6369
872.0925	910.6742	936.3063
943.9640	947.8354	951.9720
954.1029	955.1086	959.0822
963.9122	979.2669	1031.0634
1036.3963	1039.2652	1041.5690
1044.8300	1048.5812	1055.1918
1064.8171	1089.0559	1091.2510
1108.4922	1139.8208	1175.9780
1182.0067	1190.4078	1216.4751
1224.1177	1239.2002	1247.3671
1253.6192	1268.2413	1350.7827
1358.6717	1365.4708	1369.6210

H	4.59800	-1.54265	-1.77293	1374.2570	1378.0731	1389.3803
H	3.25630	-0.85795	-2.72086	1391.3091	1397.8677	1399.5456
H	3.99760	0.10521	-1.45057	1411.8275	1419.2893	1428.3580
C	4.05378	-0.77503	1.37977	1431.8128	1439.5775	1444.4802
H	5.03622	-1.12497	1.03902	1447.8247	1451.6689	1452.8850
H	3.99156	0.29810	1.15315	1454.1176	1457.1527	1460.4274
H	4.00931	-0.88736	2.46634	1460.8863	1461.5858	1464.8798
C	1.58264	-2.39277	2.71876	1470.2206	1474.0172	1477.5065
H	2.40437	-2.06270	3.35991	1480.3437	1481.5261	1488.6470
H	0.68851	-1.80473	2.97377	1505.5374	1520.0517	1551.2838
H	1.36636	-3.44354	2.94637	1586.5732	1625.7124	1676.8265
C	3.40419	3.44735	1.08410	1725.5697	1815.2556	2055.1693
H	3.73886	4.41551	1.47835	3014.7043	3024.6604	3033.6539
H	3.13106	2.80690	1.93105	3036.6625	3037.7330	3039.4066
H	4.25192	2.98987	0.55453	3039.8635	3043.7378	3101.4423
C	2.61287	4.57768	-0.99980	3102.7159	3105.4150	3115.4596
H	1.79012	4.70672	-1.71194	3120.3159	3123.6782	3125.4631
H	2.87806	5.56370	-0.59718	3127.8882	3129.7204	3140.7599
H	3.46982	4.18229	-1.55412	3143.1110	3146.6995	3147.6528
C	1.03297	4.23079	0.91005	3148.4581	3150.4305	3153.1793
H	1.30369	5.21577	1.31224	3187.3607	3206.4653	3208.8546
H	0.16138	4.36302	0.25741			
H	0.73797	3.58189	1.73985			
C	-5.73350	0.50456	-0.24800			
F	-6.15890	1.73534	0.07895			
F	-5.89673	0.36415	-1.56689			
F	-6.57457	-0.35170	0.35581			
H	-2.21361	-2.36558	2.19244			
C	0.25625	6.03410	-0.45916			
H	-0.42291	6.01154	-1.31860			
H	0.11414	6.98408	0.07070			
H	1.27908	6.00174	-0.84948			
C	-1.44736	4.92650	1.00708			
H	-1.65206	4.11353	1.71111			
H	-1.61538	5.88171	1.52049			
H	-2.17110	4.85704	0.18478			
C	0.96973	4.91672	1.66265			
H	2.00942	4.86508	1.31297			
H	0.84670	5.86169	2.20675			
H	0.79603	4.09098	2.36141			
C	-5.72069	-0.80581	-0.84573			
F	-6.33133	-0.47590	-1.99464			
F	-6.03091	-2.07831	-0.57695			
F	-6.27821	-0.04430	0.10662			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.466089 Electronic Energy = -1597.59158300
Internal Energy (E)= -1597.092429 Enthalpy (H)= -1597.091485
Gibbs Free Energy (G)=-1597.189312 Gibbs Free Energy of Solvation=-1597.23108473

St.Pt.	General Structure	Ball & Stick model
TS_6-4		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.61673	-2.14554	1.20921
C	-2.74801	-1.34146	0.81012
C	-2.97739	-1.54005	-0.61777
C	-1.93841	-2.33024	-1.11524
C	-1.03059	-2.65207	-0.00410
C	1.99375	-0.06123	0.19821
Ir	-0.88187	-0.48538	0.00482
C	3.29484	0.12445	0.66225
C	4.33423	0.22379	-0.24846
C	1.71166	-0.15807	-1.17836
C	4.06208	0.13859	-1.62372
C	2.77807	-0.05258	-2.09366
H	2.56733	-0.12378	-3.15736
H	4.88465	0.21888	-2.33006
H	-1.25866	0.50586	1.28521
O	-1.30073	1.48449	-0.61862
C	-1.72942	2.27479	0.30255
C	-2.18299	3.64925	-0.17930
O	-1.81920	1.94661	1.50064
H	3.47096	0.18377	1.73461
C	0.83984	-0.19740	1.09853
O	0.91329	-0.21196	2.30672
O	0.47614	-0.35133	-1.56564
C	0.15644	-3.54497	-0.12580
H	0.82671	-3.43596	0.73296
H	-0.14372	-4.59871	-0.19401
H	0.73533	-3.29950	-1.02343
C	-1.19430	-2.40734	2.61143
H	-1.96811	-2.98187	3.13534
H	-0.26198	-2.97750	2.64947
H	-1.01480	-1.47208	3.15243
C	-3.70861	-0.67290	1.73217
H	-4.54496	-1.34647	1.96213
H	-3.22700	-0.38652	2.67153

Frequencies

-435.9542	14.6777	20.0482
41.3032	49.5419	59.5116
62.3624	82.0262	99.7380
111.4511	127.7783	135.7341
136.9618	148.3348	158.7576
166.1125	171.7627	172.9946
191.1033	193.9484	205.4490
212.9520	213.9863	225.3015
231.0609	234.1692	236.4600
255.7899	266.5622	275.3677
279.4308	282.9801	299.3601
302.2762	311.1952	327.9747
332.3069	339.8605	351.6217
363.5229	380.0834	391.4315
413.3969	417.8398	421.6112
430.6938	434.4310	443.6972
475.7678	488.5038	527.5545
535.1671	538.0765	552.7262
581.7334	594.6148	598.4158
608.9139	618.1886	620.8708
636.9866	639.6880	652.8598
677.5633	678.1280	761.5575
774.7338	786.7302	810.3818
813.8261	834.1565	841.8180
854.3557	880.5157	934.3008
947.1559	948.8073	951.6575
952.8920	958.8537	962.4214
964.2102	965.3188	1032.3479
1040.1445	1043.0705	1044.5967
1047.1362	1053.3580	1056.7211
1086.9572	1089.4763	1099.9116
1107.3351	1141.6435	1175.8740
1181.4747	1188.6276	1230.0593
1240.9140	1252.7208	1253.2990
1267.5553	1268.0486	1353.5352
1368.9541	1372.3088	1377.1143
1378.6814	1381.1960	1389.2726
1399.4660	1399.8276	1403.6095

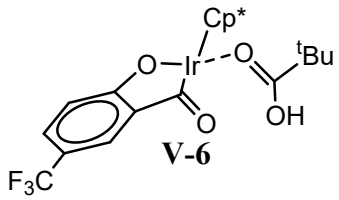
H	-4.12245	0.23962	1.28924	1406.1038	1424.9094	1429.0979
C	-4.06161	-0.85817	-1.37464	1438.6057	1440.1026	1448.7044
H	-5.05134	-1.16731	-1.01536	1448.7982	1452.9119	1455.7128
H	-3.99259	0.23134	-1.24970	1456.3516	1457.5674	1458.9009
H	-4.00669	-1.07114	-2.44567	1465.1586	1466.6805	1468.8702
C	-1.64473	-2.67790	-2.52914	1472.1672	1472.4256	1473.2303
H	-2.45526	-2.38014	-3.19990	1482.6620	1485.8485	1502.1762
H	-0.72842	-2.16501	-2.85290	1503.8681	1513.7236	1552.6074
H	-1.48238	-3.75649	-2.64339	1577.5795	1586.9946	1625.3807
C	-3.43005	3.42645	-1.04254	1674.9136	1762.1931	1817.6123
H	-3.81859	4.39096	-1.39288	3017.3748	3030.9941	3033.7669
H	-3.19944	2.80801	-1.91720	3034.8499	3037.0185	3038.4439
H	-4.22633	2.93528	-0.46556	3041.2204	3045.0488	3096.9577
C	-2.52489	4.54203	1.00619	3103.5316	3110.3523	3116.2241
H	-1.65359	4.69573	1.65195	3118.3719	3120.2201	3128.8299
H	-2.86422	5.52086	0.64450	3129.7751	3130.5928	3140.0008
H	-3.31822	4.10304	1.62023	3142.7521	3145.8639	3146.3483
C	-1.07777	4.28610	-1.02201	3150.2930	3152.8129	3156.2988
H	-1.41436	5.26304	-1.39184	3198.4274	3201.9007	3212.3225
H	-0.16987	4.44662	-0.42808			
H	-0.81746	3.65796	-1.87924			
C	5.71735	0.47953	0.24823			
F	5.89993	1.76425	0.59235			
F	5.99342	-0.24650	1.34122			
F	6.64743	0.18924	-0.67180			
H	-2.21361	-2.36558	2.19244			
C	0.25625	6.03410	-0.45916			
H	-0.42291	6.01154	-1.31860			
H	0.11414	6.98408	0.07070			
H	1.27908	6.00174	-0.84948			
C	-1.44736	4.92650	1.00708			
H	-1.65206	4.11353	1.71111			
H	-1.61538	5.88171	1.52049			
H	-2.17110	4.85704	0.18478			
C	0.96973	4.91672	1.66265			
H	2.00942	4.86508	1.31297			
H	0.84670	5.86169	2.20675			
H	0.79603	4.09098	2.36141			
C	-5.72069	-0.80581	-0.84573			
F	-6.33133	-0.47590	-1.99464			
F	-6.03091	-2.07831	-0.57695			
F	-6.27821	-0.04430	0.10662			

Statistical Thermodynamic Analysis

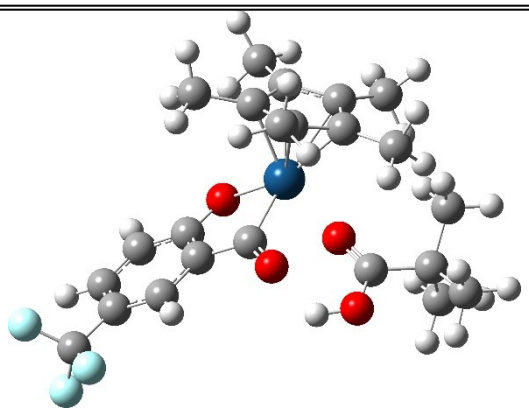
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.464569 Electronic Energy = -1597.59035475
Internal Energy (E)= -1597.09332975 Enthalpy (H)= -1597.09238675
Gibbs Free Energy (G)=-1597.18849975 Gibbs Free Energy of Solvation=-1597.2286858

St.Pt.	General Structure	Ball & Stick model

V-6



V-6



Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.39551	-2.00431	1.46153
C	-2.56609	-1.27550	1.06943
C	-2.93379	-1.70176	-0.28894
C	-1.94897	-2.57059	-0.76049
C	-0.91858	-2.70257	0.28219
C	1.95733	0.08462	0.12008
Ir	-0.83988	-0.61957	-0.09523
C	3.22080	0.41673	0.61584
C	4.32014	0.32797	-0.21628
C	1.76952	-0.30792	-1.22847
C	4.14750	-0.06735	-1.55916
C	2.90625	-0.37281	-2.06954
H	2.77363	-0.66658	-3.10764
H	5.02339	-0.12472	-2.20443
H	-0.74277	1.68725	1.65105
O	-1.46928	1.42005	-0.65972
C	-1.74533	2.34402	0.11780
C	-2.51205	3.55311	-0.38684
O	-1.39072	2.40328	1.37035
H	3.31604	0.73482	1.65135
C	0.71377	0.19569	0.87347
O	0.62290	0.77793	1.96537
O	0.56969	-0.57464	-1.65768
C	0.25894	-3.61150	0.19226
H	1.04555	-3.30805	0.89136
H	-0.01316	-4.65262	0.41110
H	0.69208	-3.57755	-0.81360
C	-0.77921	-2.00110	2.81582
H	-1.34168	-2.65063	3.49816
H	0.25510	-2.35786	2.78260
H	-0.75425	-0.98899	3.23415
C	-3.42611	-0.44750	1.96207
H	-4.21816	-1.05235	2.42482
H	-2.83939	0.00827	2.76693
H	-3.91927	0.36157	1.40830
C	-4.10341	-1.15343	-1.02858
H	-5.04593	-1.41722	-0.53112
H	-4.05565	-0.05719	-1.07967
H	-4.14667	-1.52746	-2.05563
C	-1.79983	-3.14617	-2.12430

Frequencies

17.4937	25.0226	33.1340
46.2148	58.5538	60.7370
78.8565	90.0113	111.7833
119.2645	129.7991	134.9453
149.5168	155.5280	161.1254
166.1308	170.5425	175.4267
183.1003	188.9481	200.0207
207.5620	210.8309	215.2396
223.4827	228.1728	251.5522
271.6627	273.4730	280.7607
287.1859	288.0571	307.7514
313.1587	314.1452	333.5987
343.1207	355.4342	372.9800
392.3980	398.4816	403.7072
407.5153	413.3467	419.1212
426.0504	432.1564	460.2589
489.3518	525.3949	533.0880
536.2906	547.5630	555.8968
582.7852	594.2416	605.4529
609.7499	615.1870	625.0617
633.8758	646.4839	683.2582
697.0656	765.9124	776.5779
782.7884	788.8060	803.5921
810.4217	840.5298	876.5341
896.1359	931.3610	948.5935
954.1270	954.9426	956.8779
959.5073	959.6666	961.2039
975.6132	1035.7198	1039.5994
1040.2787	1041.7868	1047.8482
1050.3632	1051.6974	1081.6285
1088.1656	1089.6737	1105.4143
1142.7494	1177.8914	1183.0014
1188.5858	1219.4717	1236.8851
1237.2281	1250.0325	1251.9425
1269.0607	1327.3227	1356.9406
1368.6732	1373.3119	1375.9249
1379.2994	1387.5457	1391.8216
1400.1630	1403.0080	1413.0994
1418.2422	1428.2663	1432.2516
1441.4937	1451.0199	1451.6739
1452.0255	1453.5551	1460.5360
1461.2751	1463.0992	1464.6183
1467.3201	1467.8821	1469.8161
1473.0012	1477.0661	1480.1980
1487.2834	1496.6072	1507.0305

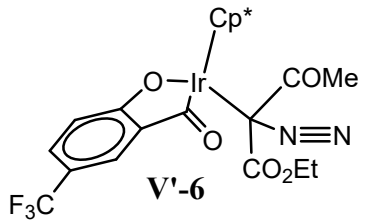
H	-2.63030	-2.86456	-2.77836	1515.8944	1531.4166	1557.2597
H	-0.87170	-2.78334	-2.58501	1593.2744	1610.4530	1660.8271
H	-1.75089	-4.24181	-2.08865	1680.7894	1741.4895	3020.2660
C	-3.53784	3.10965	-1.42736	3025.9838	3032.8080	3034.5579
H	-4.05037	3.98881	-1.83541	3035.4870	3035.7427	3042.2375
H	-3.06474	2.56787	-2.25185	3042.7533	3091.3354	3096.8477
H	-4.30016	2.45781	-0.97926	3106.0685	3110.1606	3115.1714
C	-3.20437	4.29236	0.75387	3118.7478	3126.1429	3126.7292
H	-2.48703	4.66751	1.48951	3128.1987	3134.6440	3138.0860
H	-3.75911	5.14540	0.34506	3141.6121	3141.8601	3145.7114
H	-3.91679	3.64341	1.27751	3145.9582	3147.9915	3151.1844
C	-1.46412	4.46512	-1.04186	3174.0073	3206.9306	3211.7767
H	-1.95703	5.36325	-1.43330			
H	-0.70661	4.78141	-0.31475			
H	-0.96020	3.95663	-1.87155			
C	5.69631	0.63955	0.25736			
F	6.25809	1.63175	-0.45404			
F	5.72466	1.00791	1.54279			
F	6.51769	-0.41710	0.12734			
H	-2.21361	-2.36558	2.19244			
C	0.25625	6.03410	-0.45916			
H	-0.42291	6.01154	-1.31860			
H	0.11414	6.98408	0.07070			
H	1.27908	6.00174	-0.84948			
C	-1.44736	4.92650	1.00708			
H	-1.65206	4.11353	1.71111			
H	-1.61538	5.88171	1.52049			
H	-2.17110	4.85704	0.18478			
C	0.96973	4.91672	1.66265			
H	2.00942	4.86508	1.31297			
H	0.84670	5.86169	2.20675			
H	0.79603	4.09098	2.36141			
C	-5.72069	-0.80581	-0.84573			
F	-6.33133	-0.47590	-1.99464			
F	-6.03091	-2.07831	-0.57695			
F	-6.27821	-0.04430	0.10662			

Statistical Thermodynamic Analysis

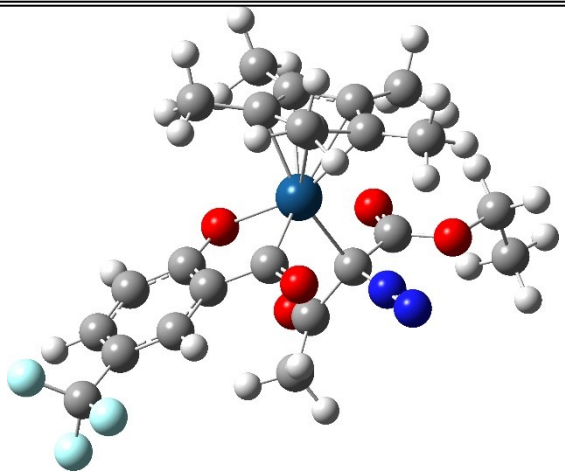
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.470082 Electronic Energy = -1597.62536139
Internal Energy (E)= -1597.12245939 Enthalpy (H)= -1597.12151539
Gibbs Free Energy (G)=-1597.21853739 Gibbs Free Energy of Solvation=-1597.25596165

St.Pt.	General Structure	Ball & Stick model

V'-6



V'-6



Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.01467	-2.55930	0.91470
C	-2.22396	-1.79169	1.01687
C	-2.80470	-1.68755	-0.32664
C	-1.89294	-2.22366	-1.24027
C	-0.73215	-2.71758	-0.49097
C	2.17337	-0.07055	0.19485
Ir	-0.67245	-0.61199	-0.03261
C	1.87231	0.07569	-1.17877
C	2.92799	0.39094	-2.06768
C	3.47255	0.09572	0.67981
C	4.20570	0.54018	-1.57668
C	4.49252	0.39398	-0.20379
H	3.65534	-0.00505	1.74746
H	5.01948	0.78333	-2.25863
H	2.70244	0.51955	-3.12302
C	-1.24545	1.54484	0.15819
C	-2.64204	1.74419	-0.37437
C	-0.18230	2.46718	-0.47952
O	-0.33712	2.84095	-1.61065
N	-1.21882	1.59734	1.54317
N	-1.13946	1.61456	2.66417
C	-4.13725	-1.10638	-0.64551
H	-4.10540	-0.47291	-1.53925
H	-4.87087	-1.90415	-0.81888
H	-4.51353	-0.49839	0.18457
C	-2.88179	-1.42121	2.30234
H	-3.54691	-0.55707	2.18718
H	-3.48124	-2.24875	2.70548
H	-2.12872	-1.15833	3.05595
C	-0.21677	-3.06639	2.06272
H	-0.06681	-2.28161	2.81252
H	-0.72684	-3.91538	2.53561
H	0.77581	-3.40084	1.74432
C	0.41842	-3.44078	-1.10110
H	1.29325	-3.42141	-0.44260
H	0.16852	-4.48916	-1.31127
H	0.71168	-2.96769	-2.04476
C	-1.99389	-2.23055	-2.72461

Frequencies

11.6492	23.7155	30.7039
39.8741	53.4127	64.0172
76.9494	83.5310	97.3059
102.2411	113.4420	120.6413
124.0375	130.5804	137.4767
142.1416	151.2847	155.4291
159.4544	166.7812	178.6690
180.7137	192.5906	198.3752
204.6784	212.6159	214.0116
218.9818	242.5162	247.9529
258.0981	260.4303	262.9778
268.4802	276.3932	286.1443
295.6407	300.3338	321.3231
339.3163	345.5903	357.3002
376.0420	381.0932	400.0021
403.9596	410.7391	417.9455
423.4440	440.8880	449.7597
461.6944	482.3865	500.4228
506.0454	525.4918	534.1588
538.4121	539.0552	547.3480
583.8505	592.4124	594.6830
601.2117	609.4983	611.7956
621.7203	632.3586	646.2295
679.4769	690.5831	763.3939
766.5010	776.0365	782.3546
801.8423	815.5721	827.3733
837.7115	868.6554	879.9055
929.9521	951.0537	953.4578
955.1060	957.2180	962.4552
991.2192	1022.7201	1034.3565
1045.8826	1048.5181	1052.0451
1060.3952	1062.4311	1065.6160
1087.5027	1089.9613	1094.6938
1107.0780	1122.5312	1134.3950
1172.9146	1177.8886	1182.8580
1185.6214	1196.6656	1217.0532
1219.4206	1248.7421	1261.5901
1329.0213	1352.2849	1373.6899
1374.7577	1376.1944	1377.9075
1387.6713	1396.1033	1399.9405
1402.3459	1417.0295	1417.3257
1431.8926	1434.8544	1441.2965
1447.4252	1447.5386	1455.3663

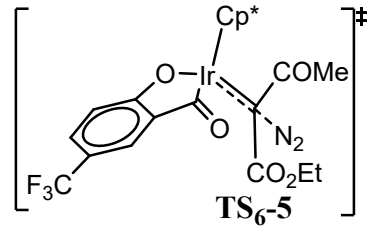
H	-2.14648	-3.24721	-3.11104	1455.7907	1464.8733	1465.7692
H	-2.82172	-1.60494	-3.07201	1469.0931	1469.6394	1473.0830
H	-1.07458	-1.83826	-3.17584	1473.5237	1476.5818	1484.6901
C	1.00441	-0.28674	1.05585	1496.4688	1507.0790	1513.4001
O	0.63894	-0.03660	-1.58247	1533.6159	1540.3843	1555.1290
O	1.04164	-0.25648	2.27938	1583.6706	1611.4185	1676.2657
O	-2.92915	1.68216	-1.53920	1745.6775	1855.0281	1897.8629
C	-4.86301	2.30363	0.22322	2265.9620	3031.6022	3032.6240
H	-5.46803	2.04783	1.09876	3033.6938	3036.3112	3037.7374
H	-5.14286	1.64788	-0.60815	3050.9803	3051.2896	3073.2948
O	-3.50961	2.00148	0.62206	3107.1582	3109.5493	3112.4090
C	-4.99031	3.75749	-0.15510	3115.9835	3122.4314	3130.0342
H	-4.37535	3.97804	-1.03302	3131.8227	3136.8016	3138.3137
H	-6.03092	3.99339	-0.40013	3142.4242	3143.8219	3144.3229
H	-4.67706	4.40493	0.67011	3146.5276	3156.6798	3180.7783
C	0.98206	2.90430	0.36834	3181.9514	3199.3145	3209.4804
H	1.86506	2.96361	-0.27492			
H	0.76690	3.91541	0.73701			
H	1.20462	2.26049	1.22191			
C	5.90100	0.57225	0.24349			
F	6.04350	0.42459	1.56526			
F	6.72639	-0.30850	-0.34755			
F	6.37329	1.79022	-0.07473			
H	-0.42291	6.01154	-1.31860			
H	0.11414	6.98408	0.07070			
H	1.27908	6.00174	-0.84948			
C	-1.44736	4.92650	1.00708			
H	-1.65206	4.11353	1.71111			
H	-1.61538	5.88171	1.52049			
H	-2.17110	4.85704	0.18478			
C	0.96973	4.91672	1.66265			
H	2.00942	4.86508	1.31297			
H	0.84670	5.86169	2.20675			
H	0.79603	4.09098	2.36141			
C	-5.72069	-0.80581	-0.84573			
F	-6.33133	-0.47590	-1.99464			
F	-6.03091	-2.07831	-0.57695			
F	-6.27821	-0.04430	0.10662			

Statistical Thermodynamic Analysis

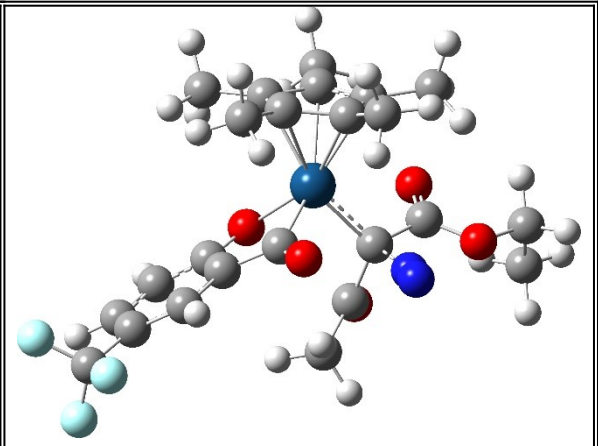
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.466560 Electronic Energy = -1819.05313672
Internal Energy (E)= -1818.55033272 Enthalpy (H)= -1818.54938972
Gibbs Free Energy (G)=-1818.65405072 Gibbs Free Energy of Solvation=-1818.69655104

St.Pt.	General Structure	Ball & Stick model

TS_6-5



TS_6-5



Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.34916	-2.76520	0.46881
C	-1.50418	-2.22997	1.14737
C	-2.50734	-1.93655	0.13508
C	-1.95398	-2.19566	-1.14482
C	-0.59381	-2.65996	-0.93481
C	2.14159	0.14817	0.19158
Ir	-0.65097	-0.58630	-0.05906
C	1.82618	0.34007	-1.17405
C	2.87359	0.68137	-2.06207
C	3.44639	0.29209	0.66770
C	4.15873	0.80195	-1.58101
C	4.45941	0.60791	-0.21837
H	3.64254	0.15246	1.72852
H	4.96827	1.05817	-2.26307
H	2.63859	0.84444	-3.11064
C	-1.49857	1.26076	0.19175
C	-2.95847	1.41869	-0.18645
C	-0.74737	2.47212	-0.39474
O	-1.20167	2.98250	-1.39248
N	-1.45885	1.50289	1.81151
N	-1.13396	1.30399	2.86366
C	-3.90420	-1.52083	0.44402
H	-4.39801	-1.07285	-0.42240
H	-4.49100	-2.39134	0.76458
H	-3.93588	-0.79293	1.26563
C	-1.68352	-2.17572	2.62598
H	-2.60374	-1.64621	2.89702
H	-1.74250	-3.18151	3.06222
H	-0.84357	-1.64723	3.09608
C	0.86766	-3.30513	1.13677
H	1.08280	-2.76602	2.06544
H	0.72903	-4.36503	1.38686
H	1.75240	-3.22519	0.49614
C	0.34851	-3.00920	-2.03303
H	1.37194	-3.12796	-1.66318
H	0.05133	-3.94688	-2.51990
H	0.36101	-2.22100	-2.79425
C	-2.59636	-2.03521	-2.47839
H	-2.91857	-3.00247	-2.88807

Frequencies

-401.3552	12.3408	22.6010
31.5078	36.5179	56.0319
65.1344	71.0231	79.0713
97.8888	107.6413	109.8383
117.3816	129.0144	137.3636
144.7806	149.2977	155.9018
161.9835	168.1824	169.5793
180.2272	186.2721	189.9393
197.1630	205.8488	210.3201
218.8607	228.9811	229.4753
240.7563	249.0351	259.2035
264.0868	275.0884	276.1379
279.7047	287.8382	300.0564
312.1211	321.3890	330.5860
350.4828	357.1482	358.9146
362.1003	401.2004	404.4262
407.8795	417.1671	422.1428
434.5599	440.3244	454.9329
482.0055	518.3167	526.0054
534.3797	537.1180	544.3727
546.4798	582.1309	591.6974
596.1736	603.0299	612.4765
627.3834	633.0550	644.3779
677.1673	688.3479	701.8321
756.2492	766.5498	776.0169
808.0173	811.2414	815.9377
839.1190	866.4627	888.9329
899.5255	926.7642	945.3678
950.5980	955.2268	956.5899
959.7508	1016.3976	1029.2053
1035.1416	1039.1319	1044.2408
1047.7559	1048.2738	1064.1948
1082.1779	1084.9391	1086.3007
1105.9447	1123.3375	1131.9529
1174.5304	1178.6463	1185.9993
1189.8553	1200.2739	1215.4387
1220.3276	1250.0223	1282.3084
1319.9225	1349.4545	1372.0588
1377.7075	1381.4609	1383.4630
1386.4395	1390.1521	1396.1681
1401.5674	1413.3555	1414.1175
1440.5468	1443.4935	1444.9745
1445.5486	1452.9792	1455.4451
1457.2221	1459.3388	1460.5994

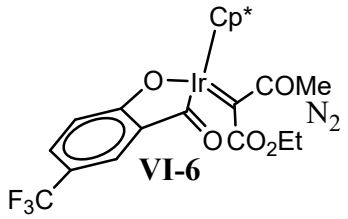
H	-3.46482	-1.37355	-2.42805	1464.0554	1468.4444	1468.6886
H	-1.89562	-1.58781	-3.19273	1474.3189	1477.9201	1480.0659
C	0.98076	-0.11450	1.05090	1485.3748	1493.3407	1496.8851
O	0.58787	0.24258	-1.57178	1514.3798	1519.7365	1550.8914
O	1.01755	-0.11034	2.27474	1552.4648	1610.2474	1674.3494
O	-3.39319	1.01082	-1.23235	1734.9390	1833.1902	1872.9194
C	-5.01405	2.43816	0.33758	2258.1524	3028.5799	3030.4653
H	-5.53255	2.61637	1.28388	3032.7252	3035.8755	3041.0574
H	-5.46450	1.57232	-0.16104	3053.6685	3058.8001	3074.0227
O	-3.66484	2.09962	0.72373	3102.7590	3104.2303	3111.0804
C	-5.00728	3.65597	-0.55229	3115.3918	3120.4893	3131.8611
H	-4.45461	3.45304	-1.47495	3134.6103	3138.0477	3141.0943
H	-6.03164	3.93749	-0.81700	3146.4000	3147.0610	3151.2391
H	-4.53708	4.50351	-0.04347	3157.8514	3160.0803	3183.1432
C	0.50382	2.98733	0.25729	3183.6603	3199.5513	3207.9245
H	1.30492	2.96905	-0.49005			
H	0.33337	4.03542	0.52598			
H	0.83643	2.43397	1.13723			
C	5.87838	0.73683	0.21345			
F	6.02744	0.59891	1.53528			
F	6.66161	-0.18401	-0.37401			
F	6.39422	1.93030	-0.12610			
H	-0.42291	6.01154	-1.31860			
H	0.11414	6.98408	0.07070			
H	1.27908	6.00174	-0.84948			
C	-1.44736	4.92650	1.00708			
H	-1.65206	4.11353	1.71111			
H	-1.61538	5.88171	1.52049			
H	-2.17110	4.85704	0.18478			
C	0.96973	4.91672	1.66265			
H	2.00942	4.86508	1.31297			
H	0.84670	5.86169	2.20675			
H	0.79603	4.09098	2.36141			
C	-5.72069	-0.80581	-0.84573			
F	-6.33133	-0.47590	-1.99464			
F	-6.03091	-2.07831	-0.57695			
F	-6.27821	-0.04430	0.10662			

Statistical Thermodynamic Analysis

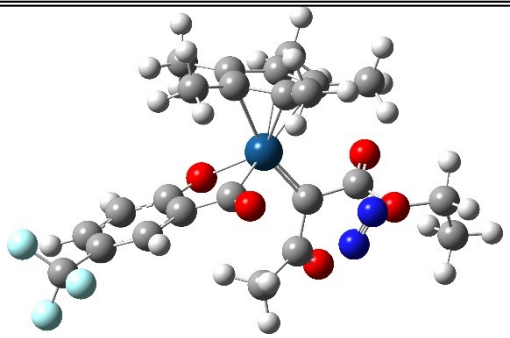
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.463722 Electronic Energy = -1819.04535893
Internal Energy (E)= -1818.54529093 Enthalpy (H)= -1818.54434693
Gibbs Free Energy (G)=-1818.64918993 Gibbs Free Energy of Solvation=-1818.68615892

St.Pt.	General Structure	Ball & Stick model

VI-6



VI-6



Cartesian co-ordinate

Atoms	X	Y	Z
C	0.06175	2.56701	0.78140
C	1.17413	1.96161	1.47545
C	2.29094	1.90400	0.55814
C	1.85970	2.45472	-0.69817
C	0.48639	2.84647	-0.55192
C	-2.14789	-0.30138	0.11772
Ir	0.63592	0.52964	-0.15112
C	-1.95473	-0.01024	-1.24602
C	-3.07453	-0.02072	-2.10610
C	-3.41221	-0.60948	0.62645
C	-4.31832	-0.31588	-1.59132
C	-4.49946	-0.61108	-0.22619
H	-3.51979	-0.83693	1.68412
H	-5.18516	-0.32561	-2.25037
H	-2.92887	0.19595	-3.16097
C	1.56271	-1.08552	-0.52403
C	3.05910	-1.11224	-0.56569
C	1.05435	-2.39121	-1.07515
O	1.77782	-2.97302	-1.86781
N	1.44100	-2.34679	2.62201
N	2.01193	-1.61080	3.21610
C	3.68840	1.55693	0.94069
H	4.30264	1.34078	0.06269
H	4.14408	2.39371	1.48550
H	3.71949	0.67896	1.59767
C	1.22087	1.64796	2.92992
H	2.14759	1.12907	3.19356
H	1.17138	2.57407	3.51730
H	0.38674	1.00309	3.22721
C	-1.26114	2.89079	1.38957
H	-1.47435	2.23320	2.23880
H	-1.28027	3.92546	1.75537
H	-2.08118	2.77319	0.67265
C	-0.36242	3.37839	-1.65296
H	-1.39683	3.52552	-1.32789
H	0.02052	4.34072	-2.01357
H	-0.37909	2.67866	-2.49779
C	2.68894	2.61480	-1.92414
H	3.28385	3.53715	-1.87764
H	3.37073	1.76696	-2.04966
H	2.05842	2.67086	-2.81730
C	-0.93513	-0.26601	0.94552
O	-0.74908	0.23894	-1.68899

Frequencies

16.6864	24.4304	29.5111
35.7536	40.4433	57.1725
62.4024	73.6988	77.4030
82.3299	88.9914	101.4969
107.7581	115.0053	116.6867
128.4376	129.6220	139.8126
143.7462	146.5733	151.6499
157.6301	167.5847	171.8482
177.3608	186.1228	192.3347
199.8066	203.4939	211.3232
222.4882	227.0614	237.7682
259.1588	269.9895	277.9990
290.3199	295.0989	303.6396
319.5268	320.3473	327.2617
327.9652	353.0962	360.1505
363.7345	368.4808	402.6701
403.9713	411.5674	418.6585
424.1890	435.4128	455.7256
477.7128	499.2579	526.9117
532.7064	540.9338	559.7183
572.0986	583.5670	588.0392
600.6308	603.9488	607.0660
632.0421	649.5129	665.0098
678.1758	683.7721	742.3019
757.0687	759.8734	773.9998
807.6873	818.1385	821.3018
842.5813	867.2251	885.6999
929.3654	943.4122	957.3323
962.2387	965.4191	978.7449
1010.1164	1016.3613	1031.5068
1037.3553	1041.0928	1042.5269
1046.5446	1047.8731	1083.0238
1090.2987	1097.6648	1114.0968
1115.2765	1125.4726	1138.1594
1176.1866	1180.0312	1188.6378
1192.3473	1226.7199	1234.7781
1249.8888	1257.2957	1290.9285
1318.7520	1349.9637	1367.3752
1377.2375	1379.4228	1382.2789
1385.5472	1392.3955	1397.0301
1401.9619	1415.2836	1415.7913
1434.5330	1436.2929	1441.9278
1447.7230	1449.0730	1451.0780
1458.7189	1464.8383	1467.8458
1469.1280	1472.8796	1473.4908
1475.2404	1480.2589	1483.3729
1489.4585	1494.7010	1501.8538

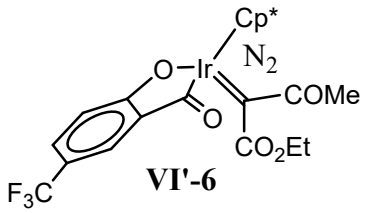
O	-0.89715	-0.54823	2.12169	1516.5636	1520.2449	1535.6362
O	3.73287	-0.48003	-1.34945	1549.3611	1619.5449	1674.2093
C	4.97121	-2.17911	0.31873	1785.0280	1805.7228	1825.3689
H	5.22996	-2.50589	1.33024	2467.8475	3030.1681	3038.1994
H	5.49404	-1.24007	0.10263	3039.9736	3041.1027	3042.2704
O	3.55398	-1.92587	0.37314	3055.4145	3062.0943	3069.1956
C	5.26683	-3.23533	-0.71682	3114.1289	3116.8593	3117.5397
H	5.00956	-2.87338	-1.71657	3119.2318	3128.1595	3130.6799
H	6.33017	-3.49645	-0.70340	3139.5221	3146.4299	3146.7330
H	4.68150	-4.13872	-0.51814	3146.9851	3152.0308	3157.4323
C	-0.27439	-2.94396	-0.66830	3159.1918	3162.7463	3173.3239
H	-1.07755	-2.40145	-1.18026	3183.0780	3210.0606	3215.9369
H	-0.31782	-3.99523	-0.96158			
H	-0.44558	-2.84162	0.40875			
C	-5.87956	-0.89851	0.25989			
F	-5.90723	-1.20836	1.55961			
F	-6.69275	0.15546	0.08174			
F	-6.43794	-1.91792	-0.41029			
H	-0.42291	6.01154	-1.31860			
H	0.11414	6.98408	0.07070			
H	1.27908	6.00174	-0.84948			
C	-1.44736	4.92650	1.00708			
H	-1.65206	4.11353	1.71111			
H	-1.61538	5.88171	1.52049			
H	-2.17110	4.85704	0.18478			
C	0.96973	4.91672	1.66265			
H	2.00942	4.86508	1.31297			
H	0.84670	5.86169	2.20675			
H	0.79603	4.09098	2.36141			
C	-5.72069	-0.80581	-0.84573			
F	-6.33133	-0.47590	-1.99464			
F	-6.03091	-2.07831	-0.57695			
F	-6.27821	-0.04430	0.10662			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.464369 Electronic Energy = -1819.09482122
Internal Energy (E)= -1818.59254922 Enthalpy (H)= -1818.59160522
Gibbs Free Energy (G)=-1818.70114922 Gibbs Free Energy of Solvation=-1818.73395724

St.Pt.	General Structure	Ball & Stick model

VI'-6



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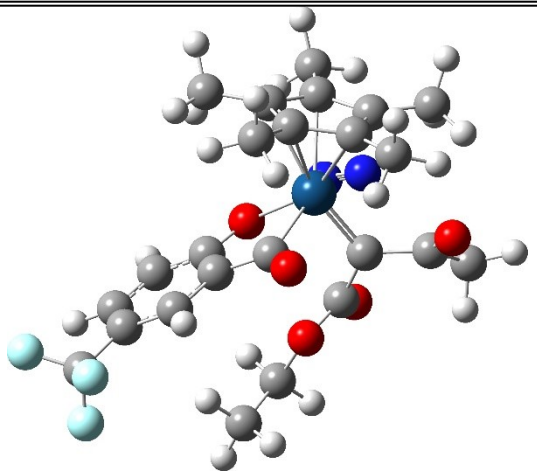


Cartesian co-ordinate

Atoms	X	Y	Z
C	1.40712	-2.62303	-0.29919
C	2.42563	-1.87157	-1.01024
C	3.20808	-1.17260	-0.02574
C	2.62185	-1.43275	1.27143
C	1.52354	-2.34062	1.08666
C	-1.79053	-0.45803	-0.20149
Ir	1.13130	-0.32261	-0.02255
C	-1.49607	0.09363	1.06241
C	-2.56718	0.36306	1.94467
C	-3.10388	-0.71755	-0.59834
C	-3.85835	0.09389	1.54670
C	-4.13867	-0.44974	0.27780
H	-3.28958	-1.11614	-1.59291
H	-4.68722	0.30324	2.22095
H	-2.34675	0.78918	2.92007
C	1.28138	1.43723	-0.72544
C	2.43972	1.87234	-1.56150
C	0.34086	2.51274	-0.29802
C	-1.87095	3.28412	-0.24696
H	-1.94110	3.15290	0.84167
H	-1.49851	4.29869	-0.43170
C	-3.17949	3.01549	-0.94019
H	-3.92287	3.75466	-0.62460
H	-3.06487	3.08824	-2.02652
H	-3.57026	2.02042	-0.69907
O	-0.90160	2.34084	-0.74432
O	0.69803	3.44209	0.39648
C	4.45989	-0.40240	-0.25780
H	4.50656	0.48318	0.38714
H	5.33370	-1.02771	-0.03438
H	4.53730	-0.06680	-1.29436
C	2.68214	-1.98840	-2.47202
H	3.37828	-1.22388	-2.82115
H	3.08636	-2.98092	-2.71198
H	1.75123	-1.85131	-3.03260
C	0.46780	-3.58215	-0.93934
H	0.22132	-3.27342	-1.95894
H	0.93089	-4.57634	-0.98866

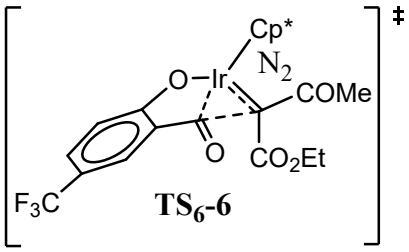
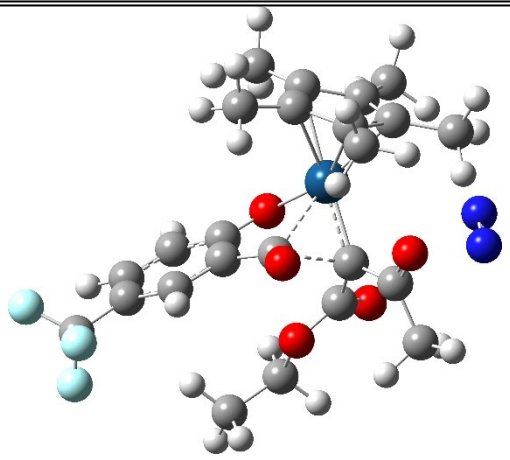
Frequencies

21.3653	31.3284	36.8741
46.1835	57.9625	61.4823
74.6897	80.9821	90.1822
100.2411	110.3043	115.8376
123.8266	129.4513	134.3186
141.7205	145.3998	155.8830
160.0170	160.5971	167.0120
174.4485	183.3273	194.8679
203.6092	206.9618	212.3609
221.4411	225.4261	231.3604
240.3303	247.1205	253.6345
267.4065	269.0407	279.9081
282.8516	285.7935	286.0955
305.9770	308.3807	320.7977
327.1819	334.4933	338.7349
364.4047	365.3233	377.3105
403.3267	409.2539	409.7047
419.4365	427.2558	434.1373
473.7055	518.7972	525.8301
532.2496	544.2832	551.3893
576.4813	581.9032	588.7494
595.1647	602.2876	610.3315
632.5047	649.5534	655.4652
664.6420	671.9454	747.4994
761.3115	772.7020	803.0187
811.5644	813.5795	818.3514
842.1054	868.0027	888.9622
932.2475	935.2587	943.7623
959.0731	961.2251	964.6532
1011.8570	1019.1253	1035.8346
1039.8894	1041.3378	1043.4652
1053.0319	1068.7998	1088.4354
1090.9217	1092.4774	1105.7952
1111.0151	1139.5770	1146.6070
1167.2957	1179.9650	1183.0179
1188.0046	1222.1991	1241.9408
1249.5414	1257.5321	1289.3077
1311.6023	1357.3225	1372.1830
1376.2974	1379.0112	1381.8069
1384.6149	1394.8155	1400.0384
1404.1331	1419.8169	1421.9534
1432.2162	1437.6900	1443.3663
1446.9251	1455.5448	1458.9914

H	-0.47084	-3.67580	-0.38246	1459.5083	1460.7916	1462.5825
C	0.62490	-2.81186	2.17705	1463.5256	1465.6147	1471.4276
H	-0.26913	-3.30013	1.77675	1475.1932	1481.5722	1488.4958
H	1.13655	-3.52754	2.83301	1493.0070	1494.8066	1497.2839
H	0.29177	-1.96796	2.79360	1503.6861	1521.3937	1548.1874
C	3.12181	-0.97136	2.59616	1553.5123	1619.8024	1675.5453
H	3.58228	-1.80141	3.14868	1781.8037	1814.1782	1832.2402
H	3.87290	-0.18239	2.49246	2464.1710	3032.4604	3038.1431
H	2.30553	-0.57355	3.21136	3040.5738	3042.3875	3042.4813
C	-0.64635	-0.65860	-1.09246	3047.7788	3057.1120	3059.5856
O	-0.26090	0.36518	1.38606	3101.1591	3105.5942	3116.0586
O	-0.69150	-1.03095	-2.23671	3119.2832	3122.6083	3133.7861
N	2.76101	2.22611	2.25689	3142.9868	3143.3012	3146.6634
N	2.09310	2.43454	3.11222	3151.3076	3157.0043	3161.8804
C	3.09977	3.18848	-1.24983	3175.6331	3180.7145	3184.3696
H	3.31853	3.28072	-0.18078	3184.6122	3206.9880	3211.1094
H	4.01180	3.26660	-1.84632			
H	2.42872	4.02107	-1.48858			
O	2.84975	1.15936	-2.46320			
C	-5.56357	-0.61876	-0.12005			
F	-6.15757	0.57307	-0.30899			
F	-5.70013	-1.31356	-1.25341			
F	-6.27658	-1.24601	0.82790			
H	-0.42291	6.01154	-1.31860			
H	0.11414	6.98408	0.07070			
H	1.27908	6.00174	-0.84948			
C	-1.44736	4.92650	1.00708			
H	-1.65206	4.11353	1.71111			
H	-1.61538	5.88171	1.52049			
H	-2.17110	4.85704	0.18478			
C	0.96973	4.91672	1.66265			
H	2.00942	4.86508	1.31297			
H	0.84670	5.86169	2.20675			
H	0.79603	4.09098	2.36141			
C	-5.72069	-0.80581	-0.84573			
F	-6.33133	-0.47590	-1.99464			
F	-6.03091	-2.07831	-0.57695			
F	-6.27821	-0.04430	0.10662			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.465282 Electronic Energy = -1819.10213724
Internal Energy (E)= -1818.59966824 Enthalpy (H)= -1818.59872424
Gibbs Free Energy (G)=-1818.70435924 Gibbs Free Energy of Solvation=-1818.73839944

St.Pt.	General Structure	Ball & Stick model
TS_6-6		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.60846	-2.53029	0.43071
C	-2.42745	-1.62681	1.23800
C	-3.31498	-0.93748	0.36031
C	-3.00920	-1.37793	-0.99716
C	-2.00471	-2.40930	-0.92451
C	1.71941	-0.34110	0.26938
Ir	-1.26216	-0.39158	-0.17364
C	1.46491	-0.32575	-1.12739
C	2.56902	-0.49390	-1.99902
C	3.01066	-0.53416	0.77309
C	3.83241	-0.68002	-1.48815
C	4.06615	-0.70704	-0.09867
H	3.16461	-0.52322	1.84936
H	4.67673	-0.81084	-2.16324
H	2.38267	-0.47180	-3.06953
C	-0.69613	1.36638	0.46923
C	-1.29453	1.99398	1.68208
C	0.04426	2.31326	-0.43121
C	2.12245	3.22496	-1.05931
H	1.96622	2.83932	-2.07588
H	1.73832	4.25227	-1.03885
C	3.56110	3.13615	-0.62403
H	4.19052	3.74911	-1.27709
H	3.67976	3.49873	0.40238
H	3.92836	2.10363	-0.66557
O	1.34936	2.42252	-0.15169
O	-0.51288	2.97546	-1.27808
C	-4.38677	0.00846	0.77264
H	-4.78757	0.56216	-0.08220
H	-5.21947	-0.53537	1.23729
H	-3.99980	0.73043	1.50142
C	-2.41468	-1.58156	2.72524
H	-3.18358	-0.90744	3.10687
H	-2.59582	-2.58797	3.12537
H	-1.45616	-1.21894	3.11010
C	-0.56969	-3.43807	0.99038
H	-0.10449	-3.00017	1.87906

Frequencies

-264.9283	32.5208	35.0338
41.9374	45.1169	54.5546
74.9357	77.9434	82.8849
90.1027	99.2828	107.5359
109.3238	115.9029	119.1914
124.3318	131.2875	133.7305
142.2964	147.1098	150.5651
159.2744	165.1212	167.5784
171.6819	181.8077	192.5798
198.3588	204.0506	209.7327
215.0759	231.7574	234.3162
242.7590	253.1918	260.4437
273.8146	279.8496	289.4615
297.2797	298.2385	310.2499
322.7291	331.8473	353.6092
361.7711	382.7373	392.3670
403.4290	403.9536	416.6565
419.1870	423.4521	447.1613
459.7511	476.0146	522.1276
533.0633	538.6428	545.0573
555.6099	574.1862	582.8067
590.7622	598.8244	607.1380
610.0883	632.2564	641.6937
650.6762	687.7083	727.1559
757.2551	767.3096	810.4208
812.5004	820.1711	834.7912
842.0929	846.6212	892.8821
925.4495	932.3588	937.7081
957.4835	964.7652	969.6713
1020.4617	1025.4635	1032.7639
1040.1262	1043.1933	1045.3052
1047.8138	1050.6476	1080.1439
1088.5166	1095.2340	1107.6239
1114.8684	1140.4276	1142.7988
1170.6647	1181.5392	1183.7100
1189.0354	1219.7571	1229.1427
1242.5037	1256.6218	1287.5214
1302.9120	1356.7350	1369.3782
1370.4582	1379.7085	1386.1974
1388.4502	1397.7378	1400.6541
1403.1415	1420.3683	1425.0236

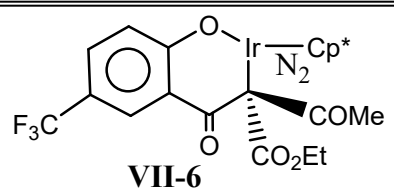
H	-1.01710	-4.39549	1.28909	1434.0355	1434.6276	1440.7803
H	0.22290	-3.65145	0.26559	1445.8995	1446.5975	1449.7893
C	-1.38442	-3.07633	-2.10159	1451.5066	1454.9814	1461.3648
H	-0.42502	-3.53447	-1.84125	1464.6276	1470.2081	1471.6905
H	-2.03799	-3.86121	-2.50219	1475.7151	1480.1151	1480.5847
H	-1.19303	-2.35357	-2.90286	1488.2972	1498.9542	1519.8660
C	-3.70153	-0.94183	-2.23968	1524.7526	1525.6125	1555.3556
H	-4.53973	-1.61189	-2.47492	1558.4470	1605.9851	1680.7157
H	-4.09990	0.07329	-2.14506	1777.5813	1831.9031	1854.1340
H	-3.01658	-0.94665	-3.09385	2466.4990	3035.7995	3039.3351
C	0.62939	-0.03547	1.18365	3040.3530	3040.9333	3042.1475
O	0.26930	-0.14008	-1.60350	3044.8541	3050.9889	3051.0019
O	0.60770	-0.12868	2.37851	3094.7444	3117.7091	3119.6971
N	-3.46610	3.09583	-0.52847	3120.8303	3121.0298	3139.2455
N	-3.77482	2.69406	-1.51040	3140.3019	3141.8678	3143.5171
C	-1.02730	3.45604	1.92394	3144.0739	3151.1935	3153.4615
H	-1.36603	4.05629	1.07165	3161.5286	3175.7655	3179.5340
H	-1.54335	3.77375	2.83182	3186.8473	3208.9303	3210.1713
H	0.05166	3.62539	2.03104			
O	-1.97012	1.33840	2.45907			
C	5.47166	-0.81698	0.37955			
F	6.17265	0.29241	0.08421			
F	5.55078	-0.99705	1.70138			
F	6.12102	-1.83358	-0.20846			
H	-0.42291	6.01154	-1.31860			
H	0.11414	6.98408	0.07070			
H	1.27908	6.00174	-0.84948			
C	-1.44736	4.92650	1.00708			
H	-1.65206	4.11353	1.71111			
H	-1.61538	5.88171	1.52049			
H	-2.17110	4.85704	0.18478			
C	0.96973	4.91672	1.66265			
H	2.00942	4.86508	1.31297			
H	0.84670	5.86169	2.20675			
H	0.79603	4.09098	2.36141			
C	-5.72069	-0.80581	-0.84573			
F	-6.33133	-0.47590	-1.99464			
F	-6.03091	-2.07831	-0.57695			
F	-6.27821	-0.04430	0.10662			

Statistical Thermodynamic Analysis

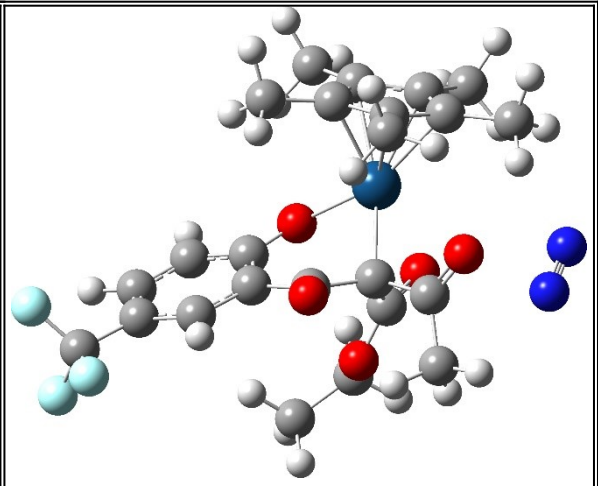
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.463514 Electronic Energy = -1819.08271476
Internal Energy (E)= -1818.58191476 Enthalpy (H)= -1818.58097076
Gibbs Free Energy (G)=-1818.68683276 Gibbs Free Energy of Solvation=-1818.72271211

St.Pt.	General Structure	Ball & Stick model

VII-6



VII-6



Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.34960	-2.40849	0.47270
C	-2.16560	-1.61258	1.36744
C	-3.24832	-1.06847	0.59915
C	-3.14171	-1.60557	-0.75417
C	-2.00920	-2.45496	-0.82774
C	1.98111	0.08461	0.38984
Ir	-1.31924	-0.42488	-0.22802
C	1.66033	-0.42818	-0.89455
C	2.72131	-0.91838	-1.69462
C	3.30092	0.03767	0.84925
C	4.01791	-0.92733	-1.23076
C	4.32066	-0.45041	0.05354
H	3.50109	0.41102	1.85041
H	4.81775	-1.31687	-1.85896
H	2.46772	-1.30290	-2.68017
C	-0.30476	1.19918	0.72101
C	-1.08692	1.99029	1.77566
C	-0.30927	1.87421	-0.59989
C	0.90778	2.88417	-2.36029
H	0.50835	2.03897	-2.93201
H	0.31839	3.77526	-2.60579
C	2.38496	3.07842	-2.57097
H	2.59136	3.28591	-3.62555
H	2.76231	3.91434	-1.97398
H	2.93057	2.17255	-2.28147
O	0.72751	2.59573	-0.95213
O	-1.28515	1.64830	-1.33857
C	-4.38794	-0.27138	1.12867
H	-4.93577	0.21877	0.31826
H	-5.09545	-0.92094	1.66114
H	-4.03467	0.50078	1.81858
C	-1.90201	-1.42955	2.82061
H	-2.58269	-0.69520	3.25478
H	-2.02356	-2.38676	3.34404
H	-0.88193	-1.06891	3.00289
C	-0.12130	-3.15982	0.84733
H	0.37944	-2.68741	1.69917
H	-0.36276	-4.19524	1.12195

Frequencies

24.6819	41.3220	42.2990
47.3226	58.9613	67.5989
73.4411	77.7426	86.8655
91.2085	101.2836	106.3207
111.9648	116.9746	124.2904
134.4359	138.0915	141.0093
155.7499	160.2383	164.3222
166.9527	172.3613	178.1227
182.5997	205.7116	210.2059
221.6357	223.8610	228.4725
233.2980	236.7502	246.0442
259.9036	268.0387	278.0064
284.6117	290.1625	297.5745
304.5615	317.7002	320.6546
332.3097	352.4528	361.3743
384.7311	391.4147	402.3893
404.8001	419.5433	425.0848
426.1233	452.3615	478.4631
498.5170	522.8496	533.0210
539.3362	540.8656	548.3325
553.3174	582.1335	585.7872
598.7692	608.5693	612.2182
641.8042	655.4218	661.2863
680.8970	735.8076	749.6357
781.8101	794.5494	808.0452
815.3885	819.2462	833.6305
842.7786	865.8687	891.6465
925.3242	943.4049	958.0375
961.0092	976.5420	991.8376
1018.7278	1033.8100	1037.0926
1042.4600	1046.3672	1047.1685
1057.1134	1079.4138	1093.7473
1095.5323	1101.9928	1114.1851
1129.7093	1139.0331	1159.8170
1178.1260	1182.0907	1189.6942
1207.8571	1219.9971	1236.8073
1251.0707	1274.5208	1293.1879
1349.8710	1364.0017	1365.7773
1369.4990	1375.7687	1384.5545
1391.6029	1395.0866	1401.8665
1402.1908	1411.2116	1430.9087
1436.8660	1441.5831	1442.2323

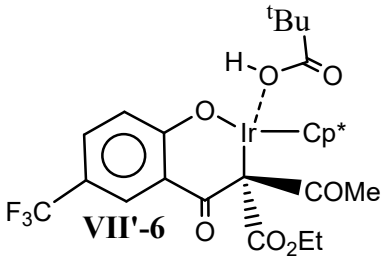
H	0.59144	-3.18429	0.01560	1443.5485	1445.3085	1449.2847
C	-1.45008	-3.15076	-2.01785	1450.4924	1460.9650	1464.5276
H	-0.42700	-2.80203	-2.21464	1464.6036	1469.5110	1470.2055
H	-1.41707	-4.23595	-1.86007	1473.2387	1474.7495	1475.3298
H	-2.04538	-2.95742	-2.91500	1484.8687	1505.3191	1507.1782
C	-4.05515	-1.22679	-1.86635	1516.2768	1525.7706	1546.2623
H	-5.02605	-1.72839	-1.76430	1552.3449	1611.9683	1672.0949
H	-4.23773	-0.14530	-1.86225	1681.9286	1739.3348	1848.3311
H	-3.63453	-1.48897	-2.84141	2467.1801	3030.9913	3034.6394
C	0.97574	0.68788	1.29092	3039.9994	3040.7237	3043.2674
O	0.44723	-0.48881	-1.38671	3046.3091	3047.4444	3062.4537
O	1.15284	0.73930	2.50701	3107.6713	3116.6456	3118.1142
N	-3.36984	3.23037	0.00906	3119.6350	3121.3052	3134.9728
N	-4.16025	2.61932	-0.46281	3138.0760	3140.1221	3141.5374
C	-0.52021	3.34517	2.09146	3141.5788	3149.1648	3151.6958
H	-0.46074	3.95433	1.18051	3176.8673	3183.7363	3184.3591
H	-1.14529	3.84745	2.83290	3186.7096	3201.1741	3212.8079
H	0.49905	3.22535	2.47552			
O	-2.08560	1.57195	2.31792			
C	5.73533	-0.50572	0.51604			
F	6.55707	0.15123	-0.32148			
F	5.90262	0.02141	1.73229			
F	6.19109	-1.76946	0.56198			
H	-0.42291	6.01154	-1.31860			
H	0.11414	6.98408	0.07070			
H	1.27908	6.00174	-0.84948			
C	-1.44736	4.92650	1.00708			
H	-1.65206	4.11353	1.71111			
H	-1.61538	5.88171	1.52049			
H	-2.17110	4.85704	0.18478			
C	0.96973	4.91672	1.66265			
H	2.00942	4.86508	1.31297			
H	0.84670	5.86169	2.20675			
H	0.79603	4.09098	2.36141			
C	-5.72069	-0.80581	-0.84573			
F	-6.33133	-0.47590	-1.99464			
F	-6.03091	-2.07831	-0.57695			
F	-6.27821	-0.04430	0.10662			

Statistical Thermodynamic Analysis

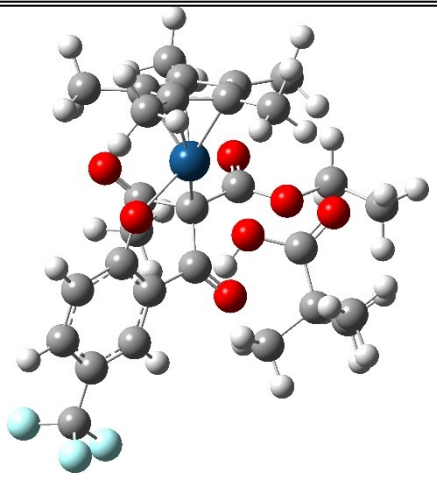
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.465993 Electronic Energy = -1819.12146791
Internal Energy (E)= -1818.61835091 Enthalpy (H)= -1818.61740791
Gibbs Free Energy (G)=-1818.72304691 Gibbs Free Energy of Solvation=-1818.76054161

St.Pt.	General Structure	Ball & Stick model

VII'-6



VII'-6



Cartesian co-ordinate

Atoms	X	Y	Z
C	2.55044	-1.78294	-1.87178
C	3.14910	-0.54673	-1.49326
C	3.39064	-0.55270	-0.05802
C	2.94043	-1.81622	0.45164
C	2.35090	-2.55078	-0.65911
O	0.27305	1.37393	-1.32388
C	0.54688	2.70288	-1.20123
O	1.68990	3.04860	-1.05044
C	-0.62226	3.67986	-1.30936
C	-1.76337	-1.16824	-0.83323
H	-0.67023	1.20612	-1.48263
C	3.46859	0.59650	-2.38551
H	3.25500	1.54901	-1.88919
H	4.53272	0.57625	-2.65588
H	2.88203	0.56264	-3.30909
C	4.12071	0.49789	0.70056
H	5.20468	0.40690	0.55063
H	3.81638	1.50214	0.38193
H	3.91935	0.40535	1.77327
C	1.74680	-3.90592	-0.58332
H	1.09861	-4.09243	-1.44511
H	2.53099	-4.67447	-0.57055
H	1.13977	-4.00195	0.32145
C	2.08426	-2.19507	-3.22377
H	2.21358	-1.39083	-3.95404
H	2.64239	-3.06819	-3.58413
H	1.01974	-2.45727	-3.20199
C	3.12893	-2.33386	1.83041
H	4.15619	-2.70717	1.93754
H	2.96098	-1.55612	2.58227
H	2.43554	-3.15108	2.04247
Ir	1.24828	-0.75926	-0.38220
C	-0.32136	4.58654	-2.50712
H	-0.33956	4.02703	-3.45120
H	-1.08014	5.37580	-2.56932
H	0.66233	5.05503	-2.40176
C	-1.98371	3.01141	-1.48528
H	-2.26672	2.42711	-0.59978

Frequencies

19.3379	36.0984	48.3922
52.2569	56.7183	57.6764
64.2781	68.2323	76.6139
85.1149	94.8344	95.9892
103.4225	111.1269	115.9834
124.1865	125.6956	131.5216
139.1163	141.8662	145.8701
149.8032	155.0111	156.7745
160.9427	169.3100	177.3798
184.2932	190.6635	198.4413
206.6736	218.9579	231.1592
235.6757	242.8828	246.9221
251.7270	261.8832	263.5564
277.7947	288.7301	292.1144
295.9256	308.8086	316.2551
324.3550	336.6791	345.5767
358.3633	371.8660	375.8411
383.2047	388.0503	392.9803
398.9843	401.9885	410.6739
421.1578	421.9195	425.8730
430.7451	441.9905	457.5393
471.4581	498.3362	517.0388
525.0963	532.6394	535.8575
539.6093	549.8236	551.8979
580.0907	583.9604	588.6440
590.3663	604.4939	614.4908
638.2973	646.8316	661.8174
669.7622	700.4892	735.4996
763.2158	769.7525	773.8661
786.8445	793.7478	811.3654
812.7781	816.6757	840.4792
875.2546	884.8535	885.9523
900.2192	936.2039	947.4321
954.5062	959.8875	961.7072
965.8551	975.4195	986.5580
1004.1903	1009.2977	1022.5379
1031.8357	1034.2394	1044.2588
1046.5612	1048.4228	1054.3931
1055.4870	1094.5127	1098.0714
1101.1623	1104.9840	1114.8378
1126.9270	1129.1839	1146.0869
1158.8404	1171.5740	1186.0457
1186.8753	1191.2776	1222.4259

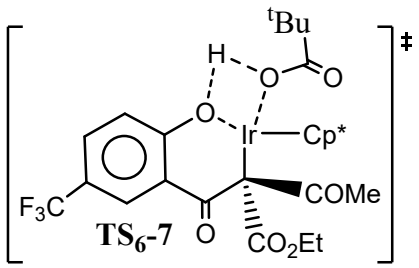
H	-2.74726	3.78717	-1.61310	1225.6120	1232.1621	1241.5910
H	-2.03557	2.38257	-2.38716	1259.2948	1266.8219	1270.8590
C	-0.62461	4.50315	-0.01818	1281.1396	1302.5320	1330.5960
H	-0.77166	3.85590	0.85616	1354.1567	1360.7982	1363.5587
H	0.32272	5.04115	0.09255	1378.8252	1383.8180	1384.8872
H	-1.44138	5.23422	-0.05591	1387.1531	1391.8057	1394.5487
O	-0.54362	-1.32583	-1.27336	1398.8096	1409.6308	1419.3420
C	-2.13457	-0.27488	0.20605	1420.5791	1423.0174	1435.2977
C	-3.49238	-0.05490	0.48258	1439.9659	1441.5161	1443.3778
C	-2.80075	-1.86219	-1.50786	1447.3566	1451.9981	1454.8309
C	-4.48343	-0.73322	-0.19607	1458.9785	1462.0748	1463.1226
C	-4.12218	-1.65229	-1.19563	1467.4984	1467.9457	1471.1754
C	-1.16074	0.47557	1.03473	1473.1746	1475.0061	1475.4885
O	-1.46446	1.57736	1.47941	1484.0897	1489.8565	1496.1305
H	-2.50682	-2.55024	-2.29650	1496.5417	1503.4121	1506.1461
H	-4.90142	-2.19427	-1.72938	1510.0559	1516.9350	1532.9091
H	-3.74089	0.66475	1.25983	1539.7744	1549.4962	1555.1970
C	0.11855	-0.23785	1.39659	1609.6727	1685.5787	1752.2088
C	-0.29041	-1.50900	2.17920	1783.2848	1832.3207	1884.9875
C	1.04529	0.55609	2.25692	3018.2791	3032.2795	3032.6047
C	2.10791	2.59363	2.69626	3034.2618	3036.8082	3037.0254
H	3.09947	2.12686	2.75500	3040.3199	3041.5288	3050.3031
H	1.68891	2.57380	3.70958	3054.1692	3057.4988	3101.6941
C	2.18305	3.98807	2.13730	3108.0342	3109.2847	3113.5051
H	2.88838	4.58589	2.72393	3118.5126	3121.6777	3123.3724
H	2.51299	3.97086	1.09280	3127.3383	3128.3736	3136.1156
H	1.20490	4.47783	2.17697	3143.9645	3144.7953	3145.9991
O	1.26976	1.80837	1.83380	3146.0452	3147.2061	3148.3665
O	1.60597	0.09886	3.24114	3151.2781	3158.3482	3160.5548
O	0.02775	-2.62932	1.84064	3172.0998	3173.7986	3181.4761
C	-1.11379	-1.28575	3.42116	3203.7332	3205.5850	3769.4249
H	-1.56397	-2.22940	3.73684			
H	-0.44121	-0.92551	4.20773			
H	-1.88734	-0.52213	3.28283			
C	-5.92918	-0.52817	0.09773			
F	-6.60144	-0.12547	-0.99442			
F	-6.52188	-1.66471	0.49812			
F	-6.13402	0.38668	1.05065			

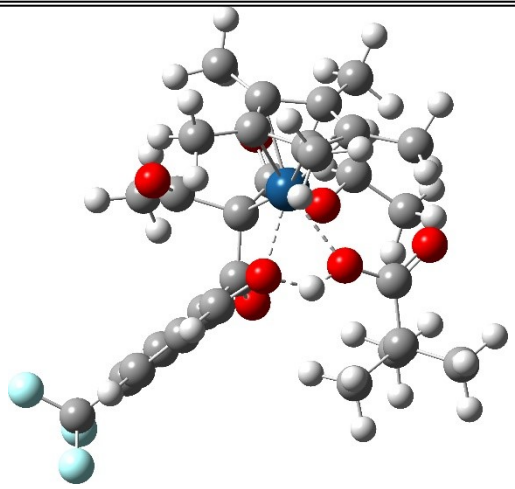
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.608730 Electronic Energy = -2056.48962968
Internal Energy (E)= -2055.83811868 Enthalpy (H)= -2055.83717568
Gibbs Free Energy (G)=-2055.95371768 Gibbs Free Energy of Solvation=-2056.0047774

St.Pt.	General Structure	Ball & Stick model

TS_6-7





Cartesian co-ordinate

Atoms	X	Y	Z
C	2.19834	-2.05500	-1.85202
C	3.13986	-1.19103	-1.24024
C	3.10166	-1.41128	0.20250
C	2.17793	-2.49244	0.46055
C	1.55514	-2.83067	-0.79594
O	0.85729	1.33428	-1.05881
C	1.40636	2.55083	-1.04225
O	2.56916	2.70063	-0.73662
C	0.47862	3.71555	-1.37792
C	-1.88747	-0.31627	-1.15559
H	-0.04118	0.88577	-1.51662
C	3.98004	-0.15197	-1.89126
H	3.82292	0.82475	-1.41658
H	5.04239	-0.41230	-1.79738
H	3.74933	-0.05063	-2.95577
C	4.01176	-0.76013	1.18265
H	5.00685	-1.22442	1.15818
H	4.12904	0.30487	0.94627
H	3.61852	-0.84247	2.20150
C	0.51887	-3.86843	-1.03563
H	-0.14840	-3.56421	-1.85073
H	0.98893	-4.81865	-1.32252
H	-0.09638	-4.02352	-0.14786
C	1.81981	-2.12413	-3.28946
H	2.29209	-1.32402	-3.86708
H	2.11786	-3.08388	-3.73012
H	0.73445	-2.02056	-3.40569
C	1.98240	-3.16255	1.77263
H	2.83653	-3.82360	1.96989
H	1.92246	-2.42858	2.58409
H	1.06797	-3.75994	1.78820
Ir	1.14033	-0.77796	-0.36484
C	1.18474	4.60276	-2.40303
H	1.29873	4.09042	-3.36700
H	0.59652	5.51277	-2.57361
H	2.17911	4.89035	-2.04790
C	-0.88176	3.27329	-1.90590
H	-1.44991	2.72390	-1.14468

Frequencies

-902.9795	1.2590	16.4976
22.9835	45.6287	55.0849
60.3119	61.2609	73.2976
76.9393	86.7426	92.2778
101.2782	109.7847	112.9431
116.6847	119.3017	123.7398
134.9393	137.6249	138.1655
142.7089	148.0898	156.8947
160.6028	167.8467	182.5259
187.5054	189.5964	192.7364
204.0504	213.5380	220.2568
223.0619	228.3451	232.5073
239.2273	250.0697	252.8598
256.6024	266.8382	277.0335
281.5553	286.2921	290.8669
302.6444	304.2973	330.4538
338.4946	342.2855	343.6036
362.9858	367.4402	371.7706
379.9835	381.7048	398.2837
404.9576	412.4350	415.2358
422.5107	429.9966	439.5468
448.8011	457.8004	499.3815
524.9177	535.4644	536.9291
544.8364	549.1787	557.7383
573.4632	584.1689	588.1583
588.8248	602.3440	605.8690
620.2616	642.0334	653.7801
658.1596	699.1557	738.5568
761.4449	770.9140	784.8565
803.6607	807.0256	810.2595
814.8267	831.8291	845.1949
873.7368	882.5659	894.7806
921.9806	935.5402	940.7741
944.2563	953.1105	953.8599
956.5683	958.4645	975.7601
1001.9369	1016.2913	1032.3721
1034.1893	1036.6382	1039.9292
1040.6984	1044.2216	1047.4945
1049.8244	1091.1447	1091.8393
1097.1602	1102.2999	1111.4191
1126.0704	1143.5632	1155.0324
1174.5658	1179.1658	1185.2078

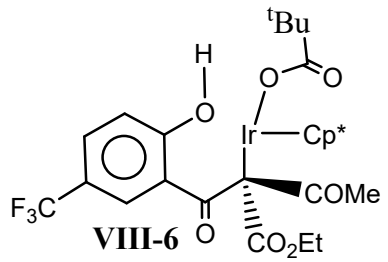
H	-1.47163	4.15813	-2.17284	1186.9588	1195.6805	1219.5677
H	-0.79736	2.65252	-2.80819	1230.4874	1233.6675	1237.7289
C	0.28541	4.48582	-0.06510	1258.9070	1264.5893	1271.5939
H	-0.16877	3.84755	0.70455	1295.0070	1314.6597	1329.1687
H	1.24676	4.85422	0.30972	1347.7559	1364.9507	1374.6924
H	-0.37614	5.34356	-0.24049	1376.0183	1377.8792	1379.6696
O	-0.63273	-0.30260	-1.62709	1381.5282	1383.6127	1390.5829
C	-2.20974	0.29494	0.06848	1393.6145	1397.9573	1402.5731
C	-3.54646	0.41621	0.44968	1410.3860	1423.3771	1433.0785
C	-2.90930	-0.86124	-1.94233	1438.5222	1441.1610	1442.0505
C	-4.55249	-0.12208	-0.33814	1445.0389	1447.5428	1448.4201
C	-4.22634	-0.77466	-1.53038	1453.3601	1456.9225	1457.7880
C	-1.16863	0.79925	1.00856	1459.1654	1460.8906	1462.8538
O	-1.32272	1.87101	1.57020	1464.7091	1465.9235	1468.0124
H	-2.63706	-1.32757	-2.88620	1473.2618	1477.9685	1480.6758
H	-5.02035	-1.19660	-2.14299	1483.3644	1488.7276	1492.4707
H	-3.78197	0.92859	1.38016	1500.0454	1505.6778	1519.3493
C	-0.05905	-0.18046	1.35421	1520.9649	1541.5369	1554.2008
C	-0.80763	-1.38247	1.96663	1633.8264	1677.3267	1774.3645
C	0.95531	0.34660	2.31691	1783.9331	1827.8547	1830.3531
C	2.36057	2.11285	2.94925	2027.5866	3025.7583	3028.7666
H	3.26213	1.48761	2.91061	3030.9139	3033.3339	3037.1097
H	1.96596	2.04283	3.97025	3038.7647	3039.7068	3040.6156
C	2.64383	3.53154	2.53828	3051.3122	3053.5955	3054.5675
H	3.39985	3.96877	3.19877	3100.0718	3101.7886	3109.5956
H	3.01045	3.56413	1.50697	3111.8576	3113.3699	3116.1493
H	1.73557	4.14012	2.60297	3117.9011	3123.4920	3126.7439
O	1.38395	1.58163	2.04142	3133.8744	3134.6787	3140.4612
O	1.41400	-0.30923	3.24103	3141.6832	3142.7962	3144.2956
O	-0.96779	-2.43025	1.37453	3146.1275	3149.3568	3163.9151
C	-1.41786	-1.17020	3.32764	3167.9185	3169.6880	3192.0038
H	-2.25172	-1.86300	3.46335	3206.0470	3208.6263	3208.8373
H	-0.65229	-1.37349	4.08378			
H	-1.74390	-0.13420	3.47638			
C	-5.98374	-0.07382	0.08472			
F	-6.78512	0.27403	-0.93297			
F	-6.41205	-1.27216	0.51011			
F	-6.19206	0.79649	1.07718			

Statistical Thermodynamic Analysis

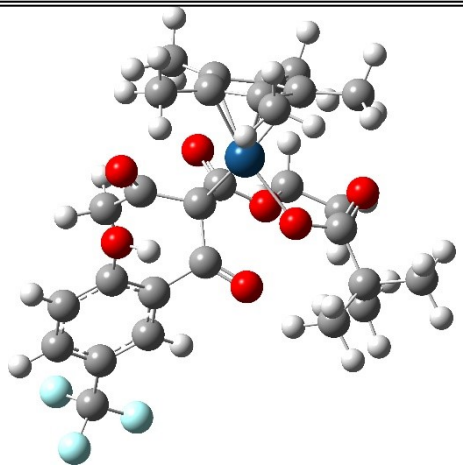
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.602135 Electronic Energy = -2056.47950788
Internal Energy (E)= -2055.83435788 Enthalpy (H)= -2055.83341488
Gibbs Free Energy (G)=-2055.95425188 Gibbs Free Energy of Solvation=-2056.00131538

St.Pt.	General Structure	Ball & Stick model

VIII-6



VIII-6



Cartesian co-ordinate

Atoms	X	Y	Z
C	2.26947	-2.15728	-1.63106
C	3.18854	-1.26538	-1.02936
C	3.03102	-1.37359	0.41946
C	2.09879	-2.46088	0.68892
C	1.57228	-2.88086	-0.56935
O	0.84930	1.16652	-1.09673
C	1.65372	2.19348	-1.01068
O	2.77448	2.16356	-0.52116
C	1.06578	3.50032	-1.55849
C	-2.07195	-0.41636	-1.27039
H	-0.40398	0.31714	-1.90513
C	4.13647	-0.35435	-1.72030
H	4.25473	0.57872	-1.16471
H	5.11464	-0.84383	-1.81978
H	3.78780	-0.09496	-2.72547
C	3.84771	-0.64313	1.42262
H	4.83439	-1.11172	1.53748
H	3.98709	0.39731	1.10382
H	3.34773	-0.64577	2.39801
C	0.53727	-3.91958	-0.81582
H	-0.22789	-3.54187	-1.50435
H	0.99180	-4.81161	-1.26696
H	0.02666	-4.20306	0.10623
C	2.01708	-2.34864	-3.08451
H	2.36666	-1.49297	-3.67043
H	2.53391	-3.24386	-3.45474
H	0.94790	-2.47761	-3.28369
C	1.81280	-3.04782	2.02436
H	2.65256	-3.68707	2.32733
H	1.68205	-2.27118	2.78585
H	0.90664	-3.65935	2.00600
Ir	1.14431	-0.76876	-0.31143
C	2.06452	4.09479	-2.55029
H	2.17376	3.45715	-3.43794
H	1.72013	5.08128	-2.88680
H	3.04968	4.20655	-2.08617
C	-0.29033	3.30755	-2.22803
H	-1.03230	2.92445	-1.51687
H	-0.65489	4.27163	-2.60596

Frequencies

27.3470	33.9527	46.6024
53.7278	59.7746	69.5418
73.0384	77.5772	83.4357
91.0941	99.7694	103.8144
109.4253	120.5336	122.2260
127.4226	132.2860	139.1733
144.2086	148.4122	151.3690
163.1274	171.8934	178.6889
182.3295	192.5699	195.9507
208.1316	212.3990	221.7173
227.1225	235.2246	237.9355
244.5136	253.3073	256.0620
268.4903	281.7096	286.1316
290.5784	293.7538	296.6108
312.1603	313.7717	319.0807
321.8407	326.5844	333.1614
355.8545	356.8902	362.1592
370.5564	373.4224	395.3600
397.4160	399.4810	405.4245
410.3317	414.7022	418.9619
426.8068	429.8688	456.7890
467.0181	478.1770	510.0952
532.8980	537.0399	540.4186
546.7480	547.8917	572.6219
582.0187	586.6348	591.2170
598.2932	602.3361	624.4061
631.6663	641.4197	653.0130
693.9885	726.0697	757.4131
774.1019	789.3390	802.6085
807.7563	808.4715	812.9356
815.0041	837.1325	852.0414
867.4387	883.2051	893.2765
912.5694	927.8666	935.9118
951.5329	954.3754	958.7813
960.2130	960.8070	974.8872
995.5302	1014.5732	1019.8424
1034.4541	1038.4178	1039.9328
1049.6651	1054.4701	1055.5850
1059.7505	1090.2773	1094.1736
1099.8175	1100.7375	1111.9894
1120.3725	1140.1862	1154.2374
1173.9597	1185.3005	1191.0914
1199.8630	1225.3318	1237.3800

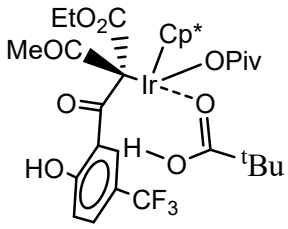
H	-0.22933	2.62000	-3.08221	1237.9103	1245.3415	1252.5644
C	0.90513	4.43763	-0.35762	1263.5832	1268.2150	1271.3038
H	0.27061	3.97892	0.41294	1284.2976	1321.8289	1345.5199
H	1.88132	4.66383	0.08456	1362.7777	1369.0484	1376.4489
H	0.44129	5.37936	-0.67943	1377.7213	1381.0228	1382.7134
O	-0.80554	-0.57831	-1.78277	1384.7085	1388.8551	1395.3130
C	-2.29265	0.37676	-0.14299	1397.6188	1400.9979	1405.0801
C	-3.60921	0.60951	0.25805	1416.7207	1425.5340	1431.7728
C	-3.12554	-1.03512	-1.93314	1440.6365	1443.6593	1446.3117
C	-4.66652	0.00266	-0.40367	1450.6870	1454.3458	1455.2912
C	-4.42317	-0.83790	-1.48952	1458.0529	1460.9941	1461.2882
C	-1.20794	0.93857	0.73786	1463.1472	1464.3258	1467.8556
O	-1.28463	2.09897	1.09324	1469.8680	1471.4376	1474.3957
H	-2.90616	-1.64543	-2.80505	1483.2354	1488.1635	1490.7694
H	-5.25657	-1.31719	-1.99848	1496.4898	1498.0697	1501.9201
H	-3.78830	1.25990	1.11092	1506.3534	1519.2372	1525.5602
C	-0.21125	-0.07276	1.26737	1532.4961	1544.5241	1560.8596
C	-1.05121	-1.24657	1.80072	1651.9772	1685.9726	1768.6019
C	0.70097	0.43976	2.33688	1776.9414	1792.1580	1827.4339
C	2.10731	2.14866	3.10655	3023.9536	3028.0962	3032.4973
H	2.90647	1.40910	3.23661	3038.6520	3039.1656	3039.5679
H	1.59110	2.23372	4.07141	3039.9613	3041.0308	3048.1431
C	2.64360	3.46573	2.61668	3048.2742	3052.5937	3099.2652
H	3.39922	3.84368	3.31354	3104.5386	3107.4199	3113.3845
H	3.09688	3.34070	1.62651	3117.6638	3119.5709	3120.9937
H	1.84456	4.21040	2.53875	3125.5493	3129.9540	3131.7213
O	1.17537	1.66502	2.12819	3139.6040	3140.2191	3141.3611
O	1.03562	-0.23331	3.30251	3144.3944	3149.9270	3156.7988
O	-1.19440	-2.28380	1.18398	3157.9770	3162.5132	3167.6088
C	-1.78267	-1.02548	3.10045	3185.7955	3186.5158	3193.7496
H	-2.68504	-1.64216	3.11498	3207.4697	3208.4514	3425.9318
H	-1.12704	-1.32630	3.92419			
H	-2.03349	0.02971	3.26168			
C	-6.08407	0.20839	0.02955			
F	-6.84177	0.64164	-0.98714			
F	-6.63403	-0.93859	0.45179			
F	-6.19018	1.09574	1.02087			

Statistical Thermodynamic Analysis

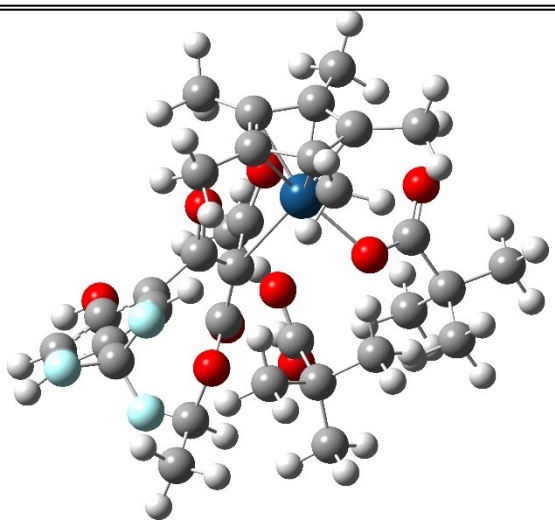
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.609393 Electronic Energy = -2056.49144140
Internal Energy (E)= -2055.8399794 Enthalpy (H)= -2055.8390354
Gibbs Free Energy (G)=-2055.9528664 Gibbs Free Energy of Solvation=-2056.00448304

St.Pt.	General Structure	Ball & Stick model

VIII'-6



VIII'-6



Cartesian co-ordinate

Atoms	X	Y	Z
H	0.38961	1.50873	0.69536
C	-2.00130	-2.09544	-2.17759
C	-1.35420	-2.80243	-1.12153
C	-2.23026	-2.78765	0.04472
C	-3.43485	-2.08268	-0.31147
C	-3.27715	-1.59764	-1.67357
C	-3.28166	1.39715	0.88969
O	-2.20196	0.67661	0.97691
O	-4.21167	1.20555	0.11251
C	-3.27540	2.61616	1.82527
O	0.09482	-0.77282	1.00954
C	0.44936	0.03655	1.86807
O	0.57621	1.32173	1.64799
C	0.78541	-0.41838	3.27470
C	-4.61336	-1.85932	0.56433
H	-5.31743	-2.69666	0.47334
H	-4.30942	-1.77949	1.61400
H	-5.11596	-0.92559	0.30027
C	-4.27859	-0.81524	-2.44273
H	-5.08347	-1.46644	-2.80820
H	-4.70295	-0.03203	-1.80672
H	-3.81219	-0.33073	-3.30587
C	-1.94513	-3.47345	1.33253
H	-0.91307	-3.28744	1.65042
H	-2.61041	-3.11970	2.12681
H	-2.07995	-4.55860	1.23599
C	-0.00144	-3.41874	-1.15117
H	0.46773	-3.37251	-0.16164
H	-0.06750	-4.47448	-1.44419
H	0.65768	-2.88782	-1.84259
C	-1.47114	-1.82331	-3.53950
H	-0.42980	-2.13792	-3.63355
H	-2.07097	-2.35014	-4.29232
H	-1.50500	-0.75029	-3.75558
C	-0.52696	-0.91398	3.89278
H	-0.33452	-1.30042	4.90116
H	-1.26072	-0.10260	3.96651

Frequencies

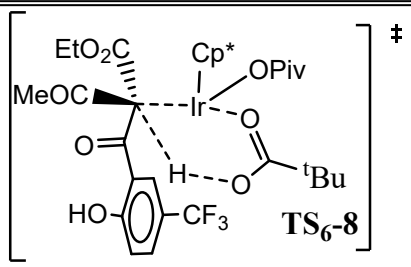
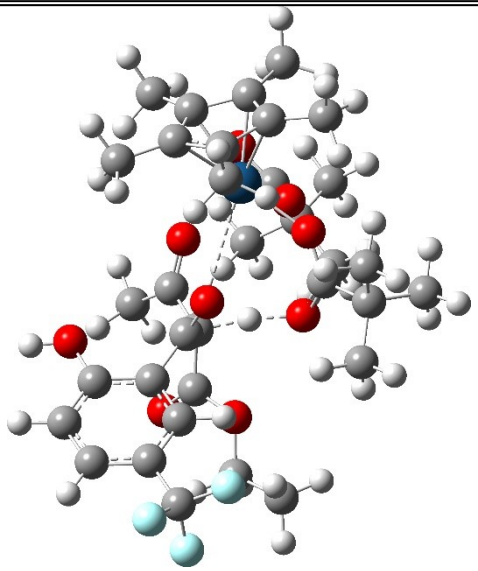
18.9285	27.1386	33.6388
45.5198	49.6119	58.2969
68.3782	71.1143	72.8976
81.6608	85.7966	91.9850
94.0563	95.7562	98.8752
101.7978	107.3448	112.4039
118.1038	123.6933	132.1596
137.4979	141.1496	143.0917
148.3595	159.3848	165.9480
170.7395	174.5857	179.3228
184.9818	195.1703	202.0716
203.6665	208.2130	214.9778
219.6454	223.0702	227.8134
232.3492	237.6024	238.8243
244.5836	255.5515	258.0648
259.9873	262.3828	270.8246
276.4134	285.3723	293.8434
297.0506	299.0225	304.6861
305.3170	315.1024	317.6946
320.5517	323.7522	327.4422
332.8489	341.2288	343.2070
349.2735	358.7904	373.6337
375.3678	389.3150	392.5757
395.2519	398.3901	410.4249
415.0655	420.6312	426.3315
428.7291	431.3854	446.6893
453.9996	469.2274	473.5889
502.5124	531.8176	536.0399
538.6505	541.3577	550.2373
559.6857	572.4474	582.3652
587.8470	592.6196	594.7017
603.6389	605.4003	621.9501
629.5247	633.0757	661.5596
685.1090	732.5127	766.4056
769.6425	770.8262	783.1220
793.1702	801.7185	806.9659
808.1096	811.9661	817.1260
819.7462	833.8009	864.9557
886.7286	899.9657	905.0395
915.8328	920.9216	924.3258
950.7394	951.1718	952.0500

H	-0.96826	-1.71342	3.28821
C	1.37049	0.70159	4.12688
H	1.59172	0.31370	5.12881
H	2.30152	1.08908	3.69915
H	0.67082	1.53797	4.23122
C	1.78575	-1.57154	3.16352
H	1.39118	-2.38613	2.54506
H	2.73324	-1.23614	2.72307
H	2.00308	-1.96788	4.16269
C	-4.70355	3.09466	2.05720
H	-5.29159	2.33593	2.58840
H	-4.70378	4.01110	2.66198
H	-5.20639	3.29540	1.10648
C	-2.48252	3.70110	1.08873
H	-2.43031	4.61557	1.69427
H	-1.45532	3.36833	0.88231
H	-2.96559	3.94847	0.13500
C	-2.60243	2.30944	3.15998
H	-2.62374	3.19928	3.80343
H	-3.12367	1.50094	3.69075
H	-1.55778	2.01159	3.01662
Ir	-1.75893	-0.76889	-0.47744
C	0.74448	1.79896	-1.35048
C	1.34726	0.48940	-1.50497
O	0.71101	-0.51618	-1.84179
C	2.82058	0.24634	-1.27915
C	3.84978	0.89298	-1.97533
C	3.15512	-0.79573	-0.42417
C	5.17899	0.51887	-1.77995
C	4.48155	-1.16044	-0.20974
H	2.34989	-1.33495	0.07156
C	5.49808	-0.49854	-0.89106
H	5.96650	1.02644	-2.33695
H	6.53487	-0.78946	-0.74302
O	3.50202	1.87331	-2.84113
H	4.28917	2.23088	-3.26607
C	-0.63162	1.96927	-1.71139
C	1.56785	2.99730	-1.11209
C	3.53701	3.73540	-0.03793
H	3.06498	4.65781	0.32279
H	3.98201	3.96584	-1.01685
C	4.54960	3.18405	0.93303
H	5.36315	3.89918	1.09219
H	4.08041	2.97458	1.89976
H	4.97540	2.24703	0.55253
O	2.54537	2.72755	-0.21319
O	1.41954	4.10976	-1.57499
C	-1.15485	3.28931	-2.20184
H	-2.22462	3.18214	-2.39883
H	-0.98343	4.07963	-1.46420
H	-0.61732	3.60879	-3.09976
O	-1.49795	1.05347	-1.65193
C	4.81080	-2.22829	0.77920
F	5.91735	-2.90238	0.44466
F	5.03162	-1.71816	2.00580
F	3.81730	-3.11830	0.91156

961.5902	966.7797	970.4259
971.3086	981.9961	994.6584
1014.6747	1031.2890	1033.9314
1041.1109	1043.4964	1044.7086
1045.1599	1047.0757	1050.0539
1051.3778	1058.8855	1062.4578
1094.4107	1099.5413	1104.6230
1110.6330	1122.0429	1136.7730
1146.0403	1168.7677	1170.3398
1184.6936	1188.8429	1196.1902
1211.9589	1237.3988	1238.4249
1244.8735	1249.1144	1252.9800
1270.6793	1273.6686	1275.3171
1284.5359	1300.6511	1318.3291
1321.3982	1327.0115	1363.4316
1364.6201	1373.6854	1375.5751
1376.0099	1379.5877	1381.0911
1382.2599	1387.7311	1391.2888
1392.0564	1393.2768	1393.4846
1398.5344	1412.6086	1417.6394
1418.7274	1421.1990	1432.0983
1435.2003	1435.9470	1442.4721
1444.0401	1448.4947	1450.3597
1450.7039	1456.5428	1457.0010
1460.5907	1463.7656	1464.5357
1465.1276	1467.2208	1468.7509
1471.8947	1472.4015	1473.6092
1474.2941	1475.0534	1478.3790
1481.1147	1484.8702	1485.0916
1488.2083	1490.0995	1492.7236
1494.4213	1502.3195	1511.2778
1513.7710	1518.1029	1537.9912
1561.8217	1580.6589	1665.8316
1675.9485	1707.7645	1758.5439
1766.3435	1831.9396	3022.1777
3024.1937	3031.2503	3032.1008
3038.1126	3038.2432	3039.4190
3040.0035	3044.4753	3044.6549
3047.2331	3048.0164	3049.0669
3057.7364	3088.0728	3098.9383
3110.8655	3112.8756	3113.7472
3117.8332	3121.1895	3121.9565
3127.4275	3130.3761	3130.9116
3132.9803	3134.1100	3135.9715
3143.2298	3145.5848	3146.5313
3149.2133	3149.4315	3150.7577
3154.9765	3155.6736	3162.6982
3165.7343	3166.2240	3169.7997
3177.5363	3180.7136	3208.8853
3218.0420	3467.3174	3894.3058

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.758082 Electronic Energy = -2403.31908432
Internal Energy (E)= -2402.50932832 Enthalpy (H)= -2402.50838432
Gibbs Free Energy (G)=-2402.64207232 Gibbs Free Energy of Solvation=-2402.70907332

St.Pt.	General Structure	Ball & Stick model
TS_6-8		

Cartesian co-ordinate

Atoms	X	Y	Z
H	0.60121	1.57163	0.12619
C	-1.94080	-1.98669	-2.20694
C	-1.24930	-2.73592	-1.21138
C	-2.11852	-2.83190	-0.04294
C	-3.36354	-2.16369	-0.35602
C	-3.23694	-1.58571	-1.67405
C	-3.40418	1.32611	0.85640
O	-2.35303	0.58743	1.05782
O	-4.29078	1.10590	0.03680
C	-3.40576	2.61716	1.69013
O	0.05014	-0.70913	0.89553
C	0.35024	0.20630	1.72523
O	0.48109	1.42211	1.42609
C	0.61960	-0.23414	3.16124
C	-4.53474	-2.04399	0.55032
H	-5.22218	-2.88494	0.39284
H	-4.21952	-2.05206	1.59945
H	-5.06194	-1.10306	0.37334
C	-4.26046	-0.81159	-2.42369
H	-4.81331	-1.46151	-3.11499
H	-4.95368	-0.31819	-1.73965
H	-3.77897	-0.01877	-3.00666

Frequencies

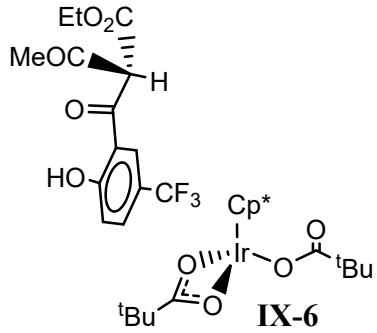
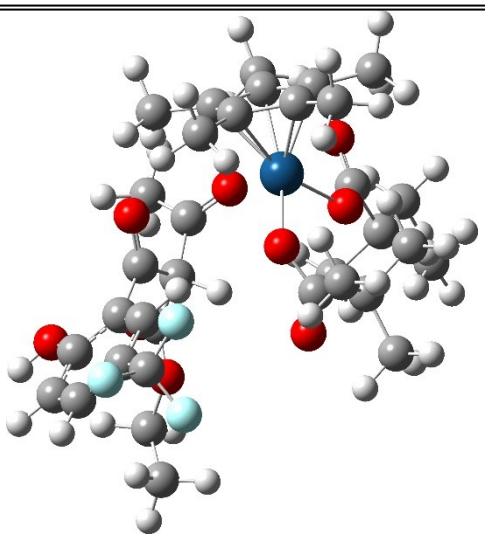
-1446.6794	-73.3996	22.3254
25.2101	39.1795	40.0132
52.4400	61.4620	65.6744
71.3231	74.7596	83.1161
85.5510	90.4189	94.2268
96.5227	103.3614	105.1576
111.1705	113.9908	122.4483
130.0253	133.4733	141.4093
146.4039	150.5167	153.9258
157.1168	161.4979	174.5053
182.4901	187.8562	193.5131
194.5223	199.0555	204.4335
206.6007	213.1447	217.2983
220.7247	222.8738	229.7255
234.3174	238.6375	249.8686
251.2469	256.9301	262.0173
271.3960	282.1278	283.9352
288.3338	291.2569	298.7912
303.9904	310.0075	317.5646
318.9648	322.5295	328.3123
331.2608	337.9109	343.3222
352.7146	364.4661	373.7278
384.6723	386.9189	396.5962
400.5386	406.5250	410.4934
421.3002	422.5468	424.2437
436.0100	439.4726	449.5717

C	-1.78638	-3.58508	1.19443	455.5612	456.9316	465.2158
H	-0.76995	-3.34511	1.52598	466.6716	519.6434	531.3582
H	-2.47219	-3.33920	2.01097	536.8823	538.7764	548.8873
H	-1.84118	-4.66688	1.01714	553.5065	568.0139	571.0376
C	0.12853	-3.29193	-1.29667	584.4491	589.2659	593.6870
H	0.61336	-3.28251	-0.31288	601.6864	602.0234	614.9724
H	0.11019	-4.33047	-1.65147	625.2138	633.3108	661.6181
H	0.75109	-2.69517	-1.97010	682.8185	689.1027	727.3703
C	-1.46736	-1.65389	-3.57487	764.5298	782.9759	792.7758
H	-0.39303	-1.80956	-3.68328	803.7013	804.8935	812.4435
H	-1.99739	-2.28110	-4.30387	815.1563	815.5825	817.7598
H	-1.67425	-0.60763	-3.82060	818.2794	823.0813	858.1835
C	-0.68302	-0.80422	3.72908	869.0247	903.2894	911.6003
H	-0.50541	-1.19939	4.73772	913.9182	922.1171	929.1098
H	-1.46122	-0.03512	3.78986	946.5955	947.6512	951.4132
H	-1.06277	-1.61418	3.09648	958.0357	960.7150	974.8362
C	1.09549	0.93399	4.01470	976.3878	988.7134	1008.5880
H	1.28493	0.59018	5.03967	1023.1603	1029.0624	1031.8284
H	2.02104	1.36489	3.61693	1034.1249	1037.2689	1041.5662
H	0.34616	1.73248	4.05157	1043.8385	1048.2640	1050.3946
C	1.68900	-1.32957	3.13252	1053.1946	1054.1868	1071.2161
H	1.34540	-2.20721	2.57337	1087.9932	1094.8406	1100.1485
H	2.62225	-0.97730	2.67343	1111.9412	1113.1777	1131.5445
H	1.92259	-1.64628	4.15692	1142.4465	1156.5626	1175.9684
C	-4.82839	3.14380	1.82954	1181.0481	1185.8552	1190.2584
H	-5.45306	2.44611	2.40132	1221.2119	1235.0199	1243.2192
H	-4.82463	4.10672	2.35734	1246.8100	1249.0543	1254.3192
H	-5.29413	3.27849	0.84888	1255.5712	1271.4852	1276.2002
C	-2.55665	3.61226	0.88882	1284.6835	1290.8573	1293.6510
H	-2.50959	4.57848	1.40867	1301.8649	1322.2924	1360.9681
H	-1.53103	3.23323	0.77471	1366.5432	1369.6575	1373.0698
H	-2.98864	3.77650	-0.10730	1374.8170	1379.2161	1379.7974
C	-2.77757	2.42370	3.06673	1384.0772	1386.1901	1387.4460
H	-2.83996	3.35976	3.63800	1388.2497	1391.7531	1392.7235
H	-3.29925	1.64599	3.64045	1399.7078	1404.4861	1410.6299
H	-1.72184	2.14361	2.98103	1413.0798	1415.4137	1420.7592
Ir	-1.72895	-0.78221	-0.39386	1421.4977	1430.9951	1435.5989
C	0.84062	1.83031	-1.13510	1442.4176	1445.8340	1447.4140
C	1.46398	0.55968	-1.60626	1448.8729	1454.5740	1455.8214
O	0.84760	-0.27159	-2.25402	1456.5341	1459.5546	1460.4727
C	2.87772	0.21041	-1.22907	1460.7005	1463.4058	1465.8349
C	3.98502	0.81487	-1.82945	1467.4836	1471.1687	1471.8968
C	3.07374	-0.85921	-0.36752	1474.6028	1475.7325	1478.2858
C	5.27319	0.36913	-1.54129	1479.7099	1483.1637	1484.5600
C	4.36000	-1.30443	-0.07182	1487.0488	1496.3509	1501.6625
H	2.19951	-1.33830	0.07187	1502.8258	1507.8088	1510.5670
C	5.46014	-0.68668	-0.65869	1516.2260	1517.7585	1541.8824
H	6.12883	0.84473	-2.02004	1544.6824	1559.0085	1666.5141
H	6.46388	-1.04250	-0.44012	1675.8406	1694.0622	1700.2348
O	3.73782	1.82796	-2.69463	1762.3250	1790.0247	1853.0378
H	4.56304	2.15321	-3.07057	3017.8890	3024.5769	3032.6056
C	-0.53339	2.03169	-1.64641	3033.1089	3034.9730	3035.8468
C	1.73257	3.02664	-1.00877	3038.9969	3039.2666	3039.8985
C	3.72156	3.75842	0.02218	3040.9922	3042.1018	3042.9384
H	3.26699	4.69910	0.35614	3046.7487	3056.7487	3091.8793
H	4.16511	3.94558	-0.96597	3101.0889	3108.7080	3112.0239
C	4.72366	3.21415	1.00713	3112.8425	3113.8387	3118.3621
H	5.55275	3.91631	1.14092	3119.5703	3119.9864	3123.0691
H	4.25424	3.04423	1.98121	3124.3613	3126.9804	3130.6394
H	5.12791	2.25694	0.65455	3131.1160	3134.5191	3135.2680
O	2.70340	2.76660	-0.11844	3142.1796	3143.2720	3146.4578

O	1.61433	4.09875	-1.55836	3148.3259	3148.7454	3154.6506
C	-0.94648	3.28145	-2.35240	3159.6498	3164.2626	3168.4963
H	-1.99325	3.19047	-2.65124	3175.5198	3190.4389	3193.8467
H	-0.81212	4.14672	-1.69477	3207.8638	3221.6841	3891.4114
H	-0.29754	3.46920	-3.21353			
O	-1.40882	1.17283	-1.46699			
C	4.56763	-2.41840	0.90099			
F	5.60657	-3.19064	0.55881			
F	4.82615	-1.95799	2.13635			
F	3.49082	-3.20842	0.99929			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.751904 Electronic Energy = -2403.30483843
Internal Energy (E)= -2402.50216143 Enthalpy (H)= -2402.50121843
Gibbs Free Energy (G)=-2402.63301343 Gibbs Free Energy of Solvation=-2402.6992633

St.Pt.	General Structure	Ball & Stick model
IX-6	 **IX-6**	

Cartesian co-ordinate

Atoms	X	Y	Z
H	0.69878	1.56459	0.02577
C	-2.09624	-1.45391	-2.39603
C	-1.41382	-2.43965	-1.62126
C	-2.25592	-2.74747	-0.47647
C	-3.47986	-1.96287	-0.58962
C	-3.36967	-1.14485	-1.76377
C	-3.29450	1.35385	1.11667
O	-2.26388	0.55947	1.18638
O	-4.26124	1.20880	0.37657
C	-3.14181	2.58686	2.01797

Frequencies

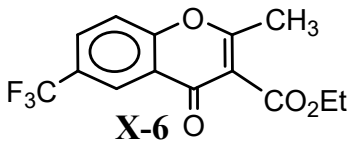
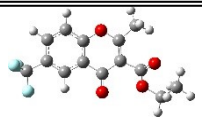
21.3094	24.0551	37.6985
42.5014	46.8922	56.5414
60.6764	63.1931	68.9573
73.6232	76.4764	79.7805
89.4496	92.5028	95.1054
100.5286	101.2853	101.3626
113.0343	118.5818	122.8670
131.0579	131.5077	136.5161
141.6385	150.9394	155.2602
164.3098	168.7880	171.6331
174.2033	178.6241	188.1470
199.6101	202.4848	213.6627
215.7688	216.9431	224.2030
229.0327	229.3565	233.2623

O	0.09241	-0.70996	0.62411	237.6694	242.4280	246.7366
C	0.37839	-0.09780	1.74788	256.8245	266.2174	272.2870
O	0.63439	1.10005	1.83023	274.3266	278.1328	284.6439
C	0.45506	-0.99863	2.98751	292.0524	295.2801	304.4579
C	-4.61249	-1.98275	0.37285	305.8684	319.4391	321.8631
H	-5.36517	-2.72099	0.06771	327.3997	332.7489	335.6446
H	-4.26429	-2.24569	1.37819	342.4125	343.4197	355.1294
H	-5.07216	-0.99216	0.43563	356.6787	366.9693	371.8464
C	-4.38012	-0.20611	-2.31789	374.7697	383.0908	391.9058
H	-4.94927	-0.68995	-3.12333	395.9280	409.5724	417.0224
H	-5.06070	0.14530	-1.54074	417.8036	419.1927	426.8844
H	-3.88964	0.68185	-2.73149	435.6244	442.3827	447.9269
C	-1.96910	-3.80116	0.53193	460.9466	463.4735	477.0695
H	-0.91050	-3.80631	0.81447	514.5712	520.2088	535.2758
H	-2.55878	-3.66340	1.44304	536.9668	546.2475	547.0155
H	-2.21155	-4.78976	0.11969	554.3772	575.7160	580.7469
C	-0.06620	-3.01843	-1.87882	582.4687	584.5902	589.8623
H	0.46417	-3.20341	-0.93640	599.4198	604.8940	620.0841
H	-0.14210	-3.97437	-2.41299	643.9119	646.2283	654.7733
H	0.55467	-2.33445	-2.46700	670.6870	703.1398	757.0729
C	-1.64247	-0.83034	-3.66559	776.4544	790.9850	797.8243
H	-0.58366	-1.00931	-3.85852	802.0861	803.5642	809.5792
H	-2.23322	-1.23728	-4.49698	813.3573	816.0117	816.5696
H	-1.80246	0.25301	-3.64238	818.5308	853.1493	861.1641
C	-0.95712	-1.48209	3.32723	900.6114	904.1421	908.6041
H	-0.92337	-2.12864	4.21460	916.5925	931.5756	945.2798
H	-1.62822	-0.63977	3.53143	948.0533	950.1878	963.0362
H	-1.38401	-2.05363	2.49531	965.6664	971.0922	972.4914
C	1.02717	-0.22026	4.16616	982.1174	986.6516	1005.0498
H	1.08937	-0.86922	5.04981	1018.1948	1027.2807	1030.4447
H	2.03186	0.15553	3.94087	1041.5334	1043.8707	1044.7246
H	0.40216	0.64446	4.41328	1048.2459	1048.7521	1053.3980
C	1.34841	-2.20005	2.68490	1053.6015	1058.8125	1073.1592
H	0.95999	-2.78764	1.84501	1097.2175	1101.6121	1109.1266
H	2.36889	-1.88567	2.43291	1111.0678	1115.9758	1135.2765
H	1.41135	-2.85375	3.56491	1142.3868	1164.9217	1175.6514
C	-4.48245	3.29279	2.16977	1185.2666	1190.7968	1220.6896
H	-5.21664	2.64461	2.66361	1230.7348	1235.7993	1237.9642
H	-4.36283	4.19976	2.77702	1248.1060	1248.4903	1254.8975
H	-4.89435	3.57401	1.19548	1263.5070	1267.8017	1272.9363
C	-2.13940	3.50504	1.30597	1276.2452	1280.5873	1289.0650
H	-1.97875	4.41665	1.89707	1304.5950	1324.6676	1350.0361
H	-1.17526	2.99459	1.18177	1366.3453	1371.4379	1374.4308
H	-2.51496	3.80290	0.31758	1375.4525	1376.9777	1378.4586
C	-2.58552	2.20704	3.38832	1379.0137	1384.8386	1386.6811
H	-2.52111	3.10080	4.02350	1387.5621	1390.5533	1393.1645
H	-3.23600	1.48264	3.89701	1400.4131	1403.5936	1408.8246
H	-1.58327	1.77590	3.29597	1414.9804	1417.8401	1427.8466
Ir	-1.77258	-0.70190	-0.36672	1429.4106	1431.3232	1435.5490
C	0.94281	1.93666	-1.00041	1438.9944	1441.3223	1442.4974
C	1.64160	0.74091	-1.62734	1444.1022	1449.9010	1452.7758
O	1.05520	0.06284	-2.44871	1454.6382	1460.0521	1462.1919
C	2.99013	0.30507	-1.15176	1462.3305	1462.6069	1470.4510
C	4.15064	1.00911	-1.48078	1471.4553	1472.1508	1473.1446
C	3.09055	-0.91594	-0.49416	1475.0919	1476.0988	1477.5826
C	5.39930	0.51940	-1.10165	1480.8319	1484.9279	1490.1040
C	4.33731	-1.41264	-0.12940	1490.3686	1491.5630	1492.8118
H	2.17432	-1.45839	-0.26268	1497.3307	1507.3539	1519.7942
C	5.48927	-0.68736	-0.42446	1521.8770	1536.9202	1544.4335
H	6.29962	1.07532	-1.36138	1559.5926	1669.0756	1681.5932
H	6.46306	-1.07999	-0.14150	1740.4703	1770.0505	1777.6472

O	3.99904	2.14356	-2.20578	1810.0827	1862.9411	2817.5415
H	4.85759	2.54039	-2.38929	3017.7359	3025.0746	3031.4522
C	-0.36731	2.12911	-1.73498	3032.5483	3033.6131	3034.2378
C	1.78241	3.17076	-0.75778	3036.7475	3037.9415	3039.1300
C	3.57304	3.97139	0.53476	3041.9753	3043.7758	3046.4684
H	2.99750	4.84626	0.86039	3048.7518	3049.7618	3098.8322
H	4.11527	4.26192	-0.37587	3099.6345	3105.2737	3109.8338
C	4.48440	3.44532	1.61130	3114.9035	3118.9004	3119.7186
H	5.20494	4.21213	1.91267	3120.2888	3120.8888	3121.5206
H	3.90444	3.14595	2.48972	3124.2030	3127.0345	3129.4659
H	5.03660	2.56698	1.25786	3134.2600	3136.9489	3139.0531
O	2.66585	2.91353	0.20744	3140.5673	3142.6859	3147.0702
O	1.66471	4.24455	-1.30075	3147.3821	3150.2291	3150.7488
C	-0.42196	3.01675	-2.92989	3157.2138	3161.1766	3168.9758
H	-1.40379	2.94488	-3.40346	3172.5569	3181.8452	3197.9697
H	-0.19458	4.04759	-2.64313	3200.8116	3204.1927	3893.1175
H	0.36859	2.71287	-3.62882			
O	-1.35520	1.49801	-1.38162			
C	4.46673	-2.71052	0.60042			
F	5.50110	-3.42965	0.14391			
F	4.68608	-2.52054	1.91103			
F	3.36928	-3.46658	0.48708			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.756624 Electronic Energy = -2403.31319626
Internal Energy (E)= -2402.50450226 Enthalpy (H)= -2402.50355926
Gibbs Free Energy (G)=-2402.63903126 Gibbs Free Energy of Solvation=-2402.7092724

St.Pt.	General Structure	Ball & Stick model
X-6	 **X-6**	

Cartesian co-ordinate

Atoms	X	Y	Z
C	0.70165	1.46686	0.10875
C	0.62019	0.09554	-0.09820
C	-0.68951	-0.55832	-0.29969
C	-1.64057	1.70293	-0.03245
O	-0.41530	2.24706	0.13174
C	1.80130	-0.65104	-0.12514
C	1.92270	2.11429	0.29638
C	3.01776	-0.02470	0.05724
C	3.07778	1.36075	0.27039
H	1.72053	-1.72097	-0.29663
H	1.93629	3.18857	0.45380
O	-0.77067	-1.74929	-0.54921
C	-1.83214	0.36497	-0.21023
C	-2.68017	2.76513	0.01103
H	-2.94661	3.06713	-1.00763
H	-3.60137	2.41286	0.47657
H	-2.28822	3.63364	0.54575
C	-3.22630	-0.12532	-0.38045
C	-4.70200	-1.91257	0.02823
H	-4.52235	-2.98744	0.11916
H	-5.07426	-1.69670	-0.97878
C	-5.65541	-1.41138	1.08507
H	-6.61258	-1.93808	1.01214
H	-5.24681	-1.58078	2.08656
H	-5.84402	-0.34162	0.95566
O	-4.10344	0.50223	-0.93740
O	-3.40261	-1.31957	0.18266
C	4.30533	-0.78966	0.04151
H	4.04475	1.83860	0.41037
F	5.15736	-0.27594	-0.85616
F	4.91884	-0.72529	1.23147
F	4.12904	-2.07694	-0.25464

Frequencies

23.7218	36.9018	44.5368
64.5874	76.0292	102.5440
130.8221	137.9469	155.5241
162.3247	202.5623	216.7223
245.9240	248.9933	269.2182
288.1418	308.2948	360.4350
390.6745	398.3965	414.9693
420.6851	442.3180	480.9545
505.5173	528.6305	553.9331
574.2293	591.3336	603.2603
622.8733	665.2602	679.5402
719.3753	753.4658	773.5255
787.3768	816.6681	838.7599
839.4308	886.8902	898.2076
947.1607	953.4255	969.2415
1017.4456	1042.9652	1049.6715
1104.1157	1115.8183	1129.7050
1141.6667	1163.9384	1195.8993
1234.8823	1236.4005	1267.1533
1272.1248	1284.9891	1314.8050
1342.2401	1365.0199	1386.2742
1393.0227	1408.9502	1415.3588
1424.9691	1455.3795	1466.9842
1472.5158	1476.8069	1490.8818
1491.5512	1539.2563	1636.9862
1679.0297	1696.6122	1807.2829
1830.3850	3050.1855	3064.8931
3075.0161	3132.4566	3140.6495
3148.7141	3157.7760	3187.3353
3192.4607	3217.0257	3222.4765

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.232536 Electronic Energy = -1139.97203811
Internal Energy (E)= -1139.72099811 Enthalpy (H)= -1139.72005411
Gibbs Free Energy (G)=-1139.78782411 Gibbs Free Energy of Solvation=-1139.8068619

2-Step C-H metalation of path-B

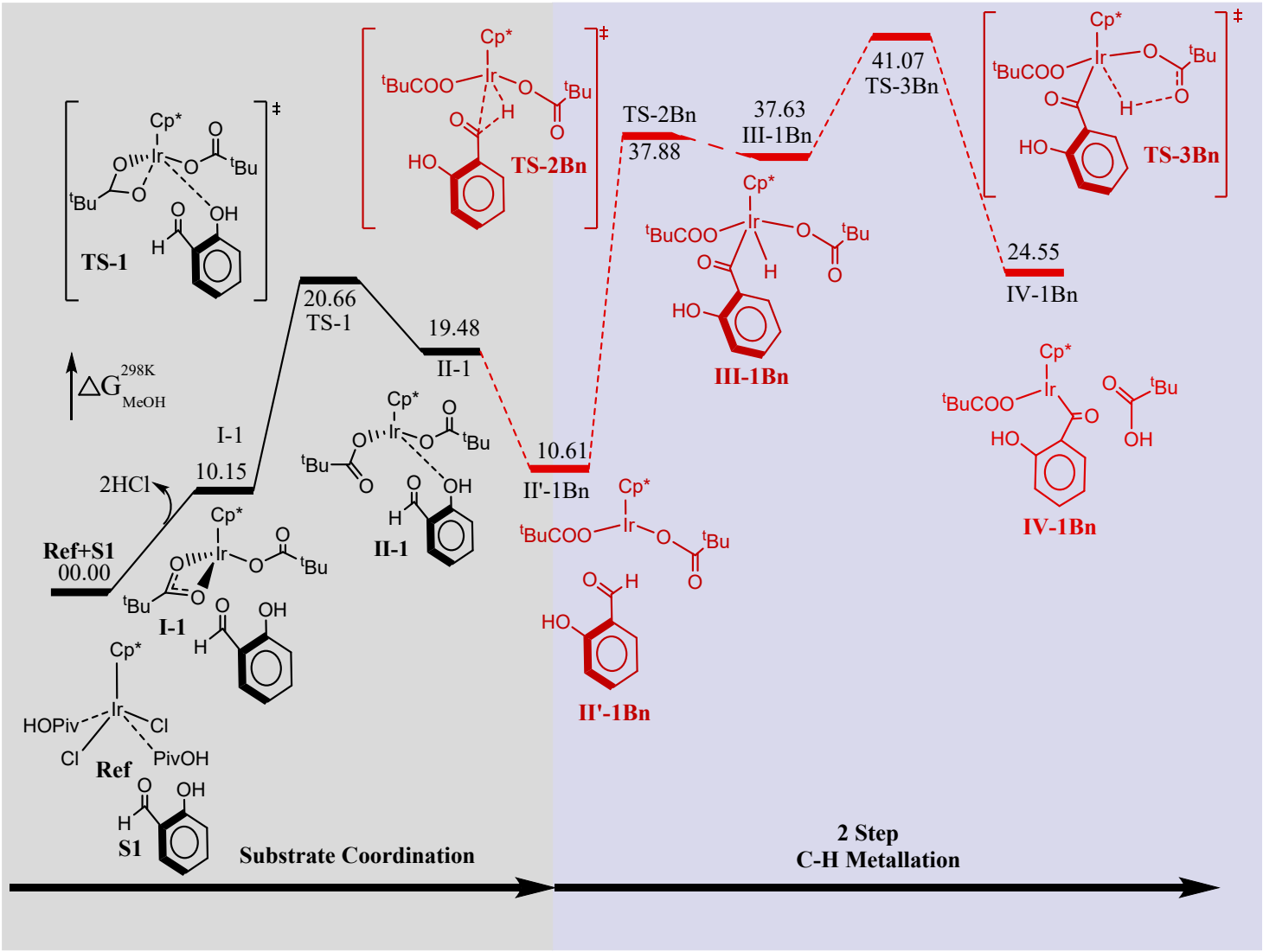
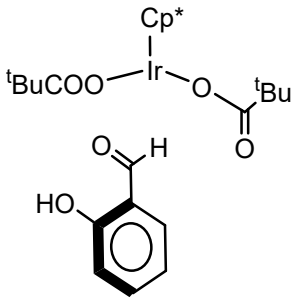
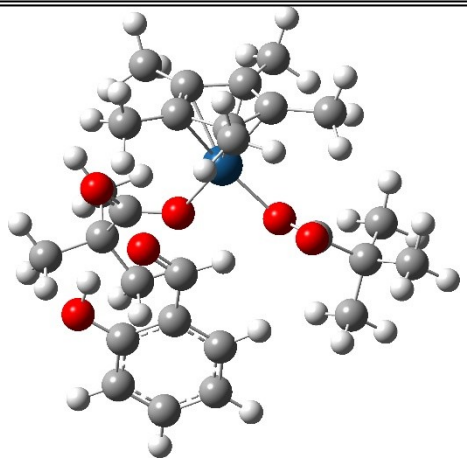


Fig-29: PES with Gibbs free energy (kcal/mol) and the structures of the stationary points for S1 using M06L functional & 6-311++G(d,p) basis set for non-metal and triple-zeta SDD for Ir metal (black and red colour represent common path and 2-step C-H metalation for Path-B respectively)

Details of coordinates from II'-1Bn to IV-1Bn are given below.

St.Pt.	General Structure	Ball & Stick model
III'-1Bn	 **II'-1Bn**	

Cartesian co-ordinate

Atoms	X	Y	Z
C	-2.14175	-1.01366	1.65460
C	-3.04402	-0.65617	0.59993
C	-2.80958	-1.57836	-0.48080
C	-1.82362	-2.56880	-0.05068
C	-1.42389	-2.22844	1.27195
C	2.39883	1.27171	1.43146
Ir	-0.97658	-0.57449	-0.11035
C	2.20095	2.53512	0.85720
C	3.23998	3.20308	0.23927
C	3.66903	0.65657	1.35817
C	4.50176	2.59644	0.19539
C	4.72125	1.34129	0.74057
H	5.69424	0.85826	0.69511
H	5.32922	3.11406	-0.28564
H	3.08433	4.18300	-0.20433
H	0.32466	1.16788	2.06610
O	-0.85548	1.35607	-0.79687
C	-1.30865	2.35512	-0.10073
C	-1.59330	3.61062	-0.93564
O	-1.46741	2.34707	1.12034
H	1.20253	2.97057	0.92178
C	1.28992	0.61558	2.09108
O	1.36922	-0.47714	2.65601
O	3.89773	-0.56401	1.84483
C	-2.50331	4.54759	-0.15057
H	-2.05103	4.82848	0.80542
H	-2.69843	5.45840	-0.73138
H	-3.46694	4.06906	0.06887
C	-0.25452	4.29910	-1.21616
H	0.43789	3.62319	-1.73215
H	-0.41349	5.18365	-1.84693
H	0.21649	4.63653	-0.28256
C	-2.25468	3.22442	-2.25760
H	-3.19795	2.68677	-2.08576
H	-2.48865	4.12636	-2.83824

Frequencies

37.7396	42.6764	47.4883
54.3861	59.0842	68.0875
75.3038	81.5836	85.0121
95.0762	98.3192	105.7102
118.1788	124.6264	135.6802
145.8634	155.2050	156.7200
161.6739	171.1244	179.8615
194.9674	208.7761	210.9795
214.3512	217.6102	226.4825
236.2821	241.6218	245.5495
252.4871	262.2124	264.7910
276.0636	282.6604	286.6914
291.8729	297.7183	301.8961
308.9611	313.1500	317.3074
323.9191	331.0840	333.7561
338.8000	349.2041	362.1841
382.2646	388.9164	391.7957
394.5596	419.5143	431.6983
436.2378	447.9093	456.3739
461.2596	470.6776	471.6153
535.4527	539.1659	545.4865
557.6894	569.7345	572.6801
574.9121	580.2135	585.2362
602.9179	626.4273	656.5079
677.1336	739.1346	787.2833
795.2542	796.9547	805.3338
807.6019	812.5954	814.5749
819.3451	879.6266	890.9601
913.6020	917.7903	946.2350
947.8797	949.7723	950.6012
955.7131	957.9712	958.8847
981.3440	984.1155	1008.1734
1024.4849	1033.8978	1036.6141
1037.4554	1038.9982	1040.2515
1042.2739	1046.4385	1051.6619
1054.7725	1063.9621	1093.5702
1104.1533	1112.9004	1132.4847
1139.7678	1170.1486	1186.2098
1192.5642	1224.0777	1234.5679

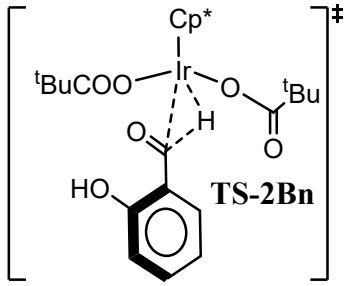
H	-1.60279	2.58106	-2.85583	1237.5260	1241.7674	1246.8055
C	-3.99767	0.48773	0.59108	1266.6375	1266.8968	1272.0649
H	-4.11904	0.89346	-0.42055	1342.5457	1351.6498	1366.3348
H	-4.98704	0.17027	0.94377	1371.2851	1375.1750	1377.0991
H	-3.64011	1.30537	1.22510	1378.3583	1383.2384	1388.4332
C	-1.99568	-0.31396	2.95636	1388.8622	1390.0905	1401.1676
H	-2.14780	0.76296	2.83522	1405.8003	1411.4651	1418.4936
H	-2.73096	-0.70221	3.67373	1424.4263	1429.1983	1432.0354
H	-0.99502	-0.47505	3.37169	1437.7144	1441.1541	1443.3803
C	-0.51642	-2.99629	2.16007	1448.5863	1449.8990	1451.4342
H	0.13240	-2.32906	2.73394	1455.2020	1458.0209	1459.0434
H	-1.12185	-3.58803	2.86058	1462.6564	1467.2284	1468.9058
H	0.12908	-3.66420	1.58834	1470.1446	1474.9217	1476.2159
C	-1.30907	-3.70299	-0.86358	1477.3667	1479.5965	1482.5468
H	-0.27376	-3.92794	-0.58735	1488.9763	1496.1363	1501.5267
H	-1.91924	-4.60363	-0.72015	1504.8783	1507.6150	1509.6947
H	-1.31636	-3.45633	-1.93148	1516.0258	1524.6033	1534.2691
C	-3.48590	-1.53456	-1.80356	1549.1951	1644.5686	1693.0806
H	-2.91913	-2.08079	-2.56333	1737.5141	1756.9275	1779.9915
H	-4.48549	-1.98368	-1.73841	2942.4283	3020.6837	3020.8939
H	-3.60033	-0.50136	-2.14965	3023.6518	3030.2839	3036.2434
H	3.05105	-0.91068	2.20550	3039.3674	3040.2856	3040.4936
O	0.85158	-0.57425	-0.92094	3041.7834	3043.5796	3044.1604
C	1.71033	-1.56285	-0.77820	3099.2755	3104.3729	3108.9782
C	2.81395	-1.56887	-1.83777	3110.0830	3115.5552	3117.7383
C	3.14184	-0.17023	-2.34911	3118.5719	3122.4463	3123.2153
H	2.26009	0.32222	-2.76923	3132.7075	3133.4613	3133.7595
H	3.53183	0.46569	-1.54496	3144.4848	3146.6289	3147.0398
H	3.91309	-0.23687	-3.12838	3153.9159	3155.3348	3157.9211
C	4.06301	-2.23511	-1.27224	3161.0602	3164.7915	3169.9505
H	3.83937	-3.24469	-0.91360	3175.6751	3181.3258	3197.0916
H	4.83792	-2.29796	-2.04733	3201.6513	3205.8107	3534.2665
H	4.46279	-1.66434	-0.42468			
C	2.25016	-2.41540	-2.98848			
H	2.01131	-3.43090	-2.64661			
H	1.34011	-1.96145	-3.40267			
H	2.98983	-2.49292	-3.79607			
O	1.62308	-2.43911	0.06873			

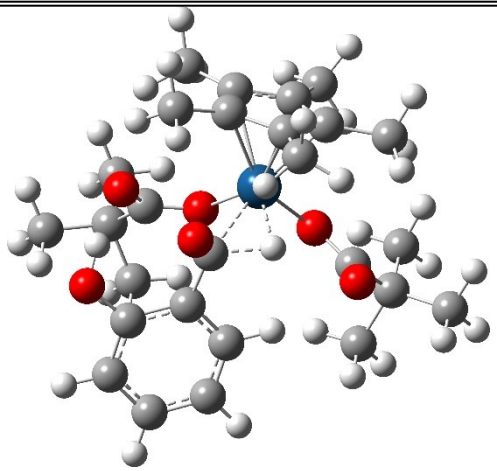
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.615576 Electronic Energy = -1607.51026459
Internal Energy (E)= -1606.85648659 Enthalpy (H)= -1606.85554359
Gibbs Free Energy (G)=-1606.96101059 Gibbs Free Energy of Solvation=-1608.01287944

St.Pt.	General Structure	Ball & Stick model

TS-2Bn





Cartesian co-ordinate

Atoms	X	Y	Z
C	1.79936	-2.11451	-1.29595
C	2.62701	-1.53914	-0.27222
C	2.04788	-1.89302	1.01936
C	0.88969	-2.69387	0.77123
C	0.69950	-2.80192	-0.65147
C	-1.77022	0.98764	-1.46486
Ir	0.65944	-0.62105	-0.15000
C	-1.28535	2.28142	-1.24089
C	-2.14011	3.37208	-1.22266
C	-3.16024	0.78512	-1.61802
C	-3.50699	3.17097	-1.41234
C	-4.01217	1.89257	-1.59439
H	-5.07758	1.70816	-1.70891
H	-4.18910	4.01835	-1.39980
H	-1.74246	4.37247	-1.07306
H	0.54682	0.37458	-1.50129
O	1.40788	1.14254	0.69456
C	1.98343	2.01702	-0.07388
C	2.52324	3.23489	0.68837
O	2.04642	1.95785	-1.30121
H	-0.21137	2.42761	-1.15049
C	-0.81993	-0.11906	-1.70984
O	-0.94140	-0.91642	-2.61097
O	-3.72813	-0.42199	-1.75895
C	3.67688	3.85241	-0.09339
H	3.36821	4.10414	-1.11212
H	4.02817	4.76282	0.40926
H	4.52283	3.15594	-0.16445
C	1.35456	4.22437	0.76475
H	0.49351	3.77852	1.28005
H	1.65772	5.12675	1.31165
H	1.03805	4.52624	-0.24230
C	2.97942	2.86421	2.09566
H	3.78910	2.12129	2.06722
H	3.36456	3.75416	2.61038
H	2.15768	2.44715	2.68586
C	3.90474	-0.79881	-0.45112
H	4.02077	-0.02483	0.31596

Frequencies

-317.5848	-35.6174	38.2066
44.3614	45.7025	50.9319
63.6406	72.3465	82.3314
86.3569	93.8394	107.4398
115.7187	126.5623	135.0315
150.1228	151.9447	165.7261
167.9358	170.1637	178.2431
181.9589	187.4904	198.3387
214.9679	217.2830	222.1725
232.7034	237.0582	244.5654
254.6290	262.0405	263.6053
274.5019	282.2576	286.8897
295.6236	304.3106	306.2170
317.3185	320.2324	323.7628
327.5537	331.1204	344.6144
349.8477	361.6076	364.4258
374.3939	375.8388	396.2043
398.9154	408.8538	414.4247
430.3377	437.1663	445.4840
459.4260	462.8375	501.8225
534.4461	536.6229	542.2024
551.2917	559.1836	563.5500
571.0717	586.9194	594.4439
598.2672	604.4318	637.9064
647.3817	658.5959	711.3165
763.5006	775.7459	795.5165
796.6634	809.2279	816.1441
818.3871	820.4854	836.7151
872.2449	888.3179	915.3332
920.7678	933.2453	945.3373
948.4858	949.4346	951.1052
952.2186	955.6467	958.7241
967.4269	981.1403	985.1935
1028.6811	1034.4697	1035.2643
1039.2587	1041.2678	1042.3061
1046.5605	1049.0871	1049.8487
1065.3183	1091.9212	1096.6732
1113.9317	1126.6860	1157.5135
1183.5339	1187.8287	1203.2262
1236.9493	1241.0295	1248.7962
1252.2660	1263.6676	1266.4890
1267.1543	1308.4102	1359.2400
1363.2796	1368.6971	1370.0104

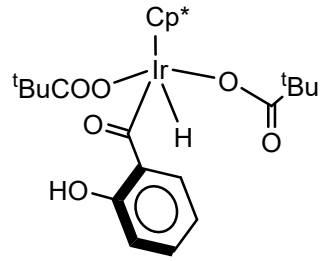
H	4.75597	-1.48632	-0.36046	1373.8075	1374.4243	1381.7803
H	3.95975	-0.30851	-1.42653	1384.5373	1387.1510	1392.4639
C	2.02104	-2.02913	-2.76425	1398.6804	1402.2064	1404.3437
H	2.71343	-1.21909	-3.01310	1411.0307	1430.0099	1434.4589
H	2.43805	-2.96984	-3.14439	1438.8109	1441.7938	1444.5087
H	1.07434	-1.83720	-3.28043	1445.3391	1449.4987	1454.4934
C	-0.35699	-3.60462	-1.32242	1455.7939	1460.9451	1462.7125
H	-0.47088	-3.30731	-2.36732	1465.7151	1467.0116	1470.0675
H	-0.10628	-4.67268	-1.28726	1473.3981	1474.8634	1478.6817
H	-1.32280	-3.45065	-0.83149	1479.1257	1481.6997	1486.9346
C	-0.02353	-3.26076	1.79592	1487.5685	1492.0897	1501.1565
H	-1.06200	-3.22840	1.45173	1503.6047	1506.1761	1508.2243
H	0.24243	-4.30683	1.99593	1517.4361	1521.4598	1522.6357
H	0.04260	-2.70906	2.73879	1534.1140	1632.1085	1673.5688
C	2.60724	-1.48822	2.33745	1708.2300	1730.2002	1767.1048
H	1.90693	-1.70161	3.15039	1857.0027	3016.6317	3020.8085
H	3.54437	-2.01926	2.54835	3024.3222	3027.7679	3031.0271
H	2.81270	-0.41126	2.35441	3035.3759	3038.5499	3041.3319
H	-3.20422	-1.08630	-1.26749	3045.0409	3046.5741	3048.9523
O	-0.89562	-0.07815	1.15278	3100.8499	3101.0760	3109.0016
C	-2.05029	-0.64536	1.08257	3109.2943	3112.0444	3116.6063
C	-3.05547	-0.12302	2.11527	3119.4191	3121.7009	3123.5385
C	-3.05028	1.40578	2.12227	3127.8533	3128.5726	3134.0798
H	-2.05270	1.80223	2.33783	3136.6097	3137.0010	3144.7243
H	-3.36893	1.80550	1.15037	3145.7096	3147.2577	3150.5320
H	-3.74954	1.77477	2.88422	3157.0976	3166.2669	3167.6050
C	-4.45148	-0.64031	1.78790	3180.6635	3183.9404	3195.4600
H	-4.48227	-1.73503	1.79416	3205.5720	3213.9481	3664.4481
H	-5.16870	-0.26644	2.53007			
H	-4.77842	-0.30746	0.79500			
C	-2.61049	-0.65219	3.48175			
H	-2.60381	-1.75097	3.49577			
H	-1.60573	-0.29282	3.73304			
H	-3.30589	-0.31245	4.26009			
O	-2.34848	-1.55168	0.29019			

Statistical Thermodynamic Analysis

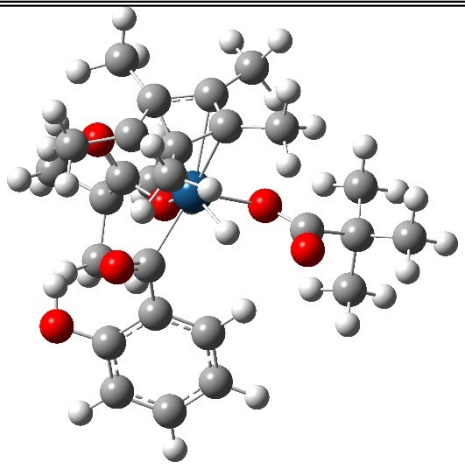
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.609181 Electronic Energy = -1607.47347569
Internal Energy (E)= -1606.82732169 Enthalpy (H)= -1606.82637869
Gibbs Free Energy (G)=-1606.92857469 Gibbs Free Energy of Solvation=-1607.96941719

St.Pt.	General Structure	Ball & Stick model

III-1Bn



III-1Bn



Cartesian co-ordinate

Atoms	X	Y	Z
C	1.65475	-2.22429	-1.26542
C	2.59233	-1.54801	-0.39011
C	2.22765	-1.85092	0.98158
C	1.04304	-2.61599	0.95423
C	0.64800	-2.82373	-0.43035
C	-1.78804	0.90487	-1.50197
Ir	0.62854	-0.58933	-0.25009
C	-1.21180	2.17431	-1.39791
C	-1.99454	3.31890	-1.42588
C	-3.19270	0.78674	-1.58889
C	-3.37882	3.19831	-1.53566
C	-3.97188	1.94705	-1.60515
H	-5.05084	1.82670	-1.66417
H	-4.00447	4.08819	-1.55279
H	-1.52894	4.29957	-1.36991
H	1.12923	0.27254	-1.49804
O	1.30254	1.18585	0.62231
C	1.99027	2.04226	-0.07351
C	2.44232	3.26491	0.73488
O	2.22069	1.96241	-1.27918
H	-0.12776	2.25831	-1.35743
C	-0.92591	-0.29815	-1.65489
O	-1.11495	-1.11245	-2.52546
O	-3.84615	-0.38610	-1.63326
C	3.70154	3.85085	0.10599
H	3.53588	4.09590	-0.94700
H	3.99846	4.76126	0.64218
H	4.53658	3.13996	0.15641
C	1.29218	4.27338	0.63136
H	0.36232	3.86112	1.04434
H	1.54245	5.18728	1.18549
H	1.11528	4.54725	-0.41685
C	2.69951	2.91404	2.19612
H	3.49896	2.16501	2.28619
H	3.02108	3.80961	2.74362
H	1.80180	2.51359	2.67736
C	3.83580	-0.83512	-0.79417
H	4.08861	-0.04810	-0.07486

Frequencies

25.4186	35.3709	41.4152
51.8978	57.3301	71.4564
76.3834	87.4476	96.6656
103.1107	111.4553	121.9204
133.6549	142.8179	148.6080
154.5532	159.8634	167.3200
169.8251	172.8562	180.6813
186.5634	187.1881	191.9834
199.0048	211.4553	222.3924
226.6448	238.1267	246.5603
257.7830	264.8877	281.7112
283.9705	285.7390	290.1640
301.6827	305.5999	317.8839
325.5627	328.3465	334.4321
341.7515	354.7067	355.3248
358.9417	371.7847	373.8008
378.0936	380.0800	393.0861
398.9230	401.4341	407.5708
440.3337	447.9793	451.5175
462.5971	480.9676	529.0427
535.0513	537.6005	556.6006
563.9590	571.3101	573.1985
593.2220	595.7308	604.4806
618.6616	629.8455	635.3573
646.6351	651.1717	740.7187
749.4918	775.8403	793.4803
796.3350	812.1540	818.7508
820.0683	823.9089	824.2705
861.1147	873.8158	895.6694
918.1603	925.1270	938.2304
946.7492	954.8586	956.7353
957.4685	963.4523	970.4762
972.5729	973.2435	988.5569
1027.5164	1034.9114	1037.4409
1042.0600	1043.0898	1043.2286
1043.7737	1052.5714	1054.8234
1064.5774	1094.3034	1099.5602
1116.5163	1122.1928	1158.3956
1181.5679	1192.2526	1197.8389
1235.9619	1241.2615	1246.9541
1250.6684	1258.1722	1265.3019
1266.3610	1305.4448	1357.8071
1361.1418	1374.1273	1376.1265

H	4.67914	-1.53685	-0.83695	1376.9212	1378.8107	1379.6268
H	3.72902	-0.35463	-1.76997	1381.7373	1388.0596	1397.5083
C	1.76232	-2.36647	-2.74169	1398.2367	1401.7910	1402.8896
H	2.46110	-1.63687	-3.16224	1412.6325	1423.6819	1426.4385
H	2.12057	-3.37128	-2.99864	1436.4427	1442.8336	1448.0250
H	0.78570	-2.21627	-3.21046	1448.5151	1456.5392	1457.9658
C	-0.44966	-3.70627	-0.90618	1458.7225	1461.2829	1462.6276
H	-0.81397	-3.36528	-1.87959	1464.8011	1468.0719	1471.2759
H	-0.08852	-4.73808	-1.00930	1473.2098	1475.5168	1480.4483
H	-1.29933	-3.68935	-0.21903	1480.7223	1482.4691	1485.6580
C	0.25580	-3.06813	2.12968	1486.8843	1492.0518	1499.7947
H	-0.80934	-3.12613	1.88382	1501.4500	1505.4393	1514.8654
H	0.58041	-4.06834	2.44512	1516.2350	1521.8730	1525.2372
H	0.37508	-2.38791	2.97882	1559.0844	1633.0221	1674.1166
C	2.92500	-1.30195	2.17641	1719.9775	1735.0889	1809.4785
H	2.56669	-1.76303	3.10097	2101.7357	3017.4567	3019.4843
H	4.00647	-1.47073	2.11356	3023.7050	3026.3961	3027.9636
H	2.75646	-0.21744	2.25066	3032.8637	3033.9946	3038.2538
H	-3.32146	-1.07481	-1.18194	3040.1978	3041.7850	3050.1588
O	-0.85474	-0.15314	1.16885	3101.6082	3102.4781	3105.0842
C	-2.03556	-0.68032	1.13929	3110.6475	3112.8102	3112.9922
C	-2.98536	-0.10452	2.19663	3116.8407	3118.9513	3120.2469
C	-2.99748	1.42191	2.08926	3122.2862	3123.7325	3129.7831
H	-1.99194	1.83776	2.21220	3131.6366	3132.7758	3140.1824
H	-3.38501	1.74885	1.11513	3145.9261	3146.7380	3149.2803
H	-3.64993	1.83967	2.86730	3150.5658	3165.0231	3175.1450
C	-4.38958	-0.65363	1.97714	3175.1680	3177.7710	3194.3989
H	-4.40782	-1.74601	2.05604	3202.8660	3212.8441	3695.6711
H	-5.07304	-0.23819	2.72881			
H	-4.76541	-0.38694	0.98165			
C	-2.46409	-0.51802	3.57558			
H	-2.43673	-1.61130	3.68144			
H	-1.45628	-0.12364	3.74779			
H	-3.12742	-0.12611	4.35733			
O	-2.39007	-1.57022	0.35819			

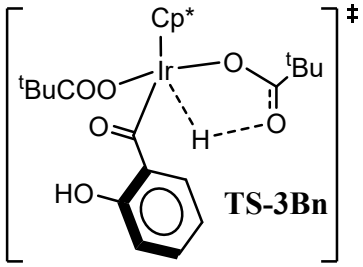
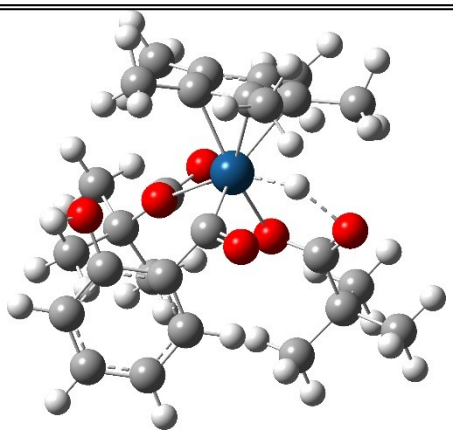
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm

Zero-point correction= 0.611190 Electronic Energy = -1607.47866916

Internal Energy (E)= -1606.82942116 Enthalpy (H)= -1606.82847816

Gibbs Free Energy (G)=-1606.93359316 Gibbs Free Energy of Solvation=-1607.96982678

St.Pt.	General Structure	Ball & Stick model
TS-3Bn		

Cartesian co-ordinate

Atoms	X	Y	Z
C	2.26403	-1.89331	-0.74631
C	2.86465	-0.84317	0.04969
C	2.43167	-0.99185	1.43115
C	1.50486	-2.03611	1.47042
C	1.31532	-2.54898	0.10942
C	-1.80929	-0.29427	-1.91953
Ir	0.70551	-0.47147	-0.21864
C	-2.25356	1.01195	-2.11421
C	-3.61273	1.30550	-2.12251
C	-2.74035	-1.31126	-1.72820
C	-4.53773	0.28088	-1.94462
C	-4.10161	-1.02411	-1.74538
H	-4.81227	-1.83336	-1.58304
H	-5.60344	0.49715	-1.95221
H	-3.94704	2.32751	-2.28244
H	1.50758	0.47694	-1.32305
O	0.33229	1.57182	0.08547
C	1.01022	2.37956	-0.64620
C	0.88302	3.84742	-0.25904
O	1.76313	1.99823	-1.56303
H	-1.51616	1.79555	-2.28369
C	-0.32986	-0.54232	-1.97858
O	0.20953	-0.68336	-3.05267
O	-2.28669	-2.58792	-1.51649
C	0.49303	-3.74487	-0.22246
H	0.35230	-3.83734	-1.30379
H	0.97374	-4.66163	0.14513
H	-0.50476	-3.66690	0.22232
C	2.64380	-2.24832	-2.14101
H	3.66986	-2.63655	-2.16220
H	1.98049	-3.01560	-2.54987
H	2.57344	-1.38428	-2.80916
C	3.96156	0.06394	-0.38833
H	4.93117	-0.35279	-0.08396
H	3.96757	0.19880	-1.47325
H	3.86152	1.05562	0.06615

Frequencies

-375.8615	-80.0690	-34.3900
-16.8034	12.3076	16.3955
26.0443	41.8810	49.1563
66.7238	72.5962	77.1078
78.0413	90.6267	103.2076
111.4238	116.1435	128.8969
144.5115	156.5209	160.7742
170.4186	175.4832	178.2546
180.7154	188.1364	198.1657
202.5218	202.9153	214.5957
224.7715	233.6893	240.2948
247.7626	248.7363	255.9849
258.0983	272.2139	275.2609
281.7250	293.1695	294.2931
302.2606	308.5437	310.4926
329.8568	334.9901	344.8495
349.9325	364.6560	373.9466
376.4203	391.4783	393.3057
418.1282	429.5083	431.5426
440.3656	446.5396	494.7631
504.4686	533.1108	538.8635
541.8119	550.4663	560.4277
571.6927	594.1216	610.0518
615.0737	620.7108	634.8620
646.3699	651.8257	683.2796
738.1932	752.3399	793.8748
794.7102	808.4818	815.4960
818.8711	827.5769	837.7482
845.2032	885.0975	909.0576
917.7994	944.2230	944.8203
946.2286	948.8176	949.0468
952.8319	955.2025	956.9981
961.7506	963.1527	977.6052
1024.4342	1031.5070	1032.5662
1037.3128	1038.3756	1044.4975
1045.4355	1047.1240	1053.0142
1063.3899	1082.8405	1087.7204
1107.5908	1107.9230	1153.2901
1175.3968	1177.7699	1189.4855
1218.6882	1232.4224	1235.7051

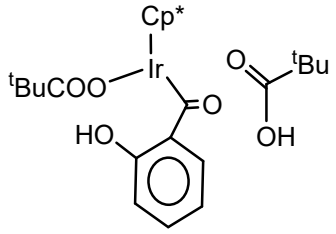
C	2.82524	-0.06344	2.52280	1236.7778	1254.8966	1265.5394
H	3.91261	-0.06032	2.67174	1269.7845	1288.9646	1298.7652
H	2.50302	0.95750	2.27714	1357.8368	1364.3141	1367.1574
H	2.33635	-0.31854	3.46522	1370.2161	1371.2363	1372.0855
C	0.70244	-2.52986	2.61576	1375.2310	1380.2968	1387.0499
H	0.95115	-2.02302	3.55051	1388.0388	1395.3853	1406.5344
H	-0.36422	-2.36530	2.41314	1407.1202	1420.9533	1424.9628
H	0.84640	-3.61092	2.74024	1429.6401	1433.6328	1436.9318
C	1.55722	3.97414	1.11368	1440.1776	1443.8724	1443.9948
H	1.52431	5.01783	1.45150	1447.8829	1448.8656	1449.6645
H	1.04862	3.34477	1.85438	1453.1658	1459.5276	1460.2991
H	2.61293	3.67201	1.06196	1461.1026	1463.0764	1466.9578
C	1.58522	4.73242	-1.27946	1467.7730	1471.2640	1471.8515
H	1.13597	4.62604	-2.27351	1474.5637	1475.0430	1480.6022
H	1.50657	5.78411	-0.97626	1492.2491	1495.1572	1499.3653
H	2.64540	4.47279	-1.36703	1502.5417	1515.9713	1534.3649
C	-0.59134	4.23247	-0.14081	1578.9867	1586.2730	1654.8852
H	-0.67376	5.28043	0.17432	1667.6601	1756.6907	1763.5965
H	-1.10763	4.13348	-1.10436	1810.0952	3016.1040	3019.0627
H	-1.10804	3.60398	0.59160	3021.7733	3028.4466	3029.8501
H	-2.82311	-3.19644	-2.03425	3030.9263	3031.9145	3034.3957
O	-1.14280	-0.57796	0.80077	3036.9953	3037.2417	3042.9836
C	-1.13971	0.00409	1.96930	3098.3490	3101.0877	3101.2810
C	-2.53058	0.24302	2.57540	3102.1009	3102.9443	3111.4114
C	-2.50641	-0.30339	4.00541	3116.0909	3118.4892	3122.4460
H	-1.69625	0.15623	4.58085	3123.3146	3128.0873	3129.3173
H	-3.46099	-0.09738	4.50706	3130.2014	3138.7452	3139.2550
H	-2.35607	-1.39257	4.01089	3140.4073	3145.8231	3147.3735
C	-3.64390	-0.42663	1.78273	3150.9363	3158.4474	3160.2548
H	-3.78357	0.05493	0.80797	3165.6558	3170.4279	3172.3387
H	-3.41894	-1.48354	1.59572	3188.6304	3203.2064	3903.5707
H	-4.59046	-0.36501	2.33671			
C	-2.73248	1.76063	2.60577			
H	-1.84316	2.25666	3.01130			
H	-2.91990	2.14780	1.59492			
H	-3.59448	2.02330	3.23388			
O	-0.14008	0.34374	2.59385			

Statistical Thermodynamic Analysis

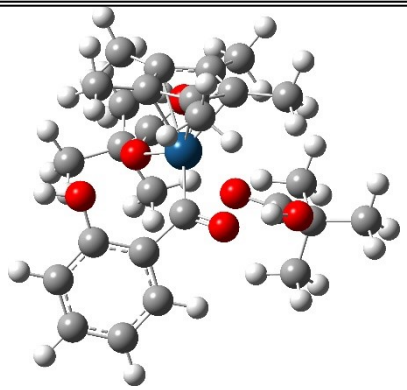
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.603853 Electronic Energy = -1607.45391349
Internal Energy (E)= -1606.81254149 Enthalpy (H)= -1606.81159749
Gibbs Free Energy (G)=-1606.91853449 Gibbs Free Energy of Solvation=-1607.96433682

St.Pt.	General Structure	Ball & Stick model

IV-1Bn



IV-1Bn



Cartesian co-ordinate

Atoms	X	Y	Z
C	0.97541	-2.79725	-0.58290
C	2.10902	-2.01358	-0.20265
C	2.03822	-1.77429	1.24789
C	0.84126	-2.31083	1.72052
C	0.11105	-2.87929	0.58151
C	-2.05944	0.05629	-1.80331
Ir	0.29478	-0.83255	-0.00170
C	-2.30129	1.30473	-2.38249
C	-3.57062	1.86984	-2.39179
C	-3.14032	-0.64495	-1.25860
C	-4.63152	1.16260	-1.83677
C	-4.41969	-0.09479	-1.28362
H	-5.25263	-0.66066	-0.86551
H	-5.63385	1.58461	-1.83717
H	-3.73060	2.85095	-2.83101
H	1.44381	0.50453	-2.43850
O	1.15126	1.24496	-0.20797
C	1.93761	1.70850	-1.03879
C	2.70799	2.97481	-0.71734
O	2.13554	1.21028	-2.23008
H	-1.45442	1.83658	-2.81256
C	-0.63187	-0.36760	-1.72484
O	0.04453	-0.21848	-2.75712
O	-2.91437	-1.88476	-0.75929
C	-1.09797	-3.73401	0.73220
H	-1.59734	-3.90018	-0.22525
H	-0.81898	-4.70973	1.15461
H	-1.82193	-3.26957	1.41079
C	0.71081	-3.39557	-1.92001
H	1.17308	-4.38750	-2.00383
H	-0.36571	-3.50458	-2.09373
H	1.10280	-2.76244	-2.72250
C	3.28883	-1.68329	-1.05119
H	4.06615	-2.45366	-0.95678
H	3.01582	-1.60657	-2.10871
H	3.73874	-0.72779	-0.75521
C	3.02870	-0.96337	2.00353
H	4.00600	-1.46264	2.04183
H	3.17073	0.01686	1.52995
H	2.68840	-0.77137	3.02349
C	0.27804	-2.24678	3.09438

Frequencies

20.7694	41.9947	49.8012
57.5807	67.0959	75.0513
80.3969	86.1306	94.2065
97.4139	118.5006	122.3450
130.7426	132.2030	141.8114
153.6291	159.1802	164.2559
173.0246	181.6381	184.6970
189.8236	193.8775	205.9385
213.4015	228.8969	232.4189
237.4643	243.0111	252.6607
264.6014	269.6255	272.2353
278.9519	298.1800	301.1858
304.7556	311.7401	316.6478
321.6732	322.1108	329.0219
330.6656	334.5823	347.5696
357.0357	372.7094	375.4053
383.8522	391.0178	395.2903
403.7643	406.9062	422.3670
426.6182	445.9943	448.2538
458.7127	488.3098	516.9662
531.5347	535.8343	548.9980
550.8069	554.2303	572.6438
574.7188	594.2749	605.2987
613.5616	621.3537	645.3417
656.6859	683.5081	751.3259
755.4480	777.8182	792.1741
796.4454	807.4937	810.3340
821.0979	834.8830	853.5018
899.1148	910.1751	918.0235
931.8330	950.6523	951.9641
953.7180	957.2308	963.1422
963.9686	965.4559	965.6561
966.6651	985.2195	1040.4019
1041.3119	1042.6442	1044.3175
1045.2489	1046.4326	1046.6605
1048.1470	1060.3886	1073.5240
1092.3054	1096.5554	1107.5159
1112.8271	1160.5310	1182.4753
1185.7777	1186.9157	1234.2922
1235.6077	1236.4518	1249.1811
1252.0572	1269.1477	1270.1931
1301.1773	1328.8428	1365.1975
1369.4271	1370.1497	1376.8676
1377.0472	1379.5602	1380.8885
1388.4546	1390.5443	1392.5379

H	0.83009	-1.55024	3.72880	1403.4012	1411.1504	1416.8235
H	-0.75921	-1.89412	3.06154	1417.1901	1432.2596	1437.4933
H	0.28207	-3.24181	3.56001	1445.3124	1449.0280	1451.3256
C	3.10897	2.95542	0.75646	1453.5355	1457.4518	1457.5536
H	3.54450	3.92268	1.03468	1462.8402	1463.7154	1464.9709
H	2.25128	2.74632	1.40517	1468.5291	1470.8828	1471.4056
H	3.86816	2.18344	0.94325	1475.3549	1476.7844	1479.4934
C	3.93865	3.12469	-1.60557	1480.6347	1483.6552	1484.3386
H	3.66975	3.18737	-2.66460	1485.6337	1490.5253	1496.6921
H	4.47598	4.04033	-1.32973	1502.4256	1508.7280	1514.6391
H	4.62662	2.27918	-1.48237	1526.7457	1535.3726	1540.4525
C	1.72849	4.12801	-0.98049	1601.3545	1632.2954	1661.1419
H	2.22504	5.08380	-0.77289	1668.6710	1748.5840	1758.0288
H	1.40036	4.13577	-2.02763	3012.8863	3019.7931	3023.1509
H	0.84433	4.04921	-0.33681	3027.5095	3028.3504	3029.0688
H	-3.71889	-2.20185	-0.33475	3030.6555	3031.0749	3031.8450
O	-1.20777	0.31434	0.90589	3034.3319	3036.9123	3038.2939
C	-0.85019	0.98687	1.95830	3096.8362	3098.4715	3099.6852
C	-1.84854	2.09569	2.32584	3100.9210	3105.8946	3107.6728
C	-1.72683	2.43494	3.80624	3110.8781	3111.3448	3115.2540
H	-0.69198	2.68014	4.06382	3117.3676	3120.1357	3121.7734
H	-2.37042	3.28902	4.05657	3134.5185	3137.4546	3137.7055
H	-2.03137	1.58592	4.43145	3143.3087	3143.4566	3143.6917
C	-3.28472	1.70832	1.98751	3150.7284	3159.5710	3165.5174
H	-3.40622	1.51239	0.91638	3169.1089	3176.2424	3179.6482
H	-3.58896	0.80488	2.53238	3189.8307	3202.8378	3891.4033
H	-3.96823	2.51931	2.27498			
C	-1.43651	3.30708	1.48063			
H	-0.42200	3.63528	1.74613			
H	-1.45720	3.05565	0.41077			
H	-2.12312	4.14684	1.65395			
O	0.19959	0.84454	2.58135			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.614973 Electronic Energy = -1607.50122544
Internal Energy (E)= -1606.84842744 Enthalpy (H)= -1606.84748344
Gibbs Free Energy (G)=-1606.95180544 Gibbs Free Energy of Solvation=-1607.99066995

Details of active catalyst generation

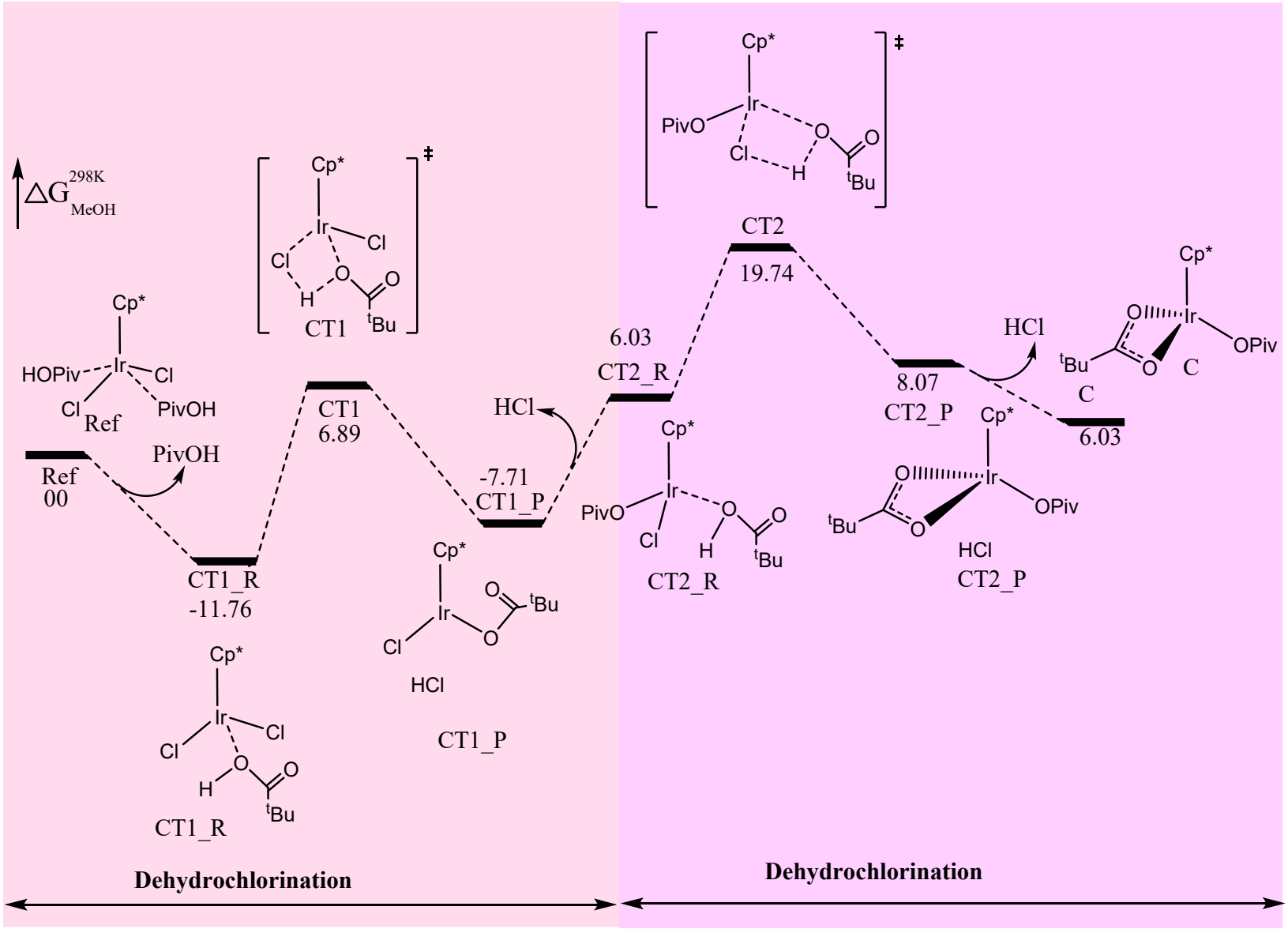


Fig-30: PES with Gibbs free energy (kcal/mol) and the structures of the stationary points using M06L functional & 6-311++G(d,p) basis set

St.Pt.	General Structure	Ball & Stick model
HCl	H-Cl	

Cartesian co-ordinate

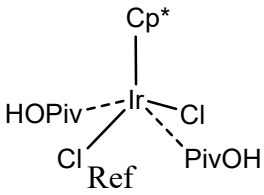
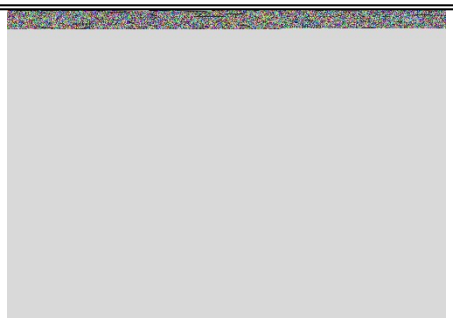
Atoms	X	Y	Z
Cl	0.00000	0.00000	0.07134
H	0.00000	0.00000	-1.21277

Frequencies

2968.6974

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.006763 Electronic Energy = -460.763827404
Internal Energy (E)= -460.754705404 Enthalpy (H)= -460.753761404
Gibbs Free Energy (G)=-460.774938404 Gibbs Free Energy of Solvation=-460.823972498

St.Pt.	General Structure	Ball & Stick model
Ref		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.43869	-2.46748	-1.12131
C	0.96918	-2.36340	-0.85390
C	1.15846	-2.37827	0.59797
C	-0.13145	-2.49607	1.21199
C	-1.12072	-2.54086	0.15188
C	3.57958	0.92595	-0.51442

Frequencies

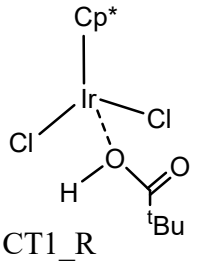
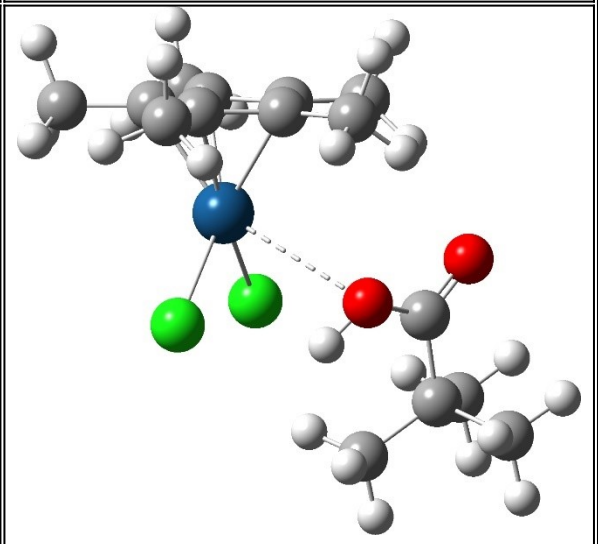
27.5259	43.2845	45.7495
57.3549	63.4097	68.3445
74.1339	75.6020	79.7309
88.0184	102.0982	105.2664
108.0363	116.4044	132.9700
143.7065	153.2902	155.8018
167.7138	185.7377	190.8915
192.0744	213.0372	216.9298
231.7302	233.5941	238.0438
253.1196	258.7785	262.8086

O	2.66155	0.69920	-1.46298
O	4.34879	0.03446	-0.22511
C	3.67740	2.32174	0.09812
Ir	-0.03408	-0.68368	0.03480
Cl	-0.45466	1.03332	-1.57444
H	1.94355	1.35639	-1.48578
Cl	0.27564	0.96085	1.74676
C	-2.58626	-2.69749	0.31869
H	-2.88800	-3.67555	-0.07998
H	-2.87898	-2.64673	1.37068
H	-3.14542	-1.91637	-0.21385
C	-1.11289	-2.48819	-2.44589
H	-0.50112	-2.00375	-3.21241
H	-1.31278	-3.51938	-2.76448
H	-2.06756	-1.95195	-2.39948
C	2.05916	-2.29966	-1.85868
H	2.92923	-1.75649	-1.47762
H	2.36633	-3.31954	-2.12677
H	1.72997	-1.78850	-2.76841
C	2.46602	-2.28452	1.29546
H	2.35056	-1.83648	2.28742
H	2.90040	-3.28523	1.42031
H	3.18078	-1.67113	0.73489
C	-0.43441	-2.53636	2.66684
H	-0.64752	-3.56275	2.99116
H	0.40403	-2.15667	3.25696
H	-1.30552	-1.91402	2.89943
C	3.82535	2.16550	1.61151
H	3.98685	3.14926	2.06974
H	2.92032	1.72716	2.05115
H	4.67806	1.52277	1.85078
C	4.95629	2.93641	-0.48563
H	4.88555	3.04644	-1.57546
H	5.11625	3.93221	-0.05370
H	5.82537	2.31055	-0.25715
C	2.48346	3.21617	-0.22353
H	1.54177	2.79921	0.15926
H	2.62511	4.19310	0.25403
H	2.38369	3.40361	-1.30187
O	-2.75014	0.34338	1.06628
C	-3.49433	0.82433	0.04885
C	-3.71641	2.33277	-0.01803
C	-5.02063	2.57583	0.75630
H	-4.92776	2.25993	1.80334
H	-5.26312	3.64572	0.74355
H	-5.85234	2.02564	0.30162
C	-3.89692	2.73557	-1.47803
H	-4.16404	3.79777	-1.53862
H	-2.96959	2.57764	-2.04038
H	-4.68697	2.14398	-1.94948
C	-2.58720	3.14531	0.61141
H	-1.61864	2.92636	0.14453
H	-2.79530	4.21314	0.47372
H	-2.50163	2.98471	1.69553
O	-4.03908	0.04257	-0.69550
H	-2.15276	1.01038	1.44893

270.6795	272.0867	292.2381
294.8269	298.0097	300.5680
306.6758	307.3415	309.9002
315.6642	319.9377	328.8673
345.7908	350.5244	369.2700
369.9029	383.7290	384.2984
387.8457	403.8652	442.5243
453.3510	459.2183	516.2333
517.4718	532.9319	538.6077
545.7126	570.7482	576.8730
587.5233	590.8061	602.4602
632.2833	641.4172	762.1902
769.9069	787.4194	788.0230
804.9882	813.2983	886.0068
888.8470	947.0384	950.7264
954.4412	954.5914	955.1189
955.9679	958.5122	973.0794
1032.1573	1033.8341	1035.4327
1037.4400	1039.5139	1040.5201
1045.1594	1045.7846	1051.9426
1089.2245	1094.8652	1108.4261
1170.0923	1177.7466	1186.1247
1188.9593	1226.0203	1227.7659
1238.5116	1240.8957	1266.2933
1266.9336	1344.5017	1358.9105
1377.8369	1381.3700	1381.6847
1382.6888	1386.5532	1387.6987
1399.2536	1403.9071	1405.9707
1413.1496	1418.0891	1427.3703
1433.1288	1442.2128	1444.5939
1448.7518	1454.0453	1455.4802
1455.8264	1459.6379	1464.6302
1464.7052	1465.9608	1466.8529
1469.9466	1470.9699	1472.1143
1480.1588	1481.4985	1484.3322
1487.1550	1492.4261	1493.9463
1501.1858	1501.9667	1507.8354
1515.5799	1533.1395	1853.5563
1867.3851	3026.4080	3026.6278
3027.9598	3029.5514	3030.2710
3036.7544	3038.3320	3039.7989
3040.1850	3044.0590	3047.7564
3107.4408	3109.9034	3110.7189
3115.4395	3118.8362	3122.7947
3123.1682	3124.9798	3126.4409
3129.6172	3129.8460	3134.0848
3139.1353	3139.7541	3143.4420
3148.6902	3150.0825	3151.6105
3151.7477	3156.4478	3159.9250
3161.3923	3717.2033	3727.0741

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.522668 Electronic Energy = -2108.56021317
Internal Energy (E)= -2108.00243717 Enthalpy (H)= -2108.00149417
Gibbs Free Energy (G)=-2108.10222217 Gibbs Free Energy of Solvation=-2109.17771283

St.Pt.	General Structure	Ball & Stick model
CT1_R	 CT1_R	

Cartesian co-ordinate

Atoms	X	Y	Z
C	-2.25895	-0.43415	1.27065
C	-1.26005	0.52042	1.67175
C	-1.26937	1.63567	0.73256
C	-2.25564	1.35527	-0.26471
C	-2.84970	0.05678	0.05057
C	2.77147	0.27063	0.87118
O	1.92923	-0.72787	1.18777
O	2.64465	1.33647	1.43332
C	3.92204	-0.03560	-0.08361
Ir	-0.76843	-0.19772	-0.30234
Cl	-0.05163	-2.44796	-0.57813
H	1.92680	-1.45283	0.53805
Cl	0.67239	0.50157	-2.03188
C	-3.90591	-0.62369	-0.74147
H	-4.90180	-0.30833	-0.40385
H	-3.81842	-0.38678	-1.80606
H	-3.83603	-1.71071	-0.63781
C	-2.57007	-1.71390	1.96012
H	-1.66070	-2.15997	2.37516
H	-3.28573	-1.55901	2.77698
H	-2.99248	-2.44606	1.26571
C	-0.38639	0.43850	2.86720
H	0.60787	0.84878	2.65991

Frequencies

34.4159	47.3928	59.6094
63.2375	72.5566	84.9610
88.3490	92.4467	104.5218
114.2073	123.7508	133.0931
137.8157	150.7858	165.7191
173.8294	181.6877	185.6055
197.9914	206.8946	213.2361
247.1738	264.7659	272.8811
292.1249	295.6948	299.0793
314.3967	320.1163	332.8673
334.2328	349.0434	365.4191
380.1280	390.8979	429.8798
447.1489	464.8246	518.0815
532.4256	535.4533	543.2803
569.8050	574.0826	584.4725
601.2335	606.6748	764.7158
782.6773	804.7970	809.9447
882.3105	943.9143	950.3570
951.5004	952.6272	968.8802
1028.3016	1029.6787	1034.1238
1035.4046	1038.0792	1039.3487
1044.5068	1088.7754	1095.0843
1105.6751	1183.5477	1187.7263
1189.4725	1234.5289	1243.4914
1263.8775	1352.2709	1370.4292
1376.3517	1376.7583	1381.7996
1390.6051	1397.1137	1404.5898

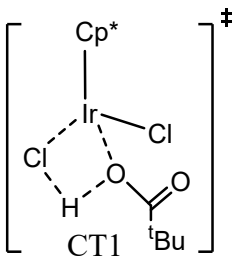
H	-0.84214	1.01065	3.68696	1406.8933	1428.9682	1430.2005
H	-0.25651	-0.59536	3.19894	1433.7308	1436.8723	1441.8929
C	-0.37643	2.82088	0.81489	1445.4979	1447.1501	1453.1739
H	-0.28900	3.31849	-0.15510	1457.3156	1460.2695	1463.5560
H	-0.76695	3.54592	1.54073	1467.8729	1471.9772	1473.6036
H	0.63330	2.52814	1.12810	1486.7556	1488.2691	1490.5697
C	-2.60239	2.20320	-1.43558	1505.1825	1507.7333	1508.4662
H	-3.46198	2.84642	-1.20871	1534.7712	1854.7695	3023.7895
H	-1.75982	2.83877	-1.72246	3029.1112	3034.5096	3037.5916
H	-2.85391	1.59070	-2.30753	3041.4716	3041.9032	3043.5228
C	4.17237	1.19050	-0.95783	3044.1718	3107.0196	3115.8248
H	5.05599	1.02078	-1.58535	3122.5287	3125.2579	3127.0008
H	3.31385	1.38388	-1.61208	3128.5062	3129.3118	3130.5480
H	4.34503	2.07805	-0.34175	3134.9086	3135.3996	3148.1696
C	5.13479	-0.28355	0.82507	3150.0526	3150.2837	3151.1692
H	4.96626	-1.14155	1.48872	3153.9285	3158.9998	3730.3291
H	6.01814	-0.49793	0.21079			
H	5.34456	0.59635	1.44339			
C	3.67493	-1.26221	-0.95895			
H	2.77117	-1.15184	-1.57295			
H	4.52505	-1.39665	-1.63820			
H	3.59869	-2.18802	-0.37076			
O	-2.75014	0.34338	1.06628			
C	-3.49433	0.82433	0.04885			
C	-3.71641	2.33277	-0.01803			
C	-5.02063	2.57583	0.75630			
H	-4.92776	2.25993	1.80334			
H	-5.26312	3.64572	0.74355			
H	-5.85234	2.02564	0.30162			
C	-3.89692	2.73557	-1.47803			
H	-4.16404	3.79777	-1.53862			
H	-2.96959	2.57764	-2.04038			
H	-4.68697	2.14398	-1.94948			
C	-2.58720	3.14531	0.61141			
H	-1.61864	2.92636	0.14453			
H	-2.79530	4.21314	0.47372			
H	-2.50163	2.98471	1.69553			
O	-4.03908	0.04257	-0.69550			
H	-2.15276	1.01038	1.44893			

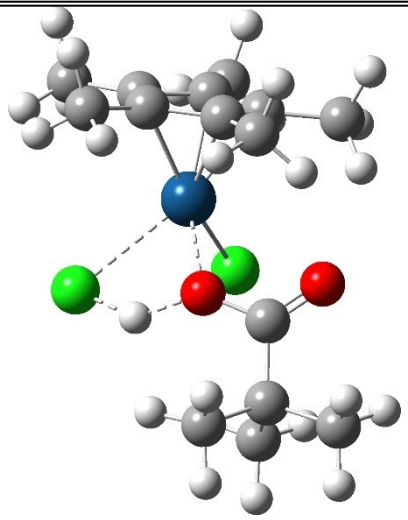
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.372463 Electronic Energy = -1761.72699708
Internal Energy (E)= -1761.32795208 Enthalpy (H)= -1761.32700808
Gibbs Free Energy (G)=-1761.41055008 Gibbs Free Energy of Solvation=-1762.21672817

St.Pt.	General Structure	Ball & Stick model

CT1





Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.93965	0.06101	1.55573
C	-1.26246	1.29908	1.31051
C	-1.53366	1.70582	-0.06106
C	-2.45375	0.73388	-0.63749
C	-2.66705	-0.28966	0.34115
C	2.34801	0.60659	0.24259
O	1.43635	-0.32974	0.47140
O	2.06562	1.78322	0.11204
C	3.77276	0.06684	0.14177
Ir	-0.56390	-0.16319	-0.11912
Cl	0.27444	-2.68448	0.11799
H	1.28532	-1.74199	0.27559
Cl	0.29229	-0.30505	-2.35227
C	-3.49447	-1.51247	0.15971
H	-4.54027	-1.31317	0.42651
H	-3.46684	-1.85871	-0.87789
H	-3.13562	-2.33204	0.78953
C	-1.93669	-0.71896	2.82242
H	-1.04740	-0.49726	3.42028
H	-2.81990	-0.48357	3.43029
H	-1.93802	-1.79653	2.62946
C	-0.37921	2.03878	2.24865
H	0.46932	2.47017	1.70837
H	-0.93884	2.84525	2.73994
H	0.01998	1.37915	3.02535
C	-1.01476	2.93971	-0.70644
H	-1.18661	2.92086	-1.78605
H	-1.50443	3.83036	-0.29157
H	0.06575	3.01600	-0.54270
C	-3.02269	0.79079	-2.00929
H	-3.88598	1.46745	-2.03991
H	-2.27475	1.14171	-2.72712
H	-3.34939	-0.19764	-2.34544
C	4.75967	1.22594	0.20439
H	5.78364	0.84910	0.08807
H	4.56160	1.95481	-0.58729
H	4.69313	1.75254	1.16384

Frequencies

-729.6578	29.5284	42.1372
61.4572	71.5220	92.5355
98.1199	106.1165	118.3936
124.6569	131.8635	135.7160
149.8199	153.2216	164.2589
177.8341	180.5372	192.2095
198.3756	220.6232	229.9455
237.6557	246.7572	275.4316
292.2828	302.1896	304.7085
308.4344	314.6267	318.9882
335.2954	351.9459	368.9278
385.6962	397.0631	429.6373
442.3228	453.8974	474.5806
534.7780	539.6156	544.4402
579.0112	587.6952	591.5975
599.4215	639.1184	688.4687
781.0952	804.9942	808.7720
816.0102	916.3181	947.8132
950.4984	952.5021	955.4880
967.0721	1030.5206	1034.2659
1037.2911	1039.8215	1040.2805
1042.2747	1045.5762	1088.5233
1094.1210	1107.8954	1184.3609
1185.8078	1228.6733	1240.1218
1262.7255	1342.7126	1376.6666
1379.3628	1385.4840	1386.7412
1391.7315	1395.6734	1397.3010
1415.1162	1431.5752	1433.8907
1436.1314	1441.3279	1443.8585
1448.9295	1455.6887	1458.6161
1461.7256	1463.2143	1465.2037
1469.6001	1471.0893	1479.0427
1484.5381	1485.0679	1490.3963
1497.1192	1503.8836	1515.2527
1534.7226	1640.3526	1809.9901
3029.3488	3031.8026	3038.6902
3039.4272	3042.4767	3042.5206
3043.4817	3043.9689	3114.3843
3120.8779	3122.1253	3122.9144
3126.7332	3127.9412	3130.2612
3130.8622	3131.1458	3132.2082

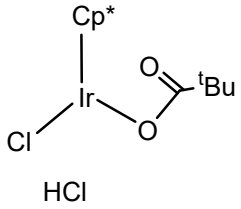
C	4.06537	-0.92304	1.26973	3144.5344	3145.7831	3152.9168
H	3.42238	-1.80906	1.22396	3153.5408	3159.3456	3162.5488
H	5.10596	-1.26383	1.19650			
H	3.93404	-0.45845	2.25516			
C	3.88548	-0.63718	-1.21582			
H	3.70867	0.06813	-2.03647			
H	4.89253	-1.05850	-1.33106			
H	3.15409	-1.44771	-1.31905			
O	-2.75014	0.34338	1.06628			
C	-3.49433	0.82433	0.04885			
C	-3.71641	2.33277	-0.01803			
C	-5.02063	2.57583	0.75630			
H	-4.92776	2.25993	1.80334			
H	-5.26312	3.64572	0.74355			
H	-5.85234	2.02564	0.30162			
C	-3.89692	2.73557	-1.47803			
H	-4.16404	3.79777	-1.53862			
H	-2.96959	2.57764	-2.04038			
H	-4.68697	2.14398	-1.94948			
C	-2.58720	3.14531	0.61141			
H	-1.61864	2.92636	0.14453			
H	-2.79530	4.21314	0.47372			
H	-2.50163	2.98471	1.69553			
O	-4.03908	0.04257	-0.69550			
H	-2.15276	1.01038	1.44893			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.366940 Electronic Energy = -1761.69247164
Internal Energy (E)= -1761.29983164 Enthalpy (H)= -1761.29888764
Gibbs Free Energy (G)=-1761.37990664 Gibbs Free Energy of Solvation=-1762.18678991

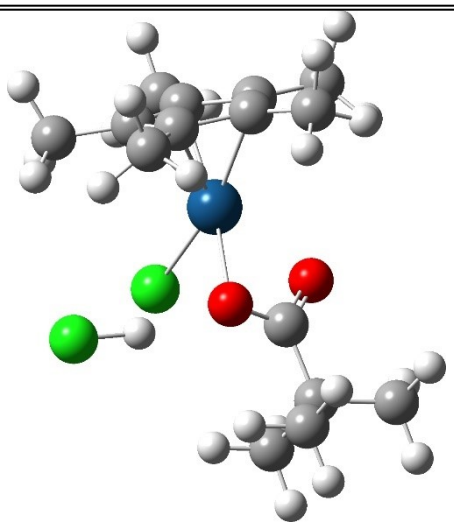
St.Pt.	General Structure	Ball & Stick model

CT1_P



HCl

CT1_P



Cartesian co-ordinate

Atoms	X	Y	Z
C	1.73462	0.46798	1.46461
C	1.69571	-0.97056	1.46526
C	2.20664	-1.41834	0.18205
C	2.58085	-0.26548	-0.59343
C	2.26313	0.91555	0.18790
C	-2.05998	-0.64747	0.11955
O	-1.50761	0.42692	0.54689
O	-1.29558	-1.56113	-0.29226
C	-3.56369	-0.74901	0.04070
Ir	0.47837	-0.19253	-0.15292
Cl	-1.19836	3.48565	0.44219
H	-1.48529	2.21268	0.32174
Cl	-0.27178	0.62588	-2.27443
C	2.49941	2.32185	-0.23456
H	3.53504	2.62237	-0.02915
H	2.30950	2.43884	-1.30610
H	1.82830	3.01225	0.28565
C	1.22491	1.35713	2.54163
H	0.43769	0.86144	3.11845
H	2.03256	1.63985	3.22818
H	0.79046	2.27237	2.12337
C	1.23606	-1.86425	2.56293
H	0.60982	-2.67456	2.17349
H	2.08859	-2.31773	3.08496
H	0.64377	-1.31705	3.30226
C	2.27839	-2.84005	-0.24599
H	2.33643	-2.92517	-1.33465
H	3.15856	-3.33293	0.18634
H	1.38673	-3.38657	0.08030
C	3.16098	-0.25387	-1.96187
H	4.24208	-0.07060	-1.92043
H	2.99269	-1.20464	-2.47618
H	2.69549	0.52750	-2.57052
C	-3.99578	-2.21114	0.04549
H	-5.08600	-2.27400	-0.05871
H	-3.53422	-2.76174	-0.78003
H	-3.71472	-2.70750	0.98238

Frequencies

29.9799	43.5778	47.6856
57.6147	60.9168	88.1149
91.7376	107.3778	121.6508
135.4741	151.6411	154.2200
162.7010	165.4226	173.2433
179.1015	182.9692	187.3983
198.5984	202.7858	215.1152
230.2641	248.8661	283.7597
305.0907	309.9246	314.0630
318.8340	326.1086	328.4440
346.3936	377.7131	391.7681
394.3107	421.9233	442.3423
451.3305	456.5477	464.5767
533.8777	538.3764	544.4922
544.9984	578.3960	580.8555
584.6274	603.5933	625.5235
792.3491	804.2344	811.9208
832.0699	937.4890	957.0809
961.5619	963.3489	963.9824
966.9999	1031.8901	1035.5815
1036.5515	1040.3177	1044.7492
1046.6737	1051.0152	1091.6300
1095.8319	1106.9001	1184.2627
1188.8876	1235.7884	1262.2698
1265.9195	1378.1191	1383.2050
1385.6530	1390.8237	1396.0291
1400.4145	1403.3341	1415.7415
1434.4307	1435.3322	1436.3043
1442.1850	1447.0797	1449.4767
1452.3974	1455.7438	1462.8099
1464.7195	1468.6887	1469.5493
1472.8948	1481.0467	1485.8549
1487.1995	1490.8825	1494.9836
1499.4035	1510.2989	1525.8033
1530.1738	1614.1625	2692.3853
3028.9105	3033.8187	3038.8016
3040.6874	3042.6021	3043.1911
3043.4342	3044.7980	3118.4971
3121.0496	3121.5970	3123.0961
3125.7558	3128.5329	3129.2240
3131.5719	3133.0939	3136.0077

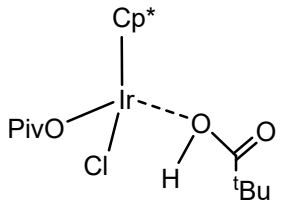
C	-4.20871	0.01000	1.19781	3145.4815	3146.9587	3148.3029
H	-3.92270	1.06743	1.19289	3151.3332	3152.5973	3164.0519
H	-5.30060	-0.05130	1.11195			
H	-3.92181	-0.41600	2.16718			
C	-3.94996	-0.09084	-1.29245			
H	-3.48093	-0.60912	-2.13671			
H	-5.03957	-0.13116	-1.41593			
H	-3.63366	0.95903	-1.32256			
O	-2.75014	0.34338	1.06628			
C	-3.49433	0.82433	0.04885			
C	-3.71641	2.33277	-0.01803			
C	-5.02063	2.57583	0.75630			
H	-4.92776	2.25993	1.80334			
H	-5.26312	3.64572	0.74355			
H	-5.85234	2.02564	0.30162			
C	-3.89692	2.73557	-1.47803			
H	-4.16404	3.79777	-1.53862			
H	-2.96959	2.57764	-2.04038			
H	-4.68697	2.14398	-1.94948			
C	-2.58720	3.14531	0.61141			
H	-1.61864	2.92636	0.14453			
H	-2.79530	4.21314	0.47372			
H	-2.50163	2.98471	1.69553			
O	-4.03908	0.04257	-0.69550			
H	-2.15276	1.01038	1.44893			

Statistical Thermodynamic Analysis

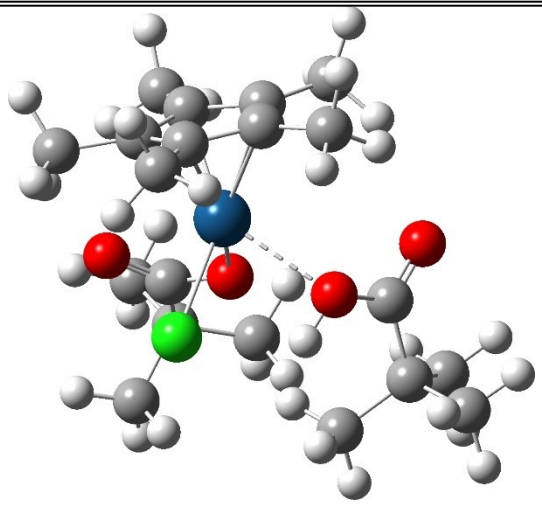
Temperature=298 K Pressure=1 atm
Zero-point correction= 0.369893 Electronic Energy = -1761.71165039
Internal Energy (E)= -1761.31540139 Enthalpy (H)= -1761.31445739
Gibbs Free Energy (G)=-1761.39747739 Gibbs Free Energy of Solvation=-1762.21005467

St.Pt.	General Structure	Ball & Stick model

CT2_R



CT2_R



Cartesian co-ordinate

Atoms	X	Y	Z
C	-2.94193	-0.60423	-0.38498
C	-2.38396	-1.39552	0.66742
C	-1.87098	-0.50708	1.70316
C	-2.11067	0.84074	1.27920
C	-2.72730	0.79591	-0.03728
C	1.78005	-2.11239	0.48358
O	0.76042	-1.95027	-0.40880
O	1.50496	-2.31938	1.63679
C	3.18568	-2.11933	-0.09742
Ir	-0.84351	-0.14081	-0.16859
Cl	-0.20965	-0.15705	-2.51934
H	1.04014	-1.67171	-1.30733
C	-1.24703	-0.95331	2.97726
H	-0.77804	-0.11560	3.50156
H	-2.00045	-1.39190	3.64464
H	-0.46774	-1.69957	2.78754
C	-1.76812	2.07084	2.04023
H	-1.60889	2.91650	1.36732
H	-2.57462	2.31139	2.74495
H	-0.84529	1.93202	2.61501
C	-3.13056	1.97712	-0.84254
H	-3.36888	1.68837	-1.87022
H	-4.01325	2.46151	-0.40504
H	-2.30222	2.69147	-0.87782
C	-3.57510	-1.09571	-1.63739
H	-3.29629	-2.13439	-1.83948
H	-4.66889	-1.04103	-1.57049
H	-3.24756	-0.50297	-2.49745
C	-2.29728	-2.87830	0.72316
H	-3.14586	-3.29149	1.28363
H	-2.30239	-3.31825	-0.27887
H	-1.37466	-3.19267	1.22176
C	3.31869	-1.17081	-1.29070
H	4.37838	-1.05739	-1.54735
H	2.81972	-1.55160	-2.19325
H	2.90164	-0.18082	-1.06947
C	4.15963	-1.73114	1.01060
H	4.07058	-2.40954	1.86429

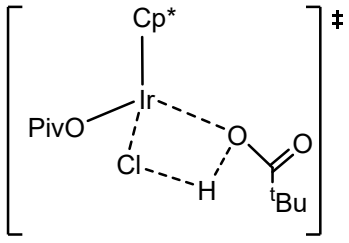
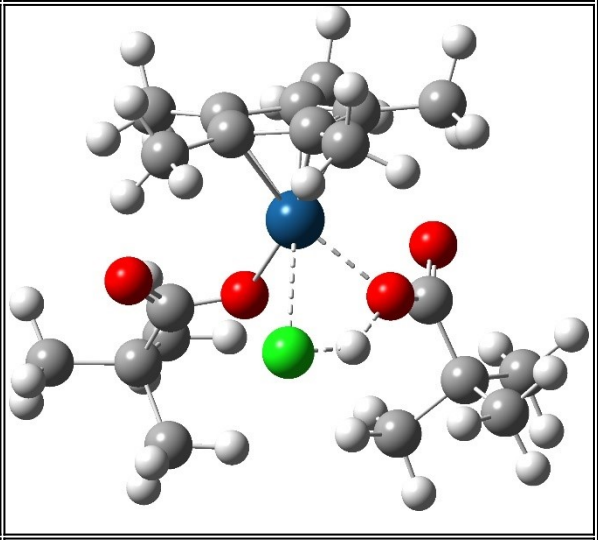
Frequencies

33.1011	43.3734	54.1865
57.0744	61.9258	72.9384
76.6727	87.9687	95.4886
98.0501	108.8918	112.0305
122.5883	147.4751	152.0071
157.1199	158.4990	168.6768
174.7096	183.1712	191.1152
195.0267	195.6830	218.8523
226.6748	229.4371	230.8211
242.5964	251.0478	268.8347
277.4127	284.3463	286.6245
288.1311	295.1276	300.6269
308.2752	310.8288	313.4190
320.9963	323.1937	372.5012
376.3831	383.0966	394.3895
401.5839	429.1355	441.5104
445.1395	474.9516	526.6450
536.0513	538.7042	541.9410
562.6161	578.4496	586.5264
590.5612	601.1963	630.0515
736.7540	766.9238	794.2305
803.9675	806.0705	807.0674
814.5964	886.6444	913.9203
942.5793	947.8300	948.8854
950.5283	952.8610	954.2191
955.4805	964.0204	1030.7355
1034.9725	1036.9326	1037.3566
1042.0694	1042.7565	1045.1771
1046.3118	1048.7597	1088.5125
1094.9590	1106.9144	1141.0226
1186.0233	1189.1066	1222.4883
1234.9702	1237.6780	1242.2159
1260.2421	1265.1064	1325.6186
1368.6599	1374.5325	1377.4949
1378.6915	1379.4094	1380.7024
1387.1289	1389.7686	1393.1334
1400.1149	1412.7023	1416.1107
1426.2900	1433.4441	1435.3018
1439.3115	1446.6005	1447.4509
1450.6792	1454.6589	1455.6377
1456.6861	1459.1907	1459.5661
1461.1092	1464.7496	1470.5570

H	5.18731	-1.77455	0.63079	1473.8391	1475.6995	1476.9770
H	3.96449	-0.71387	1.36847	1480.0924	1483.0144	1487.0909
C	3.45869	-3.56337	-0.54285	1488.8424	1495.9024	1499.3044
H	4.47105	-3.63026	-0.95973	1501.4367	1517.4290	1539.9188
H	3.38761	-4.25540	0.30445	1753.8575	1888.3837	3022.0917
H	2.75298	-3.88938	-1.31720	3024.1083	3028.2001	3031.0085
O	-0.04535	2.81923	-0.41532	3033.4840	3039.9598	3040.3089
C	0.93547	2.17307	-0.05685	3041.2756	3041.6631	3045.4197
C	2.26999	2.89999	0.16020	3047.5127	3098.8352	3104.7437
C	1.98864	4.18244	0.94182	3108.4809	3111.3577	3115.6318
H	2.90839	4.77269	1.04651	3121.9840	3122.4895	3126.6307
H	1.23341	4.78732	0.43219	3130.2663	3130.9050	3136.4874
H	1.61813	3.95504	1.95107	3136.9463	3137.8163	3140.8903
C	2.79473	3.24870	-1.23580	3142.5482	3146.5374	3152.6218
H	3.75514	3.77614	-1.16172	3154.7558	3156.4362	3160.0365
H	2.94614	2.34102	-1.83587	3171.2720	3177.6150	3599.2677
H	2.08077	3.88773	-1.76617			
C	3.30389	2.06693	0.90689			
H	3.63174	1.20506	0.31553			
H	4.19055	2.67988	1.11786			
H	2.91178	1.69347	1.86122			
O	0.95551	0.88640	0.14262			
O	-4.03908	0.04257	-0.69550			
H	-2.15276	1.01038	1.44893			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.508041 Electronic Energy = -1647.75441173
Internal Energy (E)= -1647.21300373 Enthalpy (H)= -1647.21205973
Gibbs Free Energy (G)=-1647.30870973 Gibbs Free Energy of Solvation=-1648.34556186

St.Pt.	General Structure	Ball & Stick model
CT2	 CT2	

Cartesian co-ordinate

Frequencies

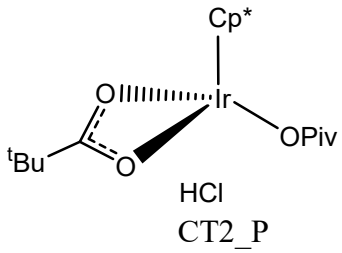
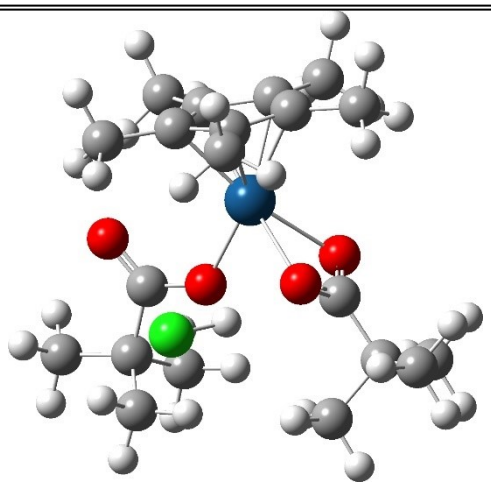
Atoms	X	Y	Z
C	-2.53931	-1.35877	-0.47244
C	-1.93873	-1.83236	0.73355
C	-1.79456	-0.70181	1.64199
C	-2.39270	0.46056	1.00240
C	-2.81075	0.07033	-0.30837
C	1.93804	-1.69742	0.49238
O	1.07795	-1.39840	-0.46571
O	1.61035	-1.81069	1.65997
C	3.37724	-1.85084	0.00545
Ir	-0.69258	-0.28541	-0.10405
Cl	0.30611	0.01761	-2.62583
H	1.06382	-0.82082	-1.78815
C	-1.23174	-0.76050	3.01563
H	-0.94250	0.23699	3.36107
H	-1.97115	-1.16558	3.71939
H	-0.33451	-1.38710	3.03531
C	-2.51654	1.80594	1.62193
H	-2.68149	2.57810	0.86860
H	-3.34528	1.81201	2.34158
H	-1.59810	2.07108	2.15748
C	-3.38200	0.98552	-1.33214
H	-3.35487	0.53327	-2.32806
H	-4.42570	1.23021	-1.09759
H	-2.79245	1.90882	-1.36417
C	-2.83234	-2.16758	-1.68653
H	-2.08220	-2.95295	-1.82508
H	-3.81827	-2.64388	-1.61381
H	-2.82230	-1.54813	-2.58866
C	-1.45162	-3.20715	1.02179
H	-2.16830	-3.74185	1.65814
H	-1.31627	-3.78578	0.10296
H	-0.48706	-3.16400	1.53950
C	3.88983	-0.43075	-0.26112
H	4.90632	-0.46834	-0.67335
H	3.24120	0.09820	-0.97113
H	3.91667	0.15379	0.66731
C	4.21715	-2.51346	1.08983
H	3.86234	-3.52940	1.30023
H	5.26407	-2.57464	0.76668
H	4.17025	-1.94709	2.02486
C	3.44343	-2.67521	-1.28027
H	4.49218	-2.81474	-1.57149
H	2.99943	-3.66911	-1.14341
H	2.93076	-2.18541	-2.11563
O	-0.70847	2.74910	-0.60740
C	0.35380	2.42877	-0.08262
C	1.43808	3.46500	0.23561
C	0.86542	4.86853	0.08436
H	1.64132	5.61522	0.29877
H	0.48798	5.03471	-0.92952
H	0.03056	5.03104	0.77677
C	2.57584	3.26031	-0.76791
H	3.34906	4.02687	-0.62469
H	3.03945	2.27535	-0.64299
H	2.20528	3.33776	-1.79834

-759.0050	34.9581	47.9795
50.1193	55.2519	67.9161
70.1595	77.0306	82.9311
95.0740	100.9005	105.6258
114.2612	120.5716	124.7597
129.5458	144.1718	151.2105
163.4125	175.8943	181.3731
185.3986	193.5461	202.7948
218.2477	221.9217	227.4345
244.1961	259.7852	263.3226
273.9950	288.3128	293.5785
304.1033	307.1638	310.9695
318.6327	324.7642	328.4710
351.1307	357.0721	372.8669
387.4421	391.3124	396.8693
414.8544	429.3957	441.4362
445.4160	452.1488	483.6606
535.2095	538.6090	543.5922
570.6367	579.1352	585.5829
592.0126	600.1084	627.5742
644.2537	775.3437	782.7089
793.9852	805.6795	807.6323
818.9714	821.0521	916.4704
917.9596	945.7929	947.3979
950.7000	951.9596	952.4950
958.1083	962.9214	971.4196
1037.1607	1037.7199	1040.0972
1040.5426	1043.3184	1044.5561
1045.0849	1045.9176	1048.5257
1091.3687	1094.3313	1108.0236
1186.1507	1186.5786	1228.4164
1241.4766	1243.3211	1247.4061
1262.9354	1266.8498	1341.0556
1365.7896	1374.0752	1376.4992
1379.8870	1380.6360	1383.7571
1386.9566	1392.8839	1394.7288
1403.4049	1410.8762	1418.1191
1424.6006	1426.6099	1437.7709
1438.8962	1441.5624	1450.9592
1452.9137	1453.4276	1454.3569
1458.9081	1461.5486	1466.1339
1467.3163	1469.8139	1470.9386
1474.9826	1476.8649	1478.9059
1482.1642	1484.4909	1489.1732
1492.0260	1496.9021	1503.9610
1507.0042	1523.8345	1532.4172
1537.9094	1761.5958	1804.9329
3020.6521	3027.2215	3028.7732
3030.8582	3032.1295	3036.9225
3038.1112	3039.1179	3039.8096
3041.5832	3043.6495	3097.4419
3108.7768	3114.3915	3115.9305
3117.3464	3121.8540	3122.0327
3122.7063	3123.5947	3126.9645
3127.3826	3129.6327	3129.8305
3140.6227	3141.9350	3144.3562
3144.9422	3145.3540	3148.3334
3153.3440	3154.2940	3168.7774

C	1.95616	3.26351	1.65867
H	2.37388	2.26090	1.79225
H	2.73627	4.00298	1.88367
H	1.15141	3.39513	2.39536
O	0.69704	1.20972	0.23368
O	-4.03908	0.04257	-0.69550
H	-2.15276	1.01038	1.44893

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.501950 Electronic Energy = -1647.72516839
Internal Energy (E)= -1647.19031939 Enthalpy (H)= -1647.18937539
Gibbs Free Energy (G)=-1647.28530539 Gibbs Free Energy of Solvation=-1648.3236582

St.Pt.	General Structure	Ball & Stick model
CT2_P		

HCl
CT2_P

Cartesian co-ordinate

Atoms	X	Y	Z
C	-2.46556	-0.03664	1.16851
C	-2.79295	0.78483	0.02733
C	-2.67581	-0.04861	-1.14152
C	-2.29175	-1.38331	-0.73275
C	-2.15938	-1.37321	0.71061
C	0.86833	2.05521	-0.35199
O	0.45865	1.63694	0.78689
O	0.32856	1.57661	-1.38453
C	2.00623	3.04925	-0.41438
Ir	-0.77423	0.03490	-0.15038
Cl	1.33745	-0.06815	3.21424
H	1.15827	0.65748	2.13773
C	-2.84908	0.41763	-2.54256
H	-2.34605	-0.25195	-3.24596

Frequencies

27.9647	32.1223	48.0102
62.8635	69.4037	70.7265
82.6674	90.6477	94.4746
100.0944	115.2797	120.9922
135.8693	145.5678	153.8847
160.2279	164.6029	170.7094
175.7430	177.5041	194.5290
203.7315	204.3202	214.9166
222.5511	232.7231	239.5196
240.8341	250.0951	274.1185
283.5581	286.3247	304.2086
309.1426	316.0350	317.3576
320.1584	325.3696	334.5310
358.8722	381.6026	383.5426
388.6787	398.0671	408.4953
423.0630	436.4493	454.2845
460.5068	463.4478	531.8323
538.9917	542.6733	547.7117

H	-3.91262	0.45793	-2.80919
H	-2.42210	1.41703	-2.67781
C	-2.15800	-2.57463	-1.61160
H	-1.31230	-3.18840	-1.28704
H	-3.07839	-3.17289	-1.58348
H	-1.98011	-2.28171	-2.65129
C	-1.85679	-2.54708	1.56988
H	-1.38140	-2.24216	2.50768
H	-2.78265	-3.08397	1.81608
H	-1.16690	-3.22069	1.05713
C	-2.39834	0.43085	2.57801
H	-2.11066	1.48598	2.63448
H	-3.37541	0.31706	3.06478
H	-1.65885	-0.13817	3.15076
C	-3.14217	2.23231	0.05021
H	-4.22159	2.38284	0.17765
H	-2.62984	2.74740	0.86982
H	-2.83981	2.72369	-0.88055
C	3.26446	2.28258	0.01068
H	4.13396	2.95097	-0.02009
H	3.16558	1.88984	1.03008
H	3.45638	1.43843	-0.66441
C	2.17446	3.58556	-1.82992
H	1.27621	4.11783	-2.16398
H	3.01942	4.28451	-1.86239
H	2.36493	2.77407	-2.54003
C	1.74134	4.18976	0.56838
H	2.58627	4.88945	0.55734
H	0.83770	4.75014	0.29698
H	1.61803	3.81238	1.58868
O	0.59597	-2.94266	-0.28860
C	1.40677	-2.02491	-0.32107
C	2.90885	-2.27750	-0.51306
C	3.17753	-3.77673	-0.53788
H	4.24644	-3.96253	-0.70639
H	2.88965	-4.24551	0.40969
H	2.60676	-4.26781	-1.33319
C	3.69252	-1.62902	0.62839
H	4.76213	-1.85304	0.51935
H	3.56753	-0.54091	0.63267
H	3.36344	-2.00800	1.60410
C	3.33050	-1.65381	-1.84667
H	3.12898	-0.57610	-1.86396
H	4.40488	-1.81123	-2.01111
H	2.79175	-2.11367	-2.68546
O	1.12084	-0.75621	-0.23162
O	-4.03908	0.04257	-0.69550
H	-2.15276	1.01038	1.44893

550.0498	575.8174	578.4004
586.5891	601.6745	617.0622
640.9695	650.1096	788.7697
798.1323	809.1642	811.6122
819.6169	831.8137	922.1119
936.3936	949.6155	952.3871
953.3412	956.3630	958.5260
961.0585	961.9903	964.9638
1034.0804	1036.5895	1038.8945
1042.0430	1043.1013	1044.8965
1045.9156	1047.5370	1048.1715
1089.4961	1098.4051	1108.1165
1185.4501	1188.7451	1239.2605
1243.5060	1246.2801	1258.7014
1262.7939	1267.7101	1364.5174
1377.8932	1379.2510	1380.0153
1380.5230	1386.9707	1388.3345
1392.3831	1394.0408	1401.5574
1414.2130	1416.9578	1433.9888
1437.1836	1440.1233	1442.1546
1447.2786	1452.4954	1453.3208
1454.6475	1455.2836	1460.8369
1461.9277	1465.5525	1466.5800
1468.1600	1473.3836	1476.6258
1477.0511	1478.7303	1482.1608
1486.9559	1488.9141	1495.0200
1503.7503	1507.3791	1512.7832
1514.8770	1522.0037	1536.9484
1618.0212	1775.8463	2692.0977
3023.3185	3030.6872	3032.2482
3032.8343	3036.9537	3038.2132
3038.4148	3039.3158	3042.2161
3043.3322	3044.0131	3107.2855
3114.2298	3115.8531	3120.6880
3122.1223	3123.5200	3124.4570
3124.6187	3124.8067	3125.5274
3129.7917	3131.8475	3134.4764
3138.5945	3139.6214	3140.6382
3141.0185	3148.7403	3153.2503
3158.2031	3174.9850	3203.1076

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.506199 Electronic Energy = -1647.74279872
Internal Energy (E)= -1647.20357972 Enthalpy (H)= -1647.20263572
Gibbs Free Energy (G)=-1647.29866272 Gibbs Free Energy of Solvation=-1648.34226797

Details mechanistic route for the generation of benzofuran

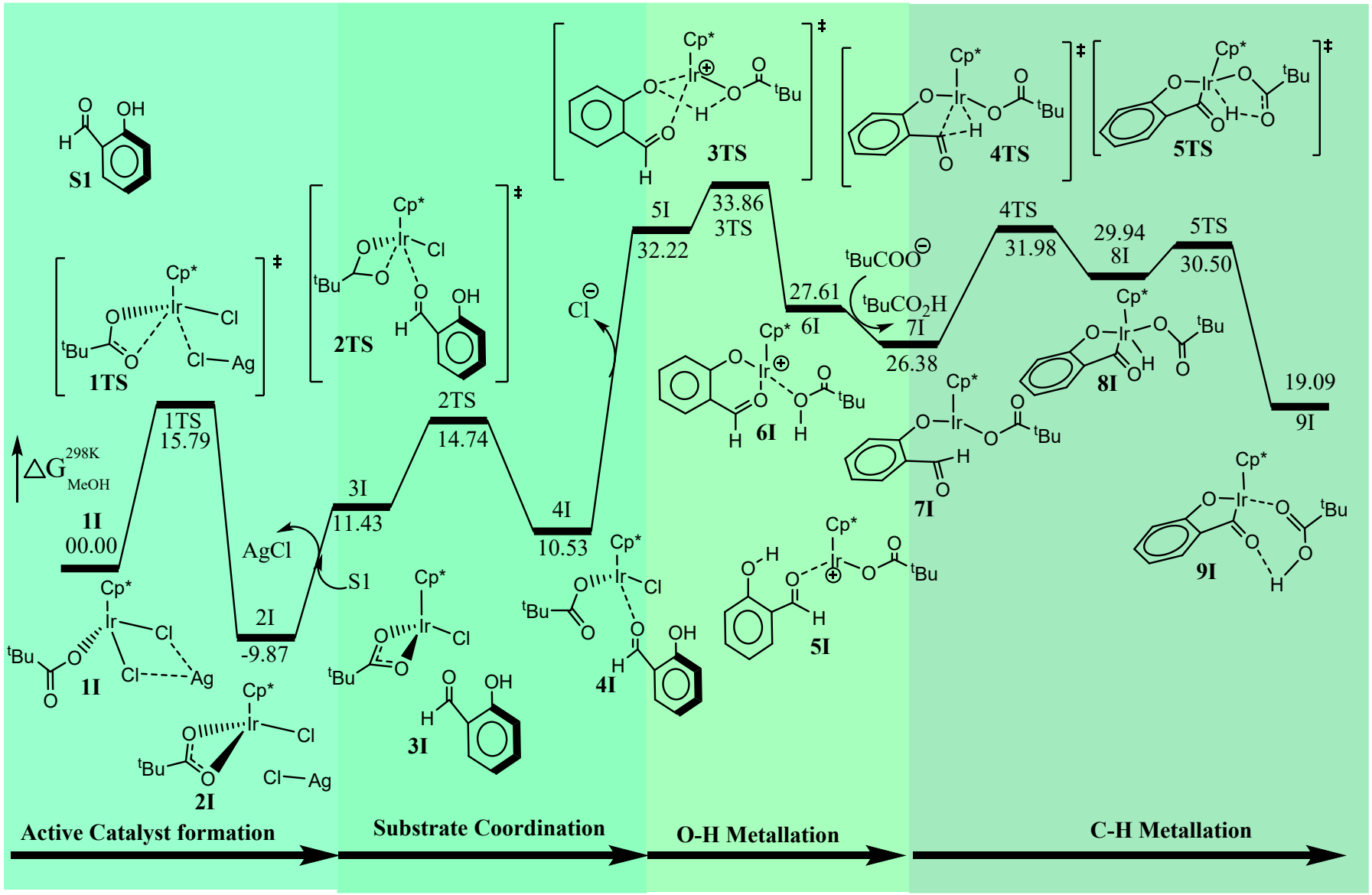


Fig-31: PES with Gibbs free energy (kcal/mol) and the structures of the stationary points for S1 using M06L functional & 6-311++G(d,p) basis set

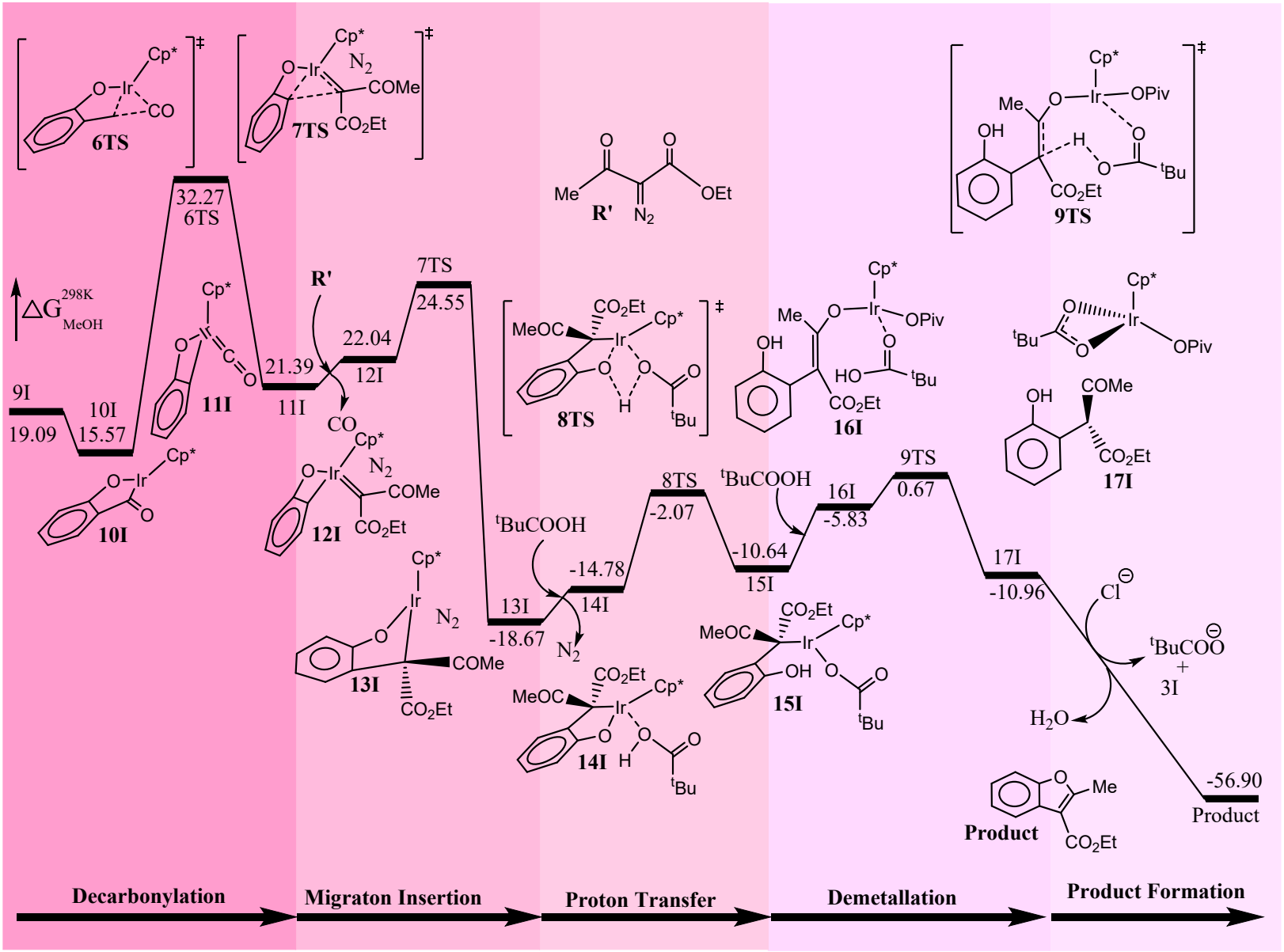
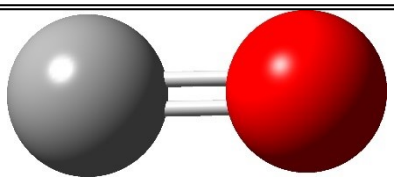


Fig-32: PES with Gibbs free energy (kcal/mol) and the structures of the stationary points for S1 using M06L functional & 6-311++G(d,p) basis set

St.Pt.	General Structure	Ball & Stick model
CO	CO	

Cartesian co-ordinate

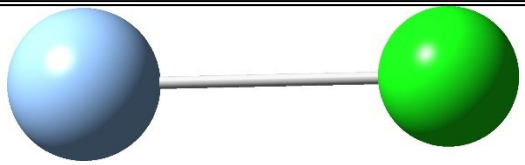
Atoms	X	Y	Z
C	0.00000	0.00000	-0.64996
O	0.00000	0.00000	0.48747

Frequencies

2224.0611

Statistical Thermodynamic Analysis

Temperature=298 K — Pressure=1 atm
Zero-point correction= 0.005067 — Electronic Energy = -113.251768950
Internal Energy (E)= -113.24434295 — Enthalpy (H)= -113.24339895
Gibbs Free Energy (G)=-113.26582895 — Gibbs Free Energy of Solvation=-113.335192888

St.Pt.	General Structure	Ball & Stick model
AgCl	AgCl	

Cartesian co-ordinate

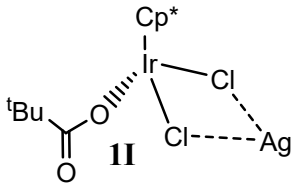
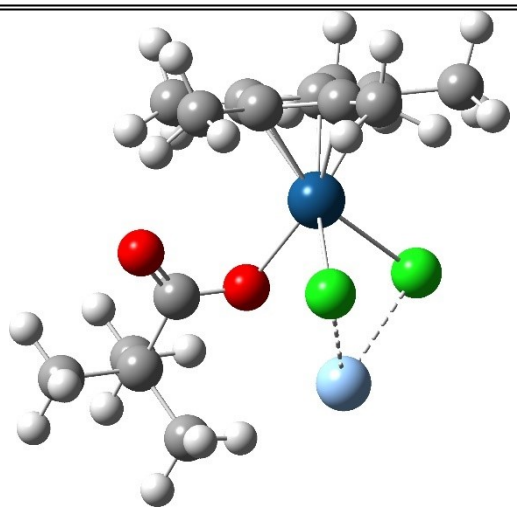
Atoms	X	Y	Z
Cl	0.00000	0.00000	-1.71920
	0.00000	0.00000	0.62184

Frequencies

333.8694

Statistical Thermodynamic Analysis

Temperature=298 K — Pressure=1 atm
Zero-point correction= 0.000761 — Electronic Energy = -605.970406417
Internal Energy (E)= -605.966907417 — Enthalpy (H)= -605.965963417
Gibbs Free Energy (G)=-605.993912417 — Gibbs Free Energy of Solvation=-606.113885444

St.Pt.	General Structure	Ball & Stick model
1I	 **1I**	

Cartesian co-ordinate

Atoms	X	Y	Z
C	-2.94660	-0.14380	0.42276
C	-2.31744	0.83854	1.29593
C	-1.76901	1.87881	0.46095
C	-1.99709	1.52393	-0.92136
C	-2.74979	0.27628	-0.93151
C	3.32637	1.48698	0.22420
C	1.82334	1.43515	-0.10966
O	1.20628	0.44028	0.46654

Frequencies

-14.0184	22.9746	38.2174
54.6006	62.5356	74.1943
86.1113	91.7525	98.7422
113.2483	128.0541	141.4376
151.5310	158.5470	166.4800
169.9182	172.6630	185.7824
190.9543	196.2360	203.2259
219.7612	222.4610	231.1290
233.8149	250.5292	270.1432
293.4163	297.5033	312.4663
321.1916	327.4270	334.2063
336.7069	357.5076	386.4458
398.6128	433.5028	440.0408

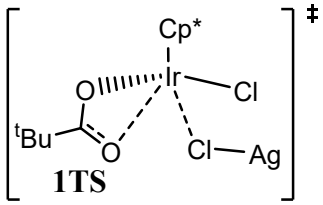
O	1.30377	2.28657	-0.81810	444.9702	457.8203	535.8530
C	-1.07245	3.09670	0.95242	537.5711	541.6101	566.0613
H	-0.46982	2.87040	1.83936	582.4914	587.6225	600.3878
H	-0.39771	3.49742	0.19293	625.2461	792.9467	803.8450
H	-1.81010	3.86068	1.23090	809.7736	814.3450	911.1369
C	-1.61136	2.33047	-2.10868	944.8129	948.5819	955.7383
H	-1.58824	1.71104	-3.01030	960.8378	968.1243	1032.1482
H	-2.32624	3.14733	-2.27334	1033.7256	1038.2896	1040.7045
H	-0.60824	2.74374	-1.96999	1044.6721	1045.4416	1051.0881
C	-3.22573	-0.44193	-2.14332	1088.8487	1098.5163	1107.5440
H	-2.57875	-0.24429	-3.00246	1185.4690	1189.0673	1237.6040
H	-3.23025	-1.52479	-1.98578	1239.8381	1258.6665	1346.6526
H	-4.24515	-0.12556	-2.39891	1367.8936	1379.5981	1382.0975
C	-3.67507	-1.35991	0.87074	1389.2550	1396.4287	1398.0327
H	-3.59654	-2.16458	0.13337	1400.3777	1411.9658	1428.6724
H	-3.26938	-1.74359	1.81129	1432.5722	1433.4602	1439.2021
H	-4.73868	-1.13342	1.02094	1446.9554	1447.6414	1453.0927
C	-2.32277	0.80656	2.78267	1454.7909	1462.0392	1466.7950
H	-1.49460	1.39258	3.19262	1469.7820	1470.6273	1475.3071
H	-3.26032	1.21798	3.17951	1481.4468	1483.6084	1487.7691
H	-2.21342	-0.21692	3.15522	1493.6309	1501.7489	1505.2479
C	3.99771	0.14922	-0.10142	1513.5196	1529.7962	1781.5484
H	3.78256	-0.16494	-1.13378	2965.9735	3024.8964	3036.6183
H	5.08824	0.23011	-0.00265	3038.2930	3039.0060	3039.4534
H	3.68557	-0.63512	0.61177	3043.1945	3045.0336	3056.4491
C	3.46828	1.78253	1.71880	3097.3474	3108.3847	3116.4716
H	4.52873	1.83946	1.99850	3123.8557	3123.9757	3127.4459
H	3.00425	2.74565	1.96842	3128.8205	3130.5380	3133.5417
H	2.98776	1.00519	2.32307	3145.7620	3150.4838	3154.4247
C	3.99350	2.58762	-0.59150	3155.8111	3164.3949	3176.9220
H	3.51994	3.55539	-0.39989			
H	5.05771	2.65844	-0.33103			
H	3.90895	2.39115	-1.66614			
Ir	-0.83352	-0.02405	0.01360			
Cl	-0.26128	-2.07685	1.38947			
Cl	0.22842	-1.14895	-1.97666			
	1.85940	-1.90470	-0.07792			

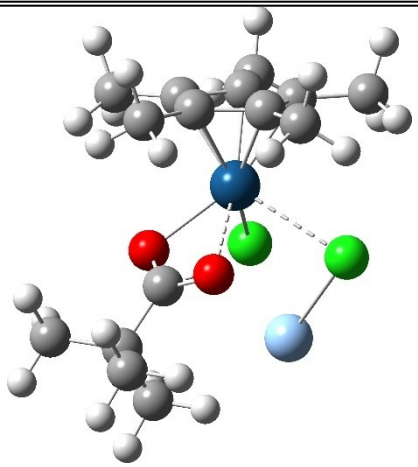
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.361577 Electronic Energy = -1906.95418222
Internal Energy (E)= -1906.56550922 Enthalpy (H)= -1906.56456522
Gibbs Free Energy (G)=-1906.64982622 Gibbs Free Energy of Solvation=-1907.50506418

St.Pt.	General Structure	Ball & Stick model

1TS





Cartesian co-ordinate

Atoms	X	Y	Z
C	2.73857	0.02147	-0.83639
C	2.24691	1.38719	-0.84856
C	1.95459	1.75908	0.52919
C	2.26036	0.62513	1.37033
C	2.74048	-0.45355	0.53145
C	-3.05927	1.80242	0.00821
C	-1.62746	1.29567	0.14714
O	-0.92007	1.23961	-0.91047
O	-1.22089	0.81778	1.23024
C	1.41151	3.06917	0.97654
H	0.76924	3.50694	0.20500
H	0.80629	2.95471	1.88061
H	2.22151	3.77835	1.18863
C	2.06573	0.56143	2.84191
H	1.74951	-0.43893	3.15149
H	2.99851	0.81762	3.36049
H	1.28538	1.25558	3.16719
C	3.19500	-1.79789	0.97571
H	2.76774	-2.05988	1.94674
H	2.86869	-2.56918	0.26952
H	4.28969	-1.83545	1.05022
C	3.20035	-0.75179	-2.01818
H	2.98883	-1.81832	-1.89876
H	2.70179	-0.42336	-2.93465
H	4.28309	-0.62612	-2.14924
C	2.07678	2.24376	-2.05109
H	1.28504	2.98301	-1.89798
H	3.00620	2.77473	-2.29407
H	1.78719	1.63854	-2.91677
C	-3.86384	0.57941	-0.46076
H	-3.81039	-0.22390	0.29656
H	-4.92511	0.83165	-0.58452
H	-3.48514	0.21043	-1.42444
C	-3.14996	2.90507	-1.04139
H	-4.19060	3.23583	-1.15440
H	-2.55145	3.77640	-0.74550
H	-2.78223	2.55856	-2.01201
C	-3.59242	2.28895	1.34922
H	-3.02336	3.15673	1.70505

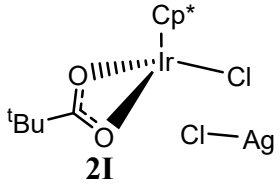
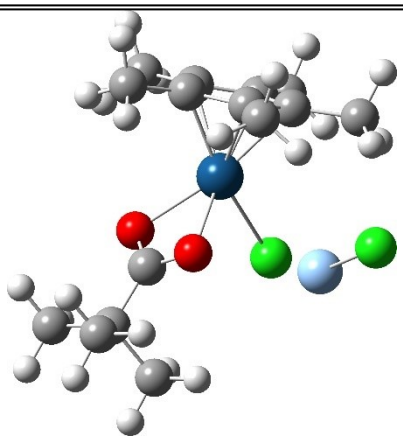
Frequencies

-101.3547	-42.7326	21.8475
46.1617	49.5477	54.7359
64.0054	65.1045	74.7556
115.1938	128.3088	147.2368
157.1794	163.0058	180.9061
186.4316	191.8300	201.4262
204.1651	218.4374	221.0051
226.7003	232.1483	241.8906
242.2710	260.4713	276.2582
279.8879	286.0505	291.6303
310.9922	322.9951	324.6351
330.0798	347.8772	379.7175
392.7959	414.3352	443.9612
458.8689	474.4880	533.3471
537.8620	540.9924	544.1115
581.7066	591.4128	600.6336
621.0984	797.5865	799.0903
807.5825	822.9337	921.6308
942.3933	952.4451	952.7916
956.4811	963.9518	1029.4916
1032.7263	1035.6357	1043.2009
1045.3283	1045.8230	1053.1287
1088.9940	1091.2784	1102.6910
1182.4510	1184.6758	1231.8510
1260.3092	1270.3828	1354.4937
1377.2822	1379.8418	1381.2725
1392.8105	1395.6046	1399.5074
1405.6170	1429.2285	1434.6002
1440.6394	1443.9550	1448.9277
1449.9847	1456.7784	1458.4046
1461.2374	1465.7750	1468.3111
1470.1921	1471.7426	1475.6319
1477.0643	1483.2052	1483.7568
1497.2579	1498.9901	1508.5106
1511.5875	1521.6653	1660.9807
2973.5764	3029.2913	3033.2157
3039.9702	3040.2984	3041.9258
3042.8260	3044.3838	3070.1529
3109.5302	3111.5674	3113.9784
3124.0986	3125.7935	3126.5019
3130.3062	3133.9109	3144.4879
3146.3846	3147.1145	3148.6687
3155.6282	3156.2595	3165.7768

H	-4.64356	2.59025	1.25219
H	-3.51542	1.50732	2.11133
Ir	0.75475	0.11300	-0.07823
Cl	-0.13004	-1.50410	-1.88551
Cl	-0.18421	-1.81252	1.69562
	-1.91725	-1.90580	-0.07913

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.361445 Electronic Energy = -1906.92308454
Internal Energy (E)= -1906.53534854 Enthalpy (H)= -1906.53440454
Gibbs Free Energy (G)=-1906.61806754 Gibbs Free Energy of Solvation=-1907.47990841

St.Pt.	General Structure	Ball & Stick model
2I	 **2I**	

Cartesian co-ordinate

Atoms	X	Y	Z
C	-2.55127	-0.93307	-0.65334
C	-2.06782	-2.08401	0.06239
C	-1.61669	-1.65045	1.37331
C	-1.85386	-0.22748	1.46581
C	-2.41737	0.22371	0.21479
C	3.55649	-1.15717	0.20018
C	2.05091	-1.06304	0.19309
O	1.31984	-1.91942	-0.39108
O	1.46582	-0.05836	0.71888
C	-1.03883	-2.52255	2.43079
H	-0.56199	-3.40509	1.99238
H	-0.27437	-1.98717	3.00350
H	-1.81102	-2.86484	3.13105
C	-1.50557	0.63519	2.62371
H	-1.20963	1.64541	2.31055
H	-2.36938	0.72193	3.29550

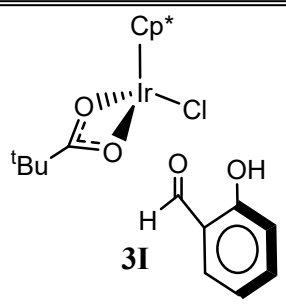
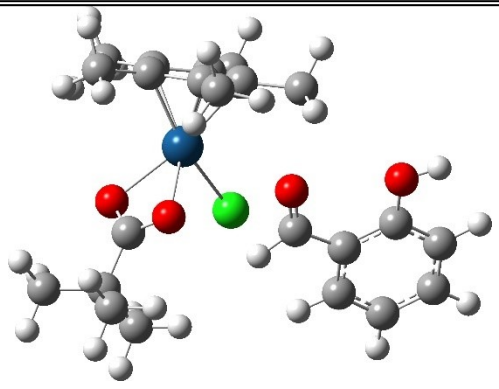
Frequencies

31.3179	34.1191	38.7207
56.2937	56.4604	63.8812
69.0372	87.8992	106.5902
126.7236	131.1198	145.3063
154.7109	162.1082	163.9259
176.1563	178.5581	186.1297
192.7037	199.1450	207.4300
213.0088	225.5437	230.5543
245.0643	264.2113	283.7131
300.2245	308.9058	311.2028
314.6653	322.4795	335.7310
341.4028	344.6824	381.8484
387.4942	417.7701	449.4484
456.8469	462.2341	530.1691
538.3436	544.5847	547.5223
582.8392	592.9252	602.4850
621.6014	795.3297	807.0486
811.0435	828.6648	933.8153
950.1690	952.8734	956.0504
959.1025	973.4117	1030.6615
1032.8688	1035.4629	1037.0121

H	-0.67397	0.20953	3.19384	1040.8438	1044.3338	1048.0566
C	-2.88403	1.60257	-0.09217	1090.4059	1096.0030	1104.7807
H	-2.33447	2.35979	0.48053	1185.9991	1188.1724	1234.2396
H	-2.76178	1.84009	-1.15430	1258.7641	1264.8367	1372.2460
H	-3.95115	1.69504	0.14961	1380.9612	1382.2846	1386.9699
C	-3.09747	-0.91173	-2.03569	1395.4082	1402.1067	1408.9562
H	-2.84310	0.02466	-2.54130	1409.6244	1434.0228	1435.3697
H	-2.68656	-1.72656	-2.63955	1439.1986	1443.3589	1448.3295
H	-4.19024	-1.00917	-2.02194	1448.6940	1452.2904	1454.1173
C	-1.96277	-3.47490	-0.45203	1461.6457	1462.3492	1463.2235
H	-0.97324	-3.89338	-0.23699	1466.3632	1471.0649	1473.6482
H	-2.71552	-4.11762	0.02120	1482.3501	1485.2053	1488.4686
H	-2.11196	-3.51494	-1.53440	1496.0164	1503.2067	1513.0523
C	4.04252	-0.12810	-0.83110	1522.8676	1540.3319	1584.1776
H	3.75406	0.88833	-0.53799	3026.2497	3031.6041	3031.6414
H	5.13638	-0.17080	-0.90271	3034.1094	3039.9960	3042.9601
H	3.62131	-0.33277	-1.82324	3044.5359	3046.0463	3109.3785
C	4.01061	-2.55449	-0.20300	3115.2383	3118.0756	3124.0542
H	5.10660	-2.59639	-0.20936	3124.7200	3125.9624	3126.4423
H	3.64431	-3.31196	0.49995	3130.7721	3132.8948	3137.1039
H	3.64621	-2.81766	-1.20115	3140.0822	3144.7882	3145.8167
C	4.08850	-0.79238	1.58549	3146.5673	3152.0371	3153.2466
H	3.75470	-1.51211	2.34348			
H	5.18522	-0.80348	1.57170			
H	3.75505	0.20477	1.88959			
Ir	-0.47528	-0.66193	-0.14042			
Cl	0.35099	0.46364	-2.18209			
Cl	-0.15236	3.84916	1.25220			
	0.51657	2.30160	-0.43352			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.362042 Electronic Energy = -1906.96460623
Internal Energy (E)= -1906.57468423 Enthalpy (H)= -1906.57374123
Gibbs Free Energy (G)=-1906.66141523 Gibbs Free Energy of Solvation=-1907.5207961

St.Pt.	General Structure	Ball & Stick model
3I		

3I

Cartesian co-ordinate **Frequencies**

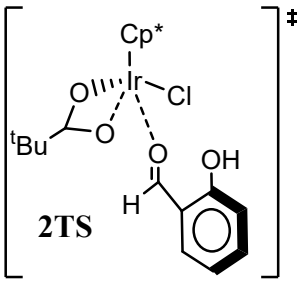
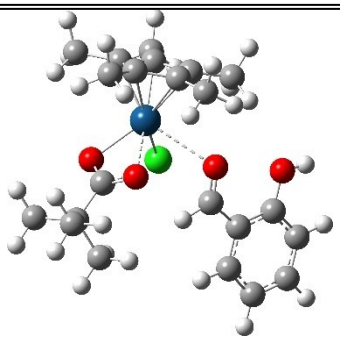
Atoms	X	Y	Z
C	1.11763	-2.41385	-0.97832
C	2.43975	-1.98392	-0.60288
C	2.44228	-1.69104	0.81761
C	1.11578	-1.95092	1.31471
C	0.28224	-2.37448	0.21042
C	-2.30446	0.60486	1.17196
C	1.53393	3.59583	0.25894
C	1.48919	2.08676	0.19628
O	2.16397	1.44236	-0.66239
O	0.69727	1.42808	0.94094
C	3.61081	-1.23685	1.61882
H	4.26118	-0.58257	1.02782
H	3.28334	-0.67134	2.49759
H	4.21169	-2.08710	1.96790
C	0.69266	-1.74991	2.72547
H	-0.38211	-1.89054	2.84375
H	1.22559	-2.45224	3.37913
H	0.91922	-0.72910	3.05413
C	-1.15186	-2.76709	0.26862
H	-1.66868	-2.28019	1.10217
H	-1.66674	-2.46228	-0.64943
H	-1.25142	-3.85588	0.37188
C	0.65825	-2.81141	-2.33544
H	-0.33136	-2.39231	-2.54340
H	1.33360	-2.43417	-3.10941
H	0.60485	-3.90390	-2.42444
C	3.60915	-1.80010	-1.50274
H	4.10045	-0.84096	-1.30359
H	4.34539	-2.59966	-1.35064
H	3.31042	-1.80509	-2.55479
O	-1.89096	-0.17884	2.00298
C	0.48342	4.07435	-0.75336
H	-0.51426	3.70375	-0.48564
H	0.45741	5.17159	-0.76768
H	0.71522	3.71123	-1.76130
C	2.91427	4.10319	-0.14535
H	2.92150	5.20044	-0.14275
H	3.68571	3.75829	0.55440
H	3.18484	3.75410	-1.14667
C	1.16729	4.08364	1.65675
H	1.88861	3.73248	2.40485
H	1.16435	5.18078	1.67679
H	0.17579	3.72633	1.95385
Ir	1.03879	-0.41334	-0.20630
H	-1.70725	1.50673	0.90509
C	-3.57185	0.50074	0.43033
C	-3.83613	1.48557	-0.52726
C	-4.52320	-0.51818	0.62847
C	-5.00270	1.48856	-1.27445
H	-3.07596	2.24974	-0.68739
C	-5.70166	-0.51458	-0.11992
C	-5.93739	0.47859	-1.06100
H	-5.18169	2.26003	-2.01781
H	-6.43693	-1.30371	0.04095
H	-6.86117	0.45856	-1.63512

30.8280	38.1817	44.1111
49.4804	63.0435	67.0704
75.1160	83.1601	94.3541
114.7961	130.5183	136.3098
144.3380	150.3681	155.5723
159.6095	170.3639	175.3779
185.1889	189.7155	207.8535
210.5251	216.6807	226.1072
235.3826	246.4662	259.4605
286.6395	287.0722	295.7450
299.0651	312.8877	315.0929
320.8404	322.9045	331.1381
334.9521	380.5195	386.2291
388.9339	418.2845	420.3993
426.4177	431.7394	439.5089
444.3845	454.2503	461.8815
465.6875	532.8976	539.8319
546.1221	551.6641	555.0442
574.3083	580.9735	584.1790
603.9730	621.3633	664.8295
730.9641	768.6647	772.5783
797.1474	808.2247	818.1885
831.9858	849.9925	880.7402
934.6831	952.9124	954.4111
960.5085	963.8571	969.0339
976.3819	987.2726	1036.6876
1038.6122	1042.9642	1045.5165
1046.2566	1047.3682	1053.8288
1059.8921	1075.2638	1097.1175
1100.3671	1114.7509	1127.6658
1160.9841	1186.1998	1187.6340
1190.8350	1233.3730	1234.2505
1264.3290	1268.1351	1322.7368
1337.4441	1380.9085	1381.5705
1383.9920	1387.6915	1393.5992
1398.1045	1400.1563	1409.8179
1411.6461	1420.4734	1436.0935
1439.4753	1442.8910	1443.9017
1453.3686	1455.6313	1457.9739
1460.6902	1464.0521	1466.6992
1469.9587	1472.5786	1480.3232
1483.6932	1493.0474	1496.6180
1497.2399	1500.8009	1503.8188
1509.1934	1522.5267	1524.0943
1543.0539	1549.4777	1603.4364
1657.3084	1678.8916	1822.8156
2913.2859	3028.9109	3031.6897
3032.5143	3033.4459	3037.3256
3039.5683	3041.4834	3043.8458
3109.9317	3114.0109	3115.5436
3117.8209	3119.9214	3120.1798
3123.4749	3128.5660	3136.8633
3138.2234	3142.2711	3147.7296
3147.9527	3148.9658	3150.2901
3153.5592	3176.3143	3185.0554
3196.8920	3204.4633	3874.9486

O	-4.28069	-1.48020	1.54393
H	-5.03545	-2.07943	1.56631
Cl	-0.60847	0.46786	-1.73358

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.478238 Electronic Energy = -1721.46542657
Internal Energy (E)= -1720.95528357 Enthalpy (H)= -1720.95433957
Gibbs Free Energy (G)=-1721.04851457 Gibbs Free Energy of Solvation=-1722.16119909

St.Pt.	General Structure	Ball & Stick model
2TS		

Cartesian co-ordinate

Atoms	X	Y	Z
C	1.84695	-2.23837	-0.76651
C	2.89774	-1.29683	-0.40899
C	2.73363	-0.94061	0.98360
C	1.57540	-1.64907	1.47549
C	1.02578	-2.45461	0.40975
C	-2.19027	0.37304	0.78431
C	0.78554	3.78035	-0.00682
C	0.91025	2.26394	0.08463
O	1.36994	1.62801	-0.91857
O	0.48753	1.66523	1.09911
C	3.59570	-0.00499	1.75494
H	3.94068	0.82080	1.12199
H	3.04754	0.43481	2.59352
H	4.48103	-0.51560	2.15589
C	1.01289	-1.50027	2.84318

Frequencies

-74.2893	16.9926	19.3227
35.2813	45.2587	49.4471
57.0078	77.4352	83.1851
96.1513	105.8529	113.2939
117.1664	137.8118	147.3059
164.3880	171.3380	176.5350
184.0006	186.6368	189.1717
203.9736	208.3708	216.4604
221.8721	224.4051	228.2977
244.4660	266.0840	279.5929
283.2644	288.1566	292.7787
300.3889	304.2539	309.3978
313.1633	331.0814	343.1468
371.9186	391.0971	401.9044
410.6905	424.3561	433.8000
447.2132	451.2300	460.3604
469.3760	533.7138	537.1215
544.3413	546.9370	552.4904
577.5833	579.9287	587.3224
603.8691	617.4633	669.7825

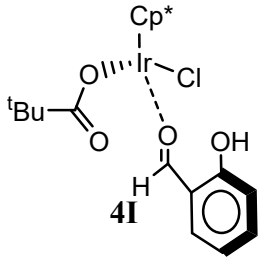
H	-0.01990	-1.85188	2.88742	727.2915	764.6848	781.9255
H	1.61489	-2.06791	3.56443	792.0579	804.2029	812.6507
H	1.00983	-0.44704	3.14339	825.7743	845.6460	884.7510
C	-0.18098	-3.32073	0.48889	926.4726	941.3738	946.6022
H	-0.91060	-2.90461	1.18950	950.1152	952.7351	961.7159
H	-0.68553	-3.36268	-0.48190	967.9825	979.1320	1030.0973
H	0.08149	-4.34176	0.79497	1031.2187	1036.7830	1041.2114
C	1.66861	-2.88342	-2.09362	1042.5836	1045.5454	1045.9701
H	0.61789	-3.12623	-2.27307	1054.0622	1073.5092	1092.0776
H	1.98081	-2.21569	-2.90261	1095.9540	1112.4689	1126.8226
H	2.25832	-3.80713	-2.15564	1161.7803	1183.5794	1187.5055
C	3.95298	-0.76674	-1.31145	1188.2276	1238.5833	1239.6792
H	4.13079	0.29552	-1.11371	1258.9519	1269.2092	1322.2101
H	4.89702	-1.30789	-1.16679	1339.4510	1368.8416	1379.0792
H	3.66210	-0.85945	-2.36178	1383.7916	1385.1646	1391.9294
O	-1.41895	-0.47149	1.19418	1394.8403	1397.6661	1402.3983
C	-0.70796	4.06455	-0.20928	1407.4803	1408.3057	1432.7166
H	-1.28579	3.73768	0.66433	1436.9270	1440.7451	1442.8461
H	-0.87215	5.14100	-0.34958	1449.9632	1451.0798	1452.8678
H	-1.08962	3.53855	-1.09551	1456.3656	1458.0256	1459.8444
C	1.57864	4.33478	-1.18351	1463.1709	1469.4274	1476.3791
H	1.45973	5.42524	-1.23247	1478.5783	1479.6188	1480.4957
H	2.64765	4.11252	-1.08304	1487.6550	1492.6870	1497.5459
H	1.23706	3.90189	-2.12904	1502.2814	1507.6238	1516.8490
C	1.25817	4.41098	1.30079	1522.0185	1544.0068	1656.1523
H	2.32864	4.22983	1.46420	1672.1042	1678.7858	1815.9414
H	1.10321	5.49741	1.27267	2928.8871	3019.9677	3027.8627
H	0.70991	4.00034	2.15457	3033.6163	3035.9747	3040.6699
Ir	1.00163	-0.39102	-0.17327	3041.4364	3041.8804	3042.7735
H	-1.84534	1.42614	0.67176	3108.3700	3111.6784	3114.0302
C	-3.58895	0.16778	0.39536	3117.2474	3121.3024	3121.3942
C	-4.33023	1.30584	0.06289	3124.7770	3128.9879	3130.9202
C	-4.20836	-1.09399	0.30539	3140.6219	3142.2700	3143.5236
C	-5.65739	1.22906	-0.32745	3151.3553	3155.4459	3157.5207
H	-3.82640	2.27138	0.11502	3168.6297	3169.1355	3172.2737
C	-5.54365	-1.17344	-0.09316	3190.0535	3207.8095	3877.7891
C	-6.25914	-0.02450	-0.40280			
H	-6.21537	2.12634	-0.57917			
H	-6.02010	-2.15168	-0.16389			
H	-7.29836	-0.11357	-0.71144			
O	-3.49848	-2.20102	0.60073			
H	-4.04754	-2.97384	0.42583			
Cl	-0.75235	-0.30978	-1.84680			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.475769 Electronic Energy = -1721.44973829
Internal Energy (E)= -1720.94179829 Enthalpy (H)= -1720.94085429
Gibbs Free Energy (G)=-1721.03740929 Gibbs Free Energy of Solvation=-1722.15591588

St.Pt.	General Structure	Ball & Stick model

4I



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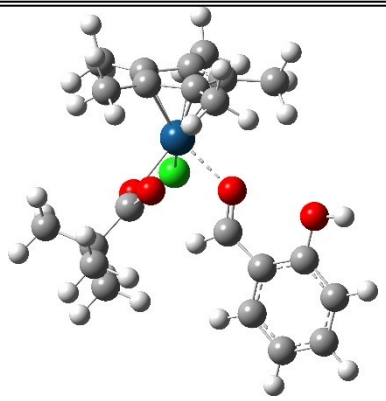


Cartesian co-ordinate

Atoms	X	Y	Z
C	2.72645	-1.71329	-0.22665
C	3.17679	-0.32941	-0.12549
C	2.65660	0.21265	1.11726
C	1.82982	-0.78539	1.73271
C	1.87526	-1.97664	0.89134
C	-1.97302	-0.42515	-0.55086
C	-0.78180	3.61684	0.08782
C	-0.25177	2.23190	0.49332
O	0.19801	1.56055	-0.52297
O	-0.26135	1.85659	1.66330
C	2.90628	1.59031	1.61865
H	3.00651	2.29519	0.78532
H	2.07887	1.93782	2.24267
H	3.83704	1.62117	2.19960
C	1.07210	-0.66371	3.00611
H	0.17789	-1.29673	2.98289
H	1.68783	-0.97403	3.86077
H	0.72702	0.36297	3.15075
C	1.10783	-3.22259	1.16539
H	0.06551	-2.98640	1.41175
H	1.09798	-3.88241	0.29296
H	1.54489	-3.77291	2.00842
C	3.06899	-2.64039	-1.33696
H	2.36233	-3.47366	-1.39493
H	3.02792	-2.12318	-2.30086
H	4.07751	-3.05105	-1.19903
C	4.11789	0.34628	-1.05914
H	3.94021	1.42611	-1.08428
H	5.16119	0.17787	-0.76022
H	3.98932	-0.02647	-2.08008
O	-1.04310	-0.89751	0.10317
C	-1.80337	3.46100	-1.03844
H	-2.67157	2.87790	-0.69745
H	-2.17326	4.44466	-1.35800
H	-1.36075	2.95351	-1.90280
C	0.41278	4.43811	-0.40452
H	0.09188	5.45128	-0.68192
H	1.17134	4.53158	0.38555
H	0.88064	3.96800	-1.27618
C	-1.42369	4.30411	1.28486
H	-0.70476	4.42480	2.10213

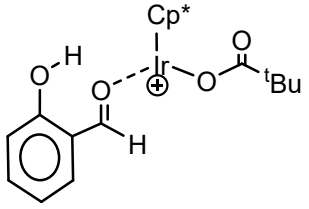
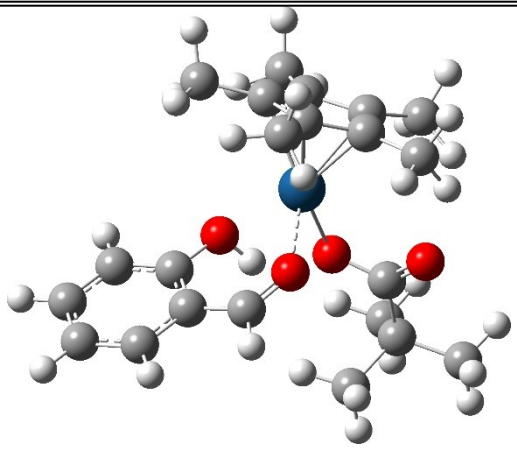
Frequencies

24.7976	25.9613	32.3343
46.7607	62.7549	64.6345
80.5297	97.3143	102.3097
107.1848	112.9931	130.1744
135.7627	137.3718	147.8971
154.3891	163.7933	174.0898
178.7845	191.9804	193.5837
198.9168	205.3382	221.0547
227.6135	240.7032	247.8473
266.9460	284.1467	288.7263
308.0077	314.2544	316.6033
320.6295	329.9544	339.5871
342.3056	347.7842	358.8091
375.1521	397.5562	420.6415
427.9543	438.7793	446.4608
450.9392	460.2762	467.0072
470.8575	538.3520	539.1529
547.7886	554.3337	569.7261
579.3698	585.9777	589.4208
602.8669	643.4101	679.3279
733.1457	765.6326	791.3951
794.5593	808.1892	811.1657
815.7050	850.7652	890.2636
914.4996	946.1980	948.0035
954.6384	962.4318	970.1441
976.4948	986.2586	1029.9681
1035.1128	1038.7512	1039.9559
1040.9456	1044.4422	1045.2712
1051.2541	1074.0001	1094.3740
1098.1006	1108.2987	1130.1190
1165.7117	1185.6485	1187.0881
1191.1247	1244.3336	1248.3500
1255.3374	1265.9221	1331.3276
1342.1429	1366.3975	1373.2747
1377.1254	1381.8705	1392.0643
1393.9952	1394.6937	1399.9389
1406.3464	1416.4944	1427.4042
1430.3079	1436.5655	1439.7894
1440.7270	1448.0446	1453.5471
1454.3199	1458.9947	1462.0269
1469.7560	1471.6000	1475.3366
1477.6585	1482.1028	1487.0207
1488.0009	1490.6999	1491.9599
1497.6389	1515.1552	1519.5099
1541.0536	1544.4493	1647.3478

H	-1.79540	5.29613	0.99518	1678.1948	1743.3638	1760.8902
H	-2.26401	3.71774	1.67358	3005.5465	3015.4757	3018.0641
Ir	1.06444	-0.32763	-0.24492	3032.9168	3036.5277	3036.8569
H	-1.75710	0.29410	-1.36140	3040.7033	3040.8757	3042.3885
C	-3.37109	-0.74435	-0.32941	3088.7780	3097.5187	3120.1691
C	-4.30745	-0.12455	-1.17019	3120.4353	3120.5851	3122.0844
C	-3.83193	-1.62739	0.67173	3122.6948	3128.7659	3133.6339
C	-5.66538	-0.35443	-1.04099	3136.6576	3136.9666	3148.6164
H	-3.93317	0.55110	-1.93833	3150.9942	3153.4054	3161.0917
C	-5.20271	-1.85523	0.80016	3165.0471	3169.8843	3176.6787
C	-6.10537	-1.22627	-0.04601	3195.6087	3217.8977	3874.8489
H	-6.37522	0.13405	-1.70157			
H	-5.55856	-2.53593	1.57337			
H	-7.16842	-1.42128	0.07520			
O	-2.93974	-2.22856	1.47830			
H	-3.41298	-2.78106	2.11164			
Cl	0.54455	-0.60687	-2.60437			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.477560 Electronic Energy = -1721.46431887
Internal Energy (E)= -1720.95455487 Enthalpy (H)= -1720.95361087
Gibbs Free Energy (G)=-1721.04929887 Gibbs Free Energy of Solvation=-1722.16261699

St.Pt.	General Structure	Ball & Stick model
5I		

Cartesian co-ordinate

Atoms	X	Y	Z
C	0.52406	-2.57454	-0.92698
C	1.78302	-1.83866	-0.93174
C	2.17124	-1.61483	0.44632
C	1.11872	-2.11805	1.28852
C	0.11316	-2.73707	0.42921

Frequencies

27.0405	32.1404	48.3983
60.9181	71.7062	80.8490
85.2810	111.8879	124.4122
129.2484	133.1331	143.5626
152.4694	157.9309	166.4776
169.0885	174.6427	178.0839
183.9164	191.0722	196.5740
201.3699	218.7208	225.0404
255.7144	275.7023	292.1449

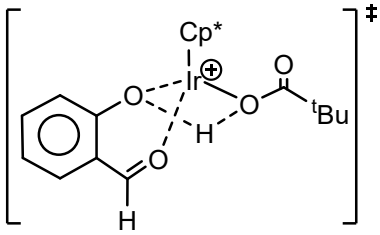
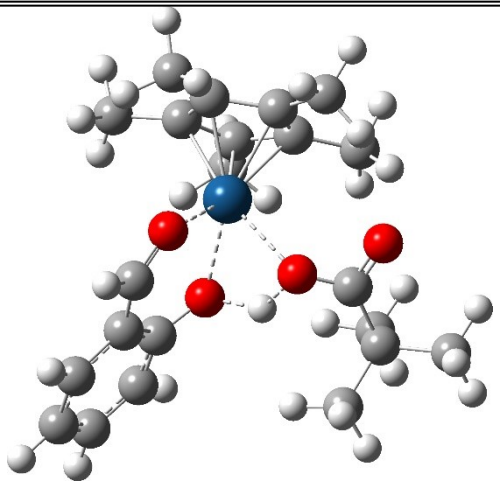
O	0.70430	1.35583	0.56264	297.0939	305.6913	309.2657
C	1.61556	2.04636	-0.10188	314.0918	317.8557	332.5171
O	2.37971	1.53479	-0.90238	347.6848	357.8245	362.2338
C	1.58748	3.54185	0.20420	391.2476	420.0072	427.7647
C	-2.71546	0.54209	0.61242	435.0407	442.0240	452.2622
H	-0.92348	1.19615	1.14623	458.9354	467.0711	471.3449
C	2.57483	-1.46078	-2.12879	532.4854	534.7027	537.2354
H	3.01562	-0.46857	-1.99758	545.1852	575.3151	584.1371
H	3.37562	-2.19149	-2.29900	589.5562	592.1815	601.4295
H	1.94949	-1.43180	-3.02592	636.3532	664.9746	720.7866
C	3.40265	-0.91855	0.89427	772.9352	778.1594	785.2192
H	3.70993	-0.16089	0.16824	799.0389	805.2719	810.3758
H	3.24960	-0.42030	1.85672	819.5331	888.5804	892.6433
H	4.21437	-1.64686	1.01545	919.9161	948.2160	950.7974
C	-1.13171	-3.38273	0.92095	953.0452	966.5671	969.2203
H	-1.88974	-3.45750	0.13591	969.8307	1012.2984	1017.9824
H	-0.91788	-4.39785	1.27818	1024.2276	1032.4747	1034.8469
H	-1.56492	-2.82404	1.75816	1035.7190	1036.8247	1040.0447
C	-0.20962	-3.00854	-2.14473	1048.3656	1061.1161	1085.8906
H	-1.26702	-3.19538	-1.93574	1096.2402	1107.6223	1134.4225
H	-0.14993	-2.24737	-2.92947	1166.7247	1187.1283	1189.5128
H	0.22280	-3.93381	-2.54430	1205.2361	1240.8682	1243.9076
C	1.07567	-2.10079	2.77396	1258.2562	1260.8741	1266.7574
H	1.41643	-3.06193	3.17900	1313.9579	1349.5530	1377.5010
H	1.71641	-1.31670	3.18634	1378.4222	1381.7867	1386.8694
H	0.05765	-1.92621	3.13811	1391.0175	1394.3372	1396.3994
Ir	0.30805	-0.61748	-0.00033	1401.0524	1416.9590	1423.0851
C	0.24748	4.08725	-0.30193	1425.5691	1432.9967	1434.9492
H	-0.59843	3.65675	0.24930	1438.9213	1443.2032	1448.3659
H	0.21134	5.17526	-0.17043	1454.6472	1456.2632	1462.1098
H	0.11435	3.87484	-1.37130	1463.0702	1465.2135	1472.1022
C	1.70961	3.77604	1.71083	1478.5508	1480.2321	1484.6904
H	2.65561	3.37872	2.09908	1485.9702	1489.7629	1490.7787
H	1.69272	4.85266	1.91948	1499.7629	1515.4964	1522.3580
H	0.88867	3.30974	2.26595	1523.9038	1540.6969	1627.1637
C	2.73234	4.23325	-0.52503	1669.0138	1723.9761	1791.8422
H	3.70205	3.84337	-0.19763	3009.0464	3026.3437	3034.7435
H	2.66472	4.08400	-1.60733	3044.8681	3045.7238	3046.6589
H	2.70692	5.30987	-0.31850	3046.9569	3047.1543	3048.8736
O	-1.46505	0.36402	1.15784	3118.5065	3121.2822	3126.0086
C	-3.80860	0.40381	1.44980	3126.5296	3128.5470	3131.6072
C	-5.09176	0.61569	0.95110	3133.1362	3133.4596	3133.9833
C	-2.89162	0.86231	-0.74901	3136.3047	3146.9017	3148.2140
C	-5.28928	0.97660	-0.38088	3150.0978	3155.1588	3159.5735
C	-4.19507	1.10271	-1.21896	3165.4434	3188.3093	3205.0826
H	-4.33360	1.36869	-2.26578	3216.1274	3223.6675	3394.5807
H	-6.29138	1.15492	-0.75846			
H	-5.94477	0.51417	1.61679			
C	-1.83523	0.86341	-1.73665			
H	-2.11646	1.27581	-2.72180			
O	-0.69076	0.40720	-1.63660			
H	-3.63680	0.15602	2.49366			
Cl	0.54455	-0.60687	-2.60437			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm

Zero-point correction= 0.476260 Electronic Energy = -1261.05929992

Internal Energy (E)= -1260.55298992	Enthalpy (H)= -1260.55204592
Gibbs Free Energy (G)=-1260.64195592	Gibbs Free Energy of Solvation=-1261.76086288

St.Pt.	General Structure	Ball & Stick model
3TS		

Cartesian co-ordinate

Atoms	X	Y	Z
C	2.44985	-1.60550	-0.44592
C	2.77428	-0.20498	-0.41775
C	2.40977	0.31328	0.89318
C	1.84583	-0.76031	1.65438
C	1.84018	-1.95394	0.82130
O	-0.54412	1.32912	-0.76785
C	-0.07862	2.61478	-0.77407
O	0.98810	2.85822	-1.27576
C	-0.97735	3.61309	-0.06202
C	-2.52102	-0.76366	0.47465
H	-1.18752	1.05202	0.03866
C	3.40752	0.59158	-1.49858
H	2.91939	1.56631	-1.60286
H	4.46762	0.75635	-1.26636
H	3.35055	0.07946	-2.46256
C	2.65157	1.70524	1.34917
H	2.50759	2.41912	0.53186
H	1.98943	1.98345	2.17527
H	3.68521	1.80325	1.70466
C	1.38726	-3.30674	1.23786
H	1.04935	-3.89713	0.38096
H	2.20835	-3.85339	1.71825
H	0.56058	-3.25043	1.95238
C	2.62871	-2.52204	-1.59956
H	1.83276	-3.27133	-1.64171
H	2.61832	-1.97683	-2.54751
H	3.58763	-3.04796	-1.51841
C	1.29673	-0.67207	3.03086

Frequencies

-351.2302	26.9127	35.3682
57.5967	71.0291	71.8204
87.2523	100.7617	109.7481
110.8950	123.1601	127.5518
145.9438	157.7965	164.8568
169.6007	175.4713	184.1172
189.2100	194.4451	210.8230
216.6216	228.5139	235.6950
240.6177	248.3746	267.5089
301.6894	306.1195	312.5164
316.3051	319.1043	334.0977
344.9866	354.0852	373.3263
386.2315	390.2064	417.9581
436.5470	443.0998	449.8747
460.5373	467.2729	504.7214
517.0007	536.1363	537.2099
543.7229	549.4919	576.6943
585.0785	587.5468	596.0190
602.6678	671.5327	704.4276
748.9347	774.4215	776.7326
789.7261	807.4422	809.3702
835.9126	878.6953	897.0534
932.5319	944.4362	955.8782
956.8504	962.4162	963.2146
971.4991	1007.6387	1011.5720
1028.1649	1030.3397	1031.1358
1033.2910	1038.0098	1040.0185
1047.8636	1057.9873	1090.6604
1094.6671	1108.6207	1146.3455
1160.4563	1167.8266	1188.4817
1191.0238	1226.1568	1234.4434
1253.1062	1263.1280	1267.6814

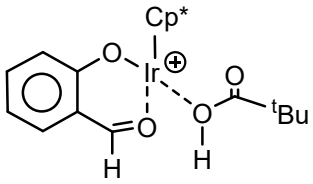
H	2.04741	-0.99865	3.76118	1304.4403	1356.4099	1381.4189
H	1.00443	0.35224	3.28079	1383.8945	1389.7075	1394.7058
H	0.41402	-1.30808	3.14806	1395.8373	1397.5004	1402.5789
Ir	0.64611	-0.46963	-0.12065	1413.7787	1421.1422	1422.2974
C	-2.45545	3.37194	-0.37677	1430.6659	1433.4482	1435.2417
H	-2.82914	2.41284	0.00525	1437.0403	1441.5600	1444.6962
H	-3.05304	4.15857	0.09750	1453.0611	1456.4635	1459.2292
H	-2.64908	3.41018	-1.45468	1459.5153	1463.3374	1466.5077
C	-0.72011	3.42135	1.44270	1473.9583	1483.5601	1485.2966
H	0.32381	3.65028	1.69165	1485.9946	1492.1281	1494.6645
H	-1.35707	4.10968	2.01019	1499.0000	1502.0574	1507.4865
H	-0.94871	2.40160	1.78517	1517.1716	1533.7810	1594.5858
C	-0.57550	5.02382	-0.47562	1674.5099	1685.6704	1878.4396
H	0.48305	5.21165	-0.27262	2263.0833	3025.3646	3030.6111
H	-0.74498	5.18689	-1.54546	3034.6218	3044.7921	3046.9684
H	-1.17281	5.75441	0.08121	3047.9637	3051.2714	3051.5291
O	-1.41160	-0.12258	0.80035	3052.3990	3112.9967	3118.5918
C	-3.60346	-0.71836	1.36874	3126.4122	3130.2511	3132.1955
C	-4.81410	-1.30227	1.04770	3134.3815	3137.4459	3137.7586
C	-2.69965	-1.44981	-0.76303	3141.1705	3141.8922	3150.7898
C	-5.00542	-1.96250	-0.17676	3153.6693	3154.1986	3155.8251
C	-3.95862	-2.02880	-1.06279	3157.3489	3173.3641	3178.5259
H	-4.07868	-2.54080	-2.01668	3194.7583	3210.2339	3224.9423
H	-5.96367	-2.41334	-0.41455			
H	-5.63514	-1.24363	1.75855			
C	-1.67447	-1.64965	-1.72989			
H	-1.99594	-2.15394	-2.65643			
O	-0.45428	-1.37981	-1.67791			
H	-3.45693	-0.19756	2.31140			
Cl	0.54455	-0.60687	-2.60437			

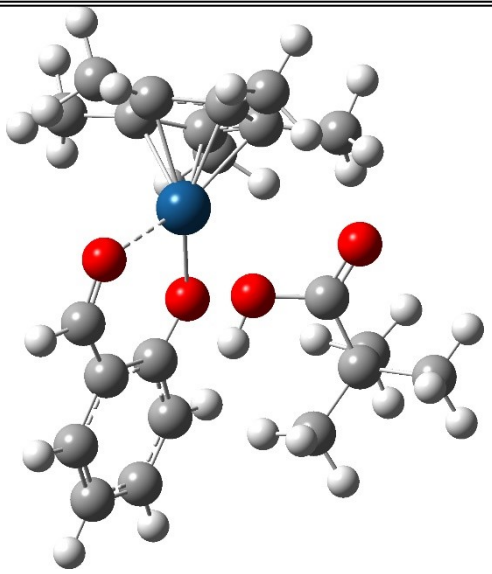
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.473107 Electronic Energy = -1261.05756969
Internal Energy (E)= -1260.55503369 Enthalpy (H)= -1260.55408969
Gibbs Free Energy (G)=-1260.64235069 Gibbs Free Energy of Solvation=-1261.7582599

St.Pt.	General Structure	Ball & Stick model

6I





Cartesian co-ordinate

Atoms	X	Y	Z
C	2.96311	-0.35813	-0.62630
C	2.60669	1.01147	-0.45195
C	2.12737	1.19133	0.91632
C	2.19739	-0.07214	1.58112
C	2.67379	-1.05678	0.61996
O	-0.97579	1.05502	-1.12785
C	-1.24931	2.33408	-0.69944
O	-0.37640	3.15563	-0.76600
C	-2.61790	2.55467	-0.07653
C	-1.83523	-1.50958	0.59140
H	-1.77581	0.50682	-1.06527
C	2.70148	2.09831	-1.45759
H	1.78844	2.70126	-1.46022
H	3.54565	2.75594	-1.21387
H	2.86033	1.70598	-2.46515
C	1.73081	2.48676	1.52518
H	1.29723	3.16712	0.78661
H	1.00336	2.34509	2.33078
H	2.61388	2.97318	1.95958
C	2.94359	-2.49098	0.89429
H	2.83844	-3.09596	-0.01134
H	3.96909	-2.61781	1.26420
H	2.26272	-2.89174	1.65095
C	3.48363	-0.99516	-1.86320
H	3.05712	-1.99290	-2.00732
H	3.24207	-0.40288	-2.74998
H	4.57416	-1.09834	-1.80989
C	1.79009	-0.35863	2.97968
H	2.65958	-0.31297	3.64660
H	1.05034	0.36476	3.33457
H	1.34457	-1.35398	3.06894
Ir	0.85738	-0.26895	-0.09665
C	-3.68794	1.60097	-0.61222
H	-3.53236	0.55266	-0.31034
H	-4.65871	1.88363	-0.19096

Frequencies

34.2818	38.7300	58.3943
68.7443	77.9035	84.5790
90.5901	90.8994	104.6115
111.8129	126.2507	135.8139
149.7370	151.8869	164.8802
174.4676	184.6815	190.1946
198.2138	202.7142	216.2307
223.0672	232.1979	248.3508
251.9838	257.3167	276.6499
288.7662	305.5440	309.2117
315.2983	327.6247	336.4413
357.1340	359.1060	381.6984
390.9317	393.2592	404.6851
436.1983	443.1041	447.0029
459.6111	475.5075	512.1138
533.7121	535.7408	543.0596
546.3290	554.5821	577.3127
584.3062	588.4999	602.9179
619.2716	650.3018	676.1801
754.6339	766.1062	776.0889
777.6339	802.6236	806.3336
809.9699	876.8512	880.4778
906.4576	948.4846	954.9191
958.8636	967.7581	968.1597
971.6724	1009.1124	1009.9801
1020.9123	1026.2657	1032.3148
1034.2739	1037.4277	1043.2866
1046.0466	1054.0537	1089.9834
1097.9282	1109.2763	1111.7499
1154.3198	1167.9355	1187.8790
1189.4193	1223.1870	1244.1531
1246.1183	1262.8920	1264.7198
1323.7675	1370.0827	1378.7550
1380.9048	1390.2599	1391.1653
1392.0719	1399.9163	1402.0356
1409.4651	1420.6131	1427.3905
1430.9618	1434.3369	1434.9684
1439.9066	1443.6979	1447.8584
1451.0604	1454.5267	1458.8102

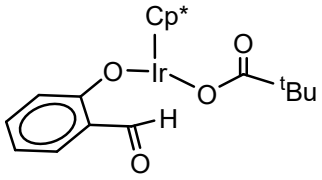
H	-3.78164	1.65526	-1.70390	1463.3881	1465.7983	1470.4366
C	-2.39751	2.31461	1.42762	1474.0280	1483.4803	1485.5935
H	-1.71893	3.07163	1.83787	1490.2292	1491.3913	1493.4409
H	-3.35635	2.39262	1.95351	1496.8921	1499.0891	1512.4482
H	-1.97221	1.31989	1.62423	1521.7372	1543.8704	1584.9159
C	-3.04203	3.99993	-0.32083	1672.9729	1685.6102	1903.7288
H	-2.27338	4.69987	0.01788	3017.3424	3032.8952	3036.4474
H	-3.22814	4.18779	-1.38438	3045.7885	3046.4831	3049.7436
H	-3.96773	4.20727	0.22761	3049.9969	3051.1659	3051.4407
O	-0.81538	-0.80643	0.98587	3102.3332	3120.0272	3127.8337
C	-2.91077	-1.67297	1.49979	3129.2579	3133.0140	3134.6797
C	-4.04294	-2.36801	1.14445	3134.9490	3136.6168	3137.1617
C	-1.96381	-2.12077	-0.70131	3140.7327	3151.1745	3153.8238
C	-4.17771	-2.96063	-0.12923	3157.6948	3160.0266	3166.0331
C	-3.14664	-2.84577	-1.02092	3175.6794	3180.5054	3189.7930
H	-3.21462	-3.30968	-2.00418	3203.9473	3220.7982	3760.9699
H	-5.07817	-3.50888	-0.38711			
H	-4.85108	-2.46589	1.86595			
C	-0.93621	-2.11332	-1.67725			
H	-1.11972	-2.72254	-2.57684			
O	0.16097	-1.50451	-1.65800			
H	-2.80335	-1.22132	2.48290			
Cl	0.54455	-0.60687	-2.60437			

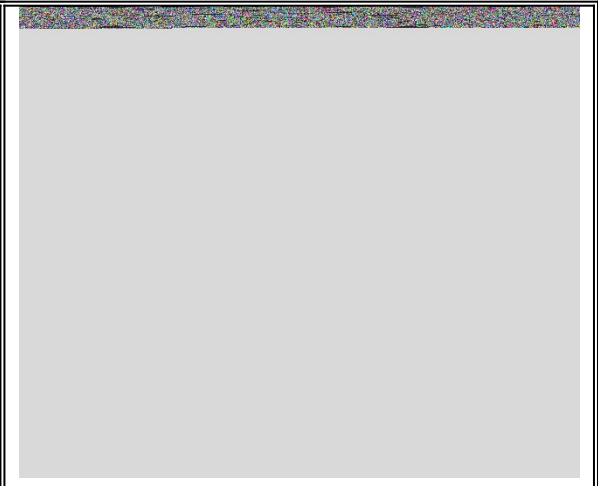
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.476845 Electronic Energy = -1261.07148317
Internal Energy (E)= -1260.56462617 Enthalpy (H)= -1260.56368217
Gibbs Free Energy (G)=-1260.65295217 Gibbs Free Energy of Solvation=-1261.76820875

St.Pt.	General Structure	Ball & Stick model

7I





Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.81921	-2.44398	-0.92848
C	0.34475	-2.74183	-0.15693
C	0.07770	-2.34623	1.21916
C	-1.30124	-1.87617	1.28402
C	-1.84896	-1.92098	-0.03534
C	-1.82374	1.95580	-0.56892
Ir	-0.07594	-0.61663	0.01999
C	-2.85462	2.85797	-0.89533
C	-3.21954	3.85203	-0.01701
C	-1.16692	2.02475	0.69065
C	-2.54055	3.95543	1.21255
C	-1.54064	3.07555	1.56325
H	-1.02558	3.14655	2.51820
H	-2.81545	4.74674	1.90806
H	-4.01024	4.55380	-0.26758
H	-0.26721	0.65704	-1.42036
O	1.90867	-0.06590	-0.01978
C	2.28866	1.04219	-0.60190
C	3.66686	1.51880	-0.13245
O	1.61695	1.69711	-1.38666
H	-3.33278	2.74952	-1.86700
C	-1.39207	0.98141	-1.54096
O	-1.96440	0.61198	-2.54852
O	-0.27167	1.16014	1.08162
C	4.30547	2.39847	-1.19995
H	3.64374	3.22570	-1.47242
H	5.25417	2.80952	-0.83005
H	4.51574	1.82607	-2.11193
C	3.38337	2.34870	1.12646
H	2.87925	1.74080	1.88769
H	4.32147	2.73527	1.54666
H	2.73253	3.19938	0.88905
C	4.58955	0.35383	0.21214
H	4.76763	-0.28501	-0.66281
H	5.56133	0.73470	0.55365
H	4.16428	-0.27045	1.00507
C	1.65451	-3.25821	-0.63838
H	2.46218	-2.57095	-0.35628

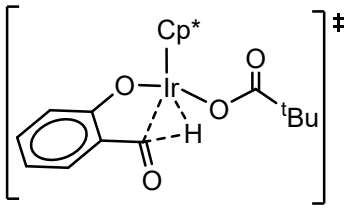
Frequencies

26.1426	36.0912	40.7567
51.7030	57.3238	65.1664
88.0946	94.8566	122.3750
135.5231	145.4921	151.7764
160.6126	164.0593	173.1818
180.9843	186.2838	194.3523
201.3308	210.3163	211.7506
226.2545	232.7383	234.8520
245.4983	256.7006	263.2800
278.3295	285.7333	303.2614
308.0613	311.2186	313.8637
324.2998	348.1144	374.7217
388.1531	415.4425	426.1663
431.8421	444.4151	457.9589
468.0659	530.7877	532.8995
536.3634	542.0544	547.3010
571.8879	583.5255	584.7920
595.2583	603.3916	619.9606
641.7659	652.3503	747.7033
764.1777	790.9007	802.9908
807.9301	816.1121	824.4970
861.2866	877.3374	914.7142
946.4611	952.9866	953.6033
954.5086	961.8969	962.2979
979.1721	1036.7718	1038.3196
1039.7383	1043.3286	1043.6827
1044.0355	1045.8542	1050.6201
1082.9737	1088.8483	1097.1529
1103.9013	1118.9666	1142.4889
1180.5967	1185.6503	1205.1460
1235.5520	1245.5773	1268.5154
1273.3959	1341.5494	1354.7659
1373.3033	1374.9698	1379.6177
1382.9655	1392.2546	1397.3656
1401.0917	1405.6029	1409.1644
1435.5646	1435.9276	1436.5137
1439.5491	1444.0995	1449.7306
1450.9281	1451.8865	1454.0150
1458.3473	1459.7093	1465.4409
1467.7208	1469.3971	1474.4286
1478.0092	1483.8030	1488.4576
1495.9945	1497.8916	1508.4595

H	1.86771	-4.24224	-0.20282	1518.8678	1523.5907	1543.1374
H	1.66853	-3.35704	-1.72737	1604.2579	1671.1504	1779.9995
C	-0.99347	-2.59408	-2.39765	1805.7272	2277.9465	3023.7688
H	-0.04371	-2.81697	-2.89201	3025.6906	3029.4207	3032.5410
H	-1.69677	-3.40669	-2.61977	3035.6126	3036.7398	3038.9883
H	-1.39299	-1.66890	-2.83356	3044.6089	3104.2203	3107.7278
C	-3.23791	-1.56820	-0.43858	3111.3802	3114.9325	3115.8425
H	-3.26481	-1.16783	-1.45686	3118.5280	3119.6986	3126.1848
H	-3.88628	-2.45302	-0.39905	3129.3354	3136.4608	3142.1952
H	-3.66347	-0.80625	0.22302	3145.8014	3147.2195	3149.1518
C	-1.98213	-1.35961	2.50056	3149.2106	3149.3228	3174.8601
H	-2.71087	-0.58314	2.24584	3184.1272	3198.4756	3207.0416
H	-2.50932	-2.16725	3.02344			
H	-1.26387	-0.91254	3.19482			
C	1.03039	-2.50775	2.34930			
H	0.75215	-1.88069	3.20142			
H	1.06037	-3.55130	2.68953			
H	2.04174	-2.21860	2.04322			
H	-2.80335	-1.22132	2.48290			
Cl	0.54455	-0.60687	-2.60437			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.462130 Electronic Energy = -1260.64913599
Internal Energy (E)= -1260.15718999 Enthalpy (H)= -1260.15624699
Gibbs Free Energy (G)=-1260.24605199 Gibbs Free Energy of Solvation=-1261.31339186

St.Pt.	General Structure	Ball & Stick model
4TS		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.95359	-1.76649	-0.89131

Frequencies

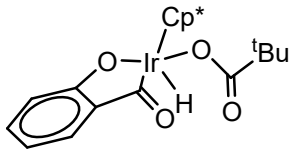
-191.9673	15.7274	30.6674
39.6229	46.0375	55.8118
69.3879	86.5315	96.6943
133.0113	137.7155	146.4286
159.6379	162.5249	168.5527

C	-0.97467	-2.53226	-0.18670
C	-1.00605	-2.13742	1.21911
C	-2.02351	-1.14434	1.36662
C	-2.58134	-0.87223	0.06660
C	-0.63507	2.52233	-0.48914
Ir	-0.41192	-0.41523	-0.03285
C	-0.96637	3.80971	-0.94348
C	-0.62833	4.91033	-0.18653
C	0.03241	2.32506	0.73908
C	0.05063	4.72139	1.03228
C	0.38186	3.46511	1.49610
H	0.90527	3.31981	2.43783
H	0.32289	5.59116	1.62796
H	-0.87355	5.91306	-0.52568
H	0.21619	0.44178	-1.33619
O	1.60306	-0.92193	0.05016
C	2.45998	-0.18335	-0.59853
C	3.90943	-0.41448	-0.15904
O	2.17428	0.67754	-1.42299
H	-1.47951	3.90495	-1.89804
C	-0.94457	1.33845	-1.26506
O	-1.61125	1.27029	-2.27379
O	0.30191	1.12189	1.16621
C	4.85879	-0.01710	-1.28189
H	4.64679	0.99794	-1.62899
H	5.89878	-0.06811	-0.93416
H	4.75602	-0.69165	-2.14090
C	4.10276	0.51173	1.04923
H	3.37671	0.27745	1.83740
H	5.11545	0.39409	1.45703
H	3.96414	1.56130	0.76152
C	4.15735	-1.86212	0.25316
H	3.97148	-2.54916	-0.58286
H	5.20316	-1.98751	0.56335
H	3.51199	-2.16061	1.08608
C	-0.04797	-3.55373	-0.74227
H	0.97766	-3.35822	-0.40547
H	-0.33575	-4.55957	-0.41066
H	-0.04660	-3.53914	-1.83598
C	-2.29814	-1.84276	-2.33773
H	-1.62189	-2.51600	-2.87258
H	-3.32190	-2.21591	-2.46766
H	-2.23135	-0.84983	-2.79919
C	-3.71253	0.04880	-0.22074
H	-3.68196	0.39619	-1.25717
H	-4.67406	-0.45099	-0.04598
H	-3.67207	0.93509	0.42262
C	-2.36442	-0.40690	2.61073
H	-2.64767	0.62799	2.39036
H	-3.20656	-0.88348	3.12824
H	-1.51184	-0.37047	3.29515
C	-0.13274	-2.71493	2.27695
H	-0.13912	-2.10180	3.18275
H	-0.45672	-3.72694	2.55259
H	0.90424	-2.76976	1.92656
H	-2.80335	-1.22132	2.48290
Cl	0.54455	-0.60687	-2.60437

172.1975	174.9609	177.8848
189.9071	192.0325	203.6136
209.7536	226.2221	247.9605
256.4651	261.4150	269.8632
274.2010	283.0996	288.9312
304.2119	307.0877	310.1645
321.2221	350.9059	351.9366
380.3235	391.1112	412.1395
426.1903	430.2801	440.1065
469.8418	495.5161	537.1969
540.9210	542.5178	552.6125
565.1215	568.8484	594.4048
596.7509	606.1040	626.2884
639.1099	653.4028	720.7664
762.1530	775.7061	791.6752
812.2329	817.0436	818.6954
843.6225	856.7250	881.2626
899.8172	922.2020	935.6541
944.8955	950.8802	951.6394
956.0720	965.1151	984.8029
1030.6651	1034.0292	1035.8324
1042.4097	1044.6116	1046.1131
1047.3934	1050.8617	1088.5628
1092.3082	1108.0654	1124.3908
1150.6662	1182.1816	1188.8914
1212.5258	1233.3184	1246.1850
1263.5094	1268.3532	1351.5455
1356.1392	1370.9465	1372.7688
1375.9575	1380.7405	1393.4935
1397.1577	1398.1652	1405.0858
1406.2422	1436.3866	1439.2234
1440.1730	1443.3579	1444.8811
1445.1157	1449.3513	1453.8461
1460.1506	1461.8811	1465.3151
1466.6762	1467.0751	1473.8420
1475.7663	1484.5707	1485.2104
1486.7514	1502.9242	1511.4942
1520.4088	1525.3637	1543.7429
1614.8406	1666.5367	1745.6099
1788.4156	1878.9342	3023.6673
3026.8917	3035.3066	3036.6602
3037.3877	3039.8155	3041.0055
3041.9344	3106.4527	3113.2483
3116.2809	3116.4040	3116.6293
3117.1752	3121.3848	3123.2180
3127.2208	3129.7330	3142.1375
3148.0833	3149.8626	3151.8305
3154.0378	3166.0939	3168.9107
3191.4141	3201.5460	3209.2786

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.458396 Electronic Energy = -1260.64392691
Internal Energy (E)= -1260.15595091 Enthalpy (H)= -1260.15500691
Gibbs Free Energy (G)=-1260.24495791 Gibbs Free Energy of Solvation=-1261.30446716

St.Pt.	General Structure	Ball & Stick model
8I		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.56745	-2.49180	-0.67850
C	0.86979	-2.43177	-0.47523
C	1.13759	-2.28063	0.94454
C	-0.08968	-2.10913	1.59030
C	-1.16165	-2.17216	0.58226
C	-2.32904	1.36530	-0.60443
Ir	-0.08232	-0.42766	-0.16820
C	-3.37893	2.10035	-1.16918
C	-4.14342	2.92503	-0.36611
C	-2.03912	1.44072	0.76970
C	-3.85619	3.00336	1.00606
C	-2.82637	2.27932	1.57975
H	-2.60456	2.34287	2.64204
H	-4.45930	3.65215	1.63905
H	-4.95700	3.50922	-0.78758
H	0.60518	-0.41627	-1.59211
O	1.14070	1.24192	-0.06822
C	2.40892	1.12579	-0.32924
C	3.20083	2.40613	-0.02878
O	2.96869	0.10138	-0.71196
H	-3.56394	2.00292	-2.23677
C	-1.50427	0.44023	-1.38625
O	-1.67387	0.15997	-2.54951
O	-1.05754	0.71789	1.26513
C	2.50323	-2.22781	1.53159
H	3.00933	-3.19636	1.42488
H	3.10704	-1.47647	1.00944

Frequencies

22.2662	30.0753	36.2542
45.6310	57.7525	80.2531
94.1109	121.2146	128.4970
141.4676	157.8219	164.6265
169.8860	178.3314	181.7525
192.7819	206.2985	210.7402
218.9661	223.7833	240.6645
242.6141	247.2857	250.7498
259.6363	265.5475	276.3580
284.5940	290.4532	299.6233
301.1185	302.2028	314.5715
323.7881	335.9066	350.6608
378.8416	391.7167	414.0327
426.9393	444.5523	448.2749
473.5332	532.5571	534.1059
541.3901	552.5382	570.5422
572.3271	594.3947	604.3193
613.0662	621.6328	643.7646
649.5053	669.4126	756.3226
765.6532	782.1791	792.9702
810.8477	813.9814	820.4792
860.5346	866.7305	890.8890
921.0103	943.6655	944.9364
955.2137	955.7229	956.6887
958.5108	971.5986	982.4701
1021.3380	1031.3654	1041.4651
1042.9466	1043.7086	1045.5833
1049.0314	1052.3049	1087.7949
1093.4995	1110.4398	1117.0866
1147.7324	1176.8672	1189.0197
1205.4348	1239.4247	1249.1822

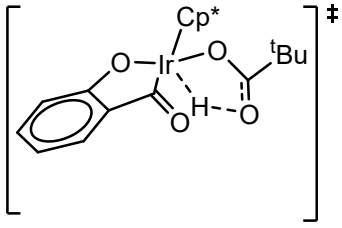
H	2.47645	-1.97629	2.59561	1266.2059	1266.7927	1341.0894
C	1.90382	-2.77382	-1.48796	1361.7507	1363.0005	1370.8247
H	2.73966	-2.07147	-1.42608	1380.2300	1385.2837	1390.3923
H	2.27600	-3.79131	-1.30851	1392.3047	1393.8550	1401.4494
H	1.49329	-2.73248	-2.50155	1417.8901	1423.6618	1430.8675
C	-1.25060	-2.87576	-1.94396	1440.7882	1444.4463	1450.1028
H	-1.02893	-3.92128	-2.19089	1451.0970	1452.3662	1458.7973
H	-2.33542	-2.76960	-1.85595	1461.9755	1462.7937	1464.2315
H	-0.93833	-2.23874	-2.77838	1465.7179	1469.2613	1476.1445
C	-2.61343	-2.12914	0.91105	1478.3575	1482.6658	1486.3576
H	-3.22271	-1.95698	0.01840	1487.3722	1489.5248	1502.2955
H	-2.93633	-3.07298	1.36929	1518.0758	1531.1723	1586.4311
H	-2.82709	-1.31879	1.61660	1628.3835	1662.1793	1756.8064
C	-0.34375	-1.78210	3.01374	1816.8579	2205.5898	3018.4750
H	-0.75177	-0.76249	3.07987	3023.6893	3030.4207	3035.9906
H	-1.08491	-2.46548	3.44603	3037.2237	3039.3467	3043.4064
H	0.56755	-1.83205	3.61564	3043.9595	3098.2099	3109.8019
C	4.52514	2.37594	-0.78262	3110.9453	3118.6322	3120.4330
H	5.11517	3.26813	-0.53526	3122.4426	3128.6345	3129.3150
H	5.10658	1.48544	-0.52472	3132.1277	3143.1684	3144.0160
H	4.36327	2.36374	-1.86707	3146.9267	3150.6300	3150.6753
C	2.40958	3.65598	-0.40261	3154.4056	3173.0657	3191.6669
H	1.46445	3.70717	0.14554	3194.9575	3202.0361	3209.7896
H	2.99962	4.55246	-0.16991			
H	2.17916	3.67369	-1.47497			
C	3.46438	2.39312	1.48127			
H	4.02366	1.49382	1.77222			
H	4.05947	3.27016	1.76784			
H	2.52330	2.41529	2.04307			
H	-2.80335	-1.22132	2.48290			
Cl	0.54455	-0.60687	-2.60437			

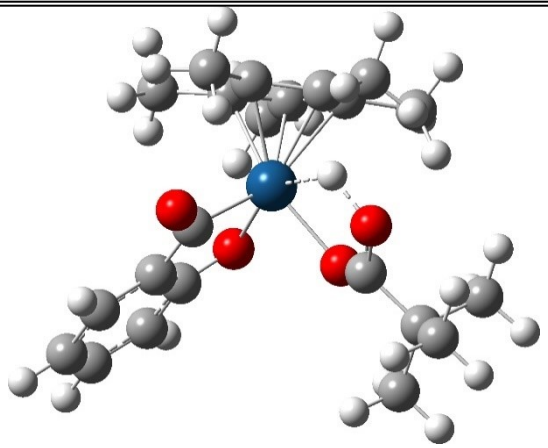
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.461420 Electronic Energy = -1260.65251733
Internal Energy (E)= -1260.16164433 Enthalpy (H)= -1260.16070133
Gibbs Free Energy (G)=-1260.24959133 Gibbs Free Energy of Solvation=-1261.30771862

St.Pt.	General Structure	Ball & Stick model

5TS





Cartesian co-ordinate

Atoms	X	Y	Z
C	0.39251	-2.31520	1.10412
C	-0.95230	-2.30024	0.57542
C	-0.88448	-2.48402	-0.87118
C	0.46080	-2.47007	-1.24389
C	1.27406	-2.28214	-0.03251
C	2.12889	1.57762	0.56236
Ir	0.11191	-0.44987	0.01711
C	3.00617	2.47662	1.18044
C	3.87194	3.22778	0.40759
C	2.11262	1.41492	-0.83487
C	3.85776	3.06882	-0.98738
C	2.99999	2.18191	-1.61320
H	2.98834	2.06305	-2.69380
H	4.53834	3.66108	-1.59710
H	4.55567	3.93553	0.86881
H	-0.91295	-0.02257	1.25448
O	-1.31384	0.97468	-0.60761
C	-2.19065	1.29790	0.27648
C	-3.30606	2.21614	-0.21480
O	-2.18589	0.86084	1.44295
H	2.97948	2.56272	2.26467
C	1.19450	0.73228	1.31375
O	1.11975	0.68556	2.52179
O	1.27975	0.55157	-1.37267
C	2.76436	-2.28992	-0.01725
H	3.15277	-1.91381	0.93466
H	3.16020	-3.30194	-0.17346
H	3.16202	-1.64358	-0.80781
C	0.75729	-2.37769	2.54542
H	0.44609	-3.33900	2.97266
H	1.83662	-2.27430	2.68701
H	0.28633	-1.56483	3.10914
C	-2.20470	-2.39608	1.37706
H	-2.50960	-3.44566	1.48396
H	-2.07314	-1.97045	2.37617
H	-3.02745	-1.85246	0.89987
C	-2.08730	-2.49965	-1.74797
H	-2.74687	-3.34206	-1.50405
H	-2.67005	-1.57711	-1.61543

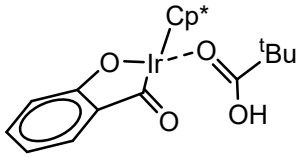
Frequencies

-318.5904	24.8504	37.7195
44.5605	60.0966	80.4685
96.8214	109.2749	127.9629
135.9322	156.1192	161.8068
168.1338	172.6133	187.5000
197.0635	200.1854	205.6622
208.5358	209.8342	217.1976
233.5929	240.8037	246.2368
251.9776	264.4110	270.5701
275.4130	279.9711	290.4461
302.3124	305.8514	310.4537
329.1813	337.5722	353.8896
372.2321	394.1635	426.2561
427.9157	436.5972	445.5730
474.4309	510.2008	535.9878
538.1655	540.9596	554.0154
572.5412	595.8151	617.9012
618.4469	628.0600	633.1282
643.0311	656.1499	677.9615
760.5140	768.9191	791.4598
809.4649	815.9883	838.0814
860.8842	862.0313	881.3889
931.2458	945.3855	948.2946
954.6126	957.3228	958.3429
958.8520	964.3589	977.0093
1031.0603	1039.7448	1040.1517
1044.4787	1047.4207	1047.9827
1050.2473	1052.8218	1087.3414
1088.4157	1107.9675	1117.2895
1147.8640	1177.0773	1186.4113
1205.9153	1239.4628	1253.0223
1265.5488	1269.6733	1344.4382
1368.8696	1374.8795	1378.8791
1384.8707	1390.0921	1390.6979
1398.5030	1399.3994	1407.4801
1427.9405	1428.9375	1435.8807
1438.3510	1447.1251	1451.5560
1452.6790	1454.3407	1455.8354
1457.8060	1460.3263	1460.9137
1462.7709	1468.6414	1470.8559
1479.0535	1480.9657	1483.3838
1489.4966	1497.5080	1506.6254
1511.6175	1518.1353	1580.4341

H	-1.82002	-2.57131	-2.80584	1593.6126	1627.0577	1662.1031
C	1.03568	-2.45320	-2.61314	1764.8781	1816.6192	3022.9560
H	0.27764	-2.64348	-3.37808	3024.2704	3030.3138	3034.5003
H	1.48098	-1.46740	-2.81090	3036.5254	3038.5573	3040.5765
H	1.82761	-3.20480	-2.71729	3040.9368	3099.6369	3101.2024
C	-4.17959	1.37192	-1.14983	3110.0920	3117.9077	3118.4677
H	-5.02455	1.97038	-1.51327	3122.0431	3125.2670	3128.2026
H	-3.60420	1.02250	-2.01492	3131.6981	3139.2051	3140.7982
H	-4.58855	0.49834	-0.62338	3142.9621	3146.9043	3149.8645
C	-4.13611	2.71504	0.96130	3150.2148	3151.0037	3172.2048
H	-3.52377	3.29462	1.66093	3189.9988	3200.3748	3205.3673
H	-4.94514	3.35976	0.59518			
H	-4.57650	1.88207	1.51882			
C	-2.71209	3.39492	-0.98389			
H	-3.52040	4.04439	-1.34374			
H	-2.05811	3.99734	-0.34179			
H	-2.12561	3.05576	-1.84261			
H	-2.80335	-1.22132	2.48290			
Cl	0.54455	-0.60687	-2.60437			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.459311 Electronic Energy = -1260.65072759
Internal Energy (E)= -1260.16259359 Enthalpy (H)= -1260.16164959
Gibbs Free Energy (G)=-1260.24823559 Gibbs Free Energy of Solvation=-1261.3068256

St.Pt.	General Structure	Ball & Stick model
9I		

Cartesian co-ordinate

Atoms	X	Y	Z
C	0.45931	-2.06640	1.35480
C	-0.89018	-2.08753	0.87420
C	-0.86450	-2.52356	-0.52957

Frequencies

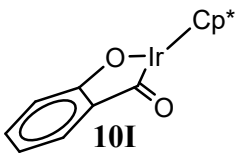
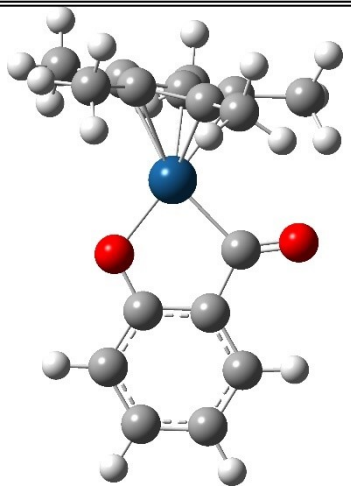
18.8734	33.7064	59.5472
66.8916	79.1068	83.5237
104.6253	126.3718	129.6155
147.2791	152.3271	159.4640
169.6575	176.3475	180.8473
188.4529	197.1381	203.8278
211.5721	223.3910	227.6976

C	0.46645	-2.65221	-0.93036
C	1.32161	-2.27695	0.20656
C	2.07282	1.68668	0.47114
Ir	0.24007	-0.48109	-0.09100
C	2.85259	2.65965	1.11153
C	3.85194	3.30670	0.41142
C	2.26138	1.37305	-0.89744
C	4.05081	2.99134	-0.94520
C	3.27647	2.05463	-1.60285
H	3.42769	1.82560	-2.65515
H	4.83634	3.50544	-1.49759
H	4.47611	4.05425	0.89415
H	-1.17183	1.21512	1.72965
O	-1.37357	0.91623	-0.67482
C	-2.21966	1.37855	0.10051
C	-3.54724	1.89904	-0.41747
O	-2.09835	1.43010	1.39923
H	2.64910	2.87987	2.15809
C	0.95039	0.98730	1.07622
O	0.43766	1.30034	2.16356
O	1.48415	0.48984	-1.46900
C	2.80953	-2.36301	0.20307
H	3.23983	-1.81615	1.04902
H	3.15439	-3.40434	0.25783
H	3.21625	-1.91573	-0.71104
C	0.87715	-1.83238	2.76372
H	0.76938	-2.74852	3.35807
H	1.92215	-1.51090	2.82059
H	0.27582	-1.04113	3.22455
C	-2.11950	-1.96880	1.70926
H	-2.40751	-2.93929	2.13670
H	-1.97288	-1.26739	2.53796
H	-2.97109	-1.60896	1.11910
C	-2.09002	-2.64775	-1.36592
H	-2.74743	-3.44455	-0.99372
H	-2.67018	-1.71373	-1.35261
H	-1.84913	-2.86778	-2.41006
C	1.00250	-2.93281	-2.28977
H	0.20253	-3.09303	-3.01880
H	1.60833	-2.08647	-2.63874
H	1.64248	-3.82457	-2.28702
C	-4.62993	0.92749	0.07145
H	-5.60939	1.26266	-0.29081
H	-4.45904	-0.08570	-0.31933
H	-4.66282	0.87918	1.16519
C	-3.80767	3.29563	0.15022
H	-3.03093	4.00259	-0.16491
H	-4.77014	3.66664	-0.22270
H	-3.84005	3.28599	1.24369
C	-3.53762	1.93911	-1.94040
H	-4.50272	2.31477	-2.30106
H	-2.74749	2.59662	-2.31846
H	-3.37186	0.94438	-2.36815
H	-2.80335	-1.22132	2.48290
Cl	0.54455	-0.60687	-2.60437

241.8458	252.7322	264.1363
265.9221	273.7274	276.3723
284.9809	296.2581	303.9757
309.9674	314.0410	324.4384
341.2129	368.9662	392.7757
396.5847	414.6553	419.6139
426.2533	445.6882	465.2976
486.4019	533.2305	537.1900
539.7705	547.7797	556.9302
568.9918	592.8122	601.9229
612.7471	623.9673	630.4002
660.2375	689.3923	761.6765
765.2527	781.4966	788.6964
802.3910	812.0628	856.6815
868.3538	896.3997	912.7404
947.9381	950.9288	951.3281
954.1202	957.9773	959.5241
965.5937	977.3441	1034.4842
1039.5182	1041.1113	1042.3330
1046.6632	1049.8433	1052.2790
1056.7546	1086.7959	1089.2490
1104.8876	1115.2311	1144.5643
1179.5468	1182.1943	1208.1185
1239.0748	1248.4011	1263.7369
1276.8931	1339.7961	1350.2689
1366.6126	1374.3936	1380.4945
1391.5894	1393.7598	1394.6950
1396.3521	1399.9691	1417.3470
1428.5177	1434.1931	1440.9895
1448.5724	1450.8282	1453.2953
1456.2571	1458.0668	1459.7786
1462.1979	1463.5180	1469.6024
1470.3223	1474.7453	1481.6574
1485.1453	1488.3064	1495.8551
1505.1630	1510.9514	1520.4603
1521.5694	1533.9806	1589.8440
1613.2034	1657.8868	1668.8237
1742.2187	3018.3892	3021.9813
3026.3916	3028.9060	3031.7469
3039.9485	3040.0483	3045.5617
3084.2274	3088.4227	3098.7110
3103.5935	3109.1884	3113.9169
3123.6733	3124.4879	3134.0904
3134.7103	3136.0598	3137.4713
3140.2030	3140.3013	3144.2242
3144.4847	3152.4007	3165.8787
3183.3405	3197.7228	3203.5312

Statistical Thermodynamic Analysis

Temperature=298 K	Pressure=1 atm
Zero-point correction= 0.465016	Electronic Energy = -1260.68475717
Internal Energy (E)= -1260.19071417	Enthalpy (H)= -1260.18977117
Gibbs Free Energy (G)=-1260.27702417	Gibbs Free Energy of Solvation=-1261.32501423

St.Pt.	General Structure	Ball & Stick model
10I	 **10I**	

Cartesian co-ordinate

Atoms	X	Y	Z
C	2.39545	-1.02205	0.50804
C	2.35158	-0.76724	-0.85807
C	1.95868	0.64463	-1.04627
C	1.93108	1.28378	0.23229
C	2.01375	0.22410	1.19524
C	-2.46840	-0.89790	-0.03417
Ir	0.25420	-0.12002	0.00557
C	-3.61205	-1.69539	-0.04806
C	-1.30643	1.21601	0.00978
C	1.86159	1.33953	-2.35810
H	1.18848	2.20029	-2.28368
H	2.84539	1.70028	-2.68946
H	1.46898	0.67310	-3.13366
C	2.54826	-1.71916	-1.98162
H	1.68155	-1.71282	-2.65356
H	3.42618	-1.44171	-2.58012

Frequencies

34.2866	40.6250	57.7737
88.2064	94.5102	128.7341
137.0140	145.8638	151.3885
160.4790	173.0750	184.4594
196.1009	199.6220	211.2624
253.3750	254.9971	268.6983
272.1059	287.1545	292.0853
303.1460	339.1185	358.7396
416.0955	427.2700	447.0304
490.4296	523.3922	535.5140
538.1719	548.2165	571.0292
587.1960	591.9919	609.0246
621.9411	638.1736	687.3955
759.4676	764.0225	804.7438
811.3871	856.1668	870.2882
886.5556	950.0381	955.1153
958.5535	977.9405	1026.0814
1028.4455	1036.8925	1040.2380
1041.6167	1045.5817	1087.1034
1088.8484	1104.6200	1106.5826

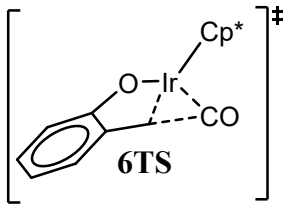
H	2.68602	-2.74477	-1.62784	1144.9073	1178.9523	1184.4965
C	2.65869	-2.31039	1.20340	1197.8339	1254.1376	1298.8676
H	2.78430	-3.13344	0.49388	1362.7100	1366.8898	1368.7244
H	3.56803	-2.25147	1.81634	1385.3008	1397.7738	1400.0342
H	1.83065	-2.57627	1.87154	1424.4657	1428.9242	1438.7508
C	1.96458	0.37474	2.67363	1446.9443	1447.6677	1448.9277
H	1.54626	-0.52067	3.14599	1455.6583	1457.6560	1461.9848
H	2.97201	0.53071	3.08398	1465.0286	1469.5958	1478.1236
H	1.34090	1.22633	2.96217	1486.3006	1495.3083	1515.4939
C	1.78693	2.74192	0.48787	1523.7672	1607.4925	1642.3331
H	2.67510	3.28074	0.13441	1654.6764	1784.8365	3030.1256
H	0.89702	3.14297	-0.00912	3030.5188	3031.7122	3032.7688
H	1.67439	2.94665	1.55716	3040.7415	3103.7938	3105.1627
C	-2.59971	0.49800	0.00803	3114.6672	3115.5197	3126.9079
O	-1.23415	-1.42790	-0.06714	3142.7401	3143.5287	3145.4692
C	-4.86167	-1.08100	-0.01525	3148.3986	3149.7078	3168.3363
C	-4.99501	0.30850	0.02739	3187.4013	3199.3314	3203.4975
C	-3.85313	1.10133	0.03611			
H	-3.50811	-2.77690	-0.08413			
H	-5.75501	-1.70317	-0.02457			
H	-5.98298	0.76130	0.05126			
H	-3.90710	2.18786	0.06446			
O	-1.22212	2.42990	-0.02854			
H	-1.84913	-2.86778	-2.41006			
C	1.00250	-2.93281	-2.28977			
H	0.20253	-3.09303	-3.01880			
H	1.60833	-2.08647	-2.63874			
H	1.64248	-3.82457	-2.28702			
C	-4.62993	0.92749	0.07145			
H	-5.60939	1.26266	-0.29081			
H	-4.45904	-0.08570	-0.31933			
H	-4.66282	0.87918	1.16519			
C	-3.80767	3.29563	0.15022			
H	-3.03093	4.00259	-0.16491			
H	-4.77014	3.66664	-0.22270			
H	-3.84005	3.28599	1.24369			
C	-3.53762	1.93911	-1.94040			
H	-4.50272	2.31477	-2.30106			
H	-2.74749	2.59662	-2.31846			
H	-3.37186	0.94438	-2.36815			
H	-2.80335	-1.22132	2.48290			
Cl	0.54455	-0.60687	-2.60437			

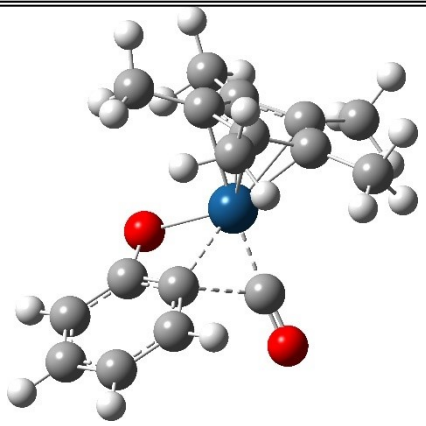
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.314298 Electronic Energy = -913.830301823
Internal Energy (E)= -913.494968823 Enthalpy (H)= -913.494024823
Gibbs Free Energy (G)=-913.565381823 Gibbs Free Energy of Solvation=-914.348801078

St.Pt.	General Structure	Ball & Stick model

6TS





Cartesian co-ordinate

Atoms	X	Y	Z
C	1.28872	1.33967	1.02046
C	1.27760	0.07861	1.68228
C	1.94986	-0.87568	0.82820
C	2.49210	-0.15951	-0.31173
C	2.03875	1.18079	-0.22044
C	-2.18859	0.78203	-0.62767
Ir	0.19594	-0.11367	-0.29440
C	-3.50640	1.23741	-0.63427
C	-0.69691	-1.52671	-1.13419
C	2.23786	-2.30045	1.16042
H	2.30534	-2.91327	0.25531
H	3.18939	-2.39677	1.69953
H	1.45276	-2.73379	1.78839
C	0.61529	-0.23096	2.97916
H	0.28836	-1.27537	3.01737
H	1.29957	-0.06213	3.82027
H	-0.27193	0.39209	3.13140
C	0.67693	2.61537	1.48806
H	-0.09452	2.43321	2.24338
H	1.42807	3.28501	1.92787
H	0.19739	3.14604	0.65828
C	2.24624	2.27959	-1.20437
H	1.28318	2.70209	-1.51506
H	2.84497	3.08823	-0.76594
H	2.75993	1.92544	-2.10275
C	3.33947	-0.75688	-1.38125
H	4.39075	-0.80857	-1.06775
H	3.01734	-1.77474	-1.62513
H	3.29461	-0.17103	-2.30433
C	-1.81943	-0.33593	0.13403
O	-1.11328	1.26724	-1.25533
C	-4.42168	0.52720	0.14383
C	-4.05273	-0.58268	0.90913
C	-2.72616	-1.02492	0.91844
H	-3.80076	2.10708	-1.21718
H	-5.46185	0.84878	0.15319
H	-4.80323	-1.10460	1.49845
H	-2.43153	-1.89433	1.50671
O	-1.19682	-2.45759	-1.61139
H	-1.84913	-2.86778	-2.41006

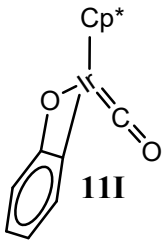
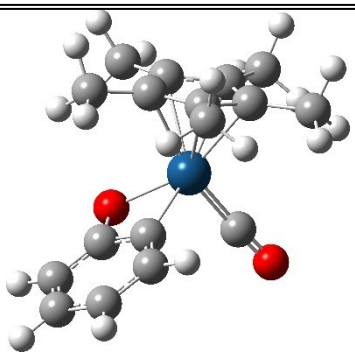
Frequencies

-135.0912	-18.0931	57.7381
78.0007	96.3665	109.4008
110.8689	122.5660	145.3942
155.4727	163.3089	175.5177
178.0852	183.3882	188.1989
208.3230	249.2344	263.6676
269.2361	287.6812	298.8802
309.3492	327.9896	370.0638
377.0172	406.6408	431.0345
471.3869	513.6462	527.2675
539.1117	541.8896	547.1066
551.3061	561.4194	579.0248
595.4879	601.2763	612.2204
665.1503	731.8924	760.8886
810.1406	811.9320	854.2639
856.6309	934.8238	951.2237
953.1457	966.4414	1022.0500
1029.4784	1035.5150	1036.8525
1037.9965	1040.2533	1046.2617
1084.0609	1087.7278	1105.0766
1119.4060	1153.8574	1184.3048
1185.4834	1255.1315	1311.8204
1377.6231	1382.9170	1385.4849
1394.8184	1397.1100	1400.3517
1438.3868	1438.9990	1445.4338
1447.5467	1448.0760	1451.0536
1456.0782	1459.9844	1463.3396
1468.4817	1473.3423	1475.5032
1481.6197	1490.7409	1499.8375
1523.5763	1555.1247	1622.0198
1643.4397	2089.5875	3033.4610
3034.2630	3036.4884	3039.2012
3039.8692	3113.9187	3115.0167
3115.2074	3119.4000	3120.4446
3137.6396	3139.4952	3141.5711
3143.1505	3148.7705	3151.1846
3167.0471	3187.7994	3195.3925

C	1.00250	-2.93281	-2.28977
H	0.20253	-3.09303	-3.01880
H	1.60833	-2.08647	-2.63874
H	1.64248	-3.82457	-2.28702
C	-4.62993	0.92749	0.07145
H	-5.60939	1.26266	-0.29081
H	-4.45904	-0.08570	-0.31933
H	-4.66282	0.87918	1.16519
C	-3.80767	3.29563	0.15022
H	-3.03093	4.00259	-0.16491
H	-4.77014	3.66664	-0.22270
H	-3.84005	3.28599	1.24369
C	-3.53762	1.93911	-1.94040
H	-4.50272	2.31477	-2.30106
H	-2.74749	2.59662	-2.31846
H	-3.37186	0.94438	-2.36815
H	-2.80335	-1.22132	2.48290
Cl	0.54455	-0.60687	-2.60437

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.312396 Electronic Energy = -913.810416360
Internal Energy (E)= -913.47801236 Enthalpy (H)= -913.47706836
Gibbs Free Energy (G)=-913.54487836 Gibbs Free Energy of Solvation=-914.322185125

St.Pt.	General Structure	Ball & Stick model
11l	 **11l**	

Cartesian co-ordinate

Atoms	X	Y	Z
C	0.77523	1.69426	0.59139
C	1.00604	0.70786	1.60782
C	1.98806	-0.21392	1.10174
C	2.46432	0.28556	-0.17993
C	1.70762	1.43779	-0.49474
C	-2.21512	0.23379	-0.91129
Ir	0.20404	-0.29932	-0.23953

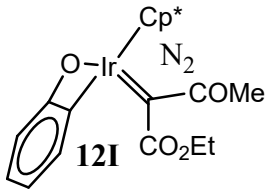
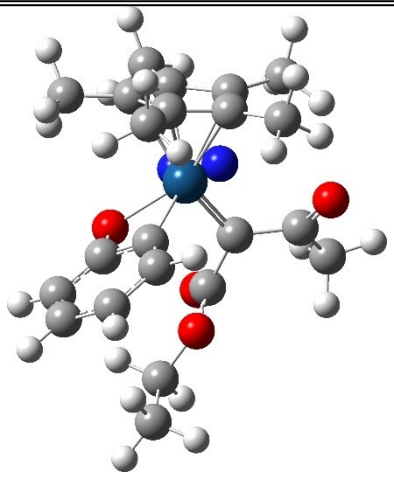
Frequencies

36.0251	50.2654	64.3570
75.6952	86.7686	131.2367
139.3810	145.4080	146.6288
155.6537	164.8460	175.8328
180.3732	207.4484	219.1681
239.4161	252.3317	280.6218
283.9124	299.3546	306.4361
319.2110	332.7144	367.6371
408.0762	412.0554	420.6785
511.5627	521.7275	537.9980
544.9971	549.8826	552.5672

C	-3.55188	0.53814	-1.13832	555.6639	566.8528	581.0262
C	0.12726	-2.08798	-0.76230	594.2492	599.7596	612.1908
C	2.58400	-1.36239	1.84282	662.2423	728.0291	756.9619
H	2.87509	-2.16925	1.16150	812.4840	817.3829	844.7082
H	3.48229	-1.05229	2.39252	853.7248	912.8793	953.8559
H	1.87806	-1.78402	2.56496	955.2858	962.7588	1022.3021
C	0.33747	0.63877	2.93530	1024.3916	1030.4408	1032.9577
H	0.28572	-0.39142	3.30271	1036.2853	1040.3791	1051.9779
H	0.88915	1.23297	3.67501	1083.0042	1091.3483	1108.6568
H	-0.68665	1.02178	2.88617	1108.9752	1149.3179	1181.6129
C	-0.16362	2.85054	0.64529	1185.3718	1248.1849	1286.7069
H	-0.96239	2.68499	1.37467	1376.5481	1382.6792	1392.2229
H	0.35890	3.77732	0.91658	1396.5760	1397.8313	1402.0403
H	-0.64260	3.00342	-0.32835	1437.3395	1437.9021	1445.1090
C	1.75130	2.24453	-1.74394	1445.8276	1449.8898	1451.9606
H	0.76528	2.25056	-2.22561	1454.8905	1465.3572	1468.7525
H	2.02436	3.28445	-1.52461	1472.9329	1474.5696	1476.6318
H	2.47599	1.84732	-2.46022	1482.9418	1489.9812	1506.5163
C	3.55259	-0.33193	-0.98961	1515.8860	1558.3669	1618.9123
H	4.53972	0.00187	-0.64306	1658.5231	2111.9345	3034.9915
H	3.53410	-1.42490	-0.91925	3036.3797	3037.1255	3038.3674
H	3.46421	-0.07197	-2.04878	3042.6276	3112.4526	3114.0134
C	-1.79235	-0.33524	0.29046	3116.7184	3116.8933	3124.2830
O	-1.14179	0.40754	-1.71056	3142.9294	3144.3135	3145.1752
C	-4.44644	0.24362	-0.10187	3146.8846	3147.6298	3150.9190
C	-4.02885	-0.33076	1.09591	3168.2816	3183.3480	3192.9689
C	-2.67277	-0.63830	1.30496			
H	-3.88514	0.97985	-2.07489			
H	-5.50299	0.46738	-0.24072			
H	-4.75792	-0.54775	1.87398			
H	-2.35112	-1.10038	2.23864			
O	0.13774	-3.20857	-1.04438			
H	-1.84913	-2.86778	-2.41006			
C	1.00250	-2.93281	-2.28977			
H	0.20253	-3.09303	-3.01880			
H	1.60833	-2.08647	-2.63874			
H	1.64248	-3.82457	-2.28702			
C	-4.62993	0.92749	0.07145			
H	-5.60939	1.26266	-0.29081			
H	-4.45904	-0.08570	-0.31933			
H	-4.66282	0.87918	1.16519			
C	-3.80767	3.29563	0.15022			
H	-3.03093	4.00259	-0.16491			
H	-4.77014	3.66664	-0.22270			
H	-3.84005	3.28599	1.24369			
C	-3.53762	1.93911	-1.94040			
H	-4.50272	2.31477	-2.30106			
H	-2.74749	2.59662	-2.31846			
H	-3.37186	0.94438	-2.36815			
H	-2.80335	-1.22132	2.48290			
Cl	0.54455	-0.60687	-2.60437			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.313341 Electronic Energy = -913.828197029
Internal Energy (E)= -913.493578029 Enthalpy (H)= -913.492634029
Gibbs Free Energy (G)=-913.564116029 Gibbs Free Energy of Solvation=-914.339512542

St.Pt.	General Structure	Ball & Stick model
12l	 **12I**	

Cartesian co-ordinate

Atoms	X	Y	Z
C	1.60218	-2.23136	-0.33890
C	2.09003	-1.16462	-1.19692
C	2.66802	-0.15815	-0.34916
C	2.42283	-0.54805	1.01883
C	1.79344	-1.84783	1.00631
C	-1.79462	-1.05176	0.91318
Ir	0.43851	-0.21143	0.00480
C	-2.97231	-1.65906	1.33632
C	-0.24404	1.43601	-0.61915
C	0.39968	2.30511	-1.65155
C	-1.46912	2.00294	0.02555
C	-3.78907	1.72976	0.27727
H	-3.64594	1.38907	1.31156
H	-3.94639	2.81500	0.29891
C	-4.89813	0.98818	-0.41836
H	-5.84532	1.13730	0.11014
H	-5.01851	1.34109	-1.44791
H	-4.67517	-0.08531	-0.44307
O	-2.57974	1.44038	-0.44340
O	-1.43316	2.88174	0.85901
C	3.48467	1.00045	-0.79692
H	3.44480	1.82894	-0.08137
H	4.53518	0.69733	-0.89725
H	3.14427	1.37824	-1.76488
C	2.17874	-1.21947	-2.68225
H	2.15534	-0.21247	-3.10600
H	3.10107	-1.72303	-3.00213
H	1.33295	-1.76970	-3.10901
C	1.01617	-3.51287	-0.81298
H	0.54877	-3.40494	-1.79613
H	1.80284	-4.27354	-0.90111

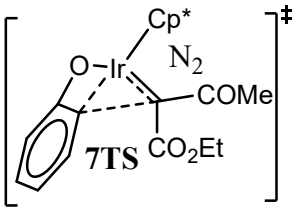
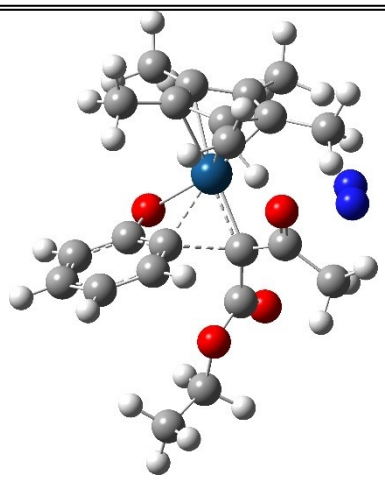
Frequencies

-29.6787	30.7622	37.6631
46.0186	60.6223	63.4016
78.6994	80.8520	93.4169
98.8961	105.4710	129.4931
130.4476	133.6266	143.1721
149.3475	155.6738	169.4382
174.4210	182.3774	186.6979
208.9187	218.0614	221.6470
225.5821	230.7912	238.7967
250.1199	259.5384	272.7869
274.8915	283.5480	298.2314
309.0958	310.6356	319.3553
328.9470	337.2700	343.5116
357.2867	370.7254	373.9893
398.9744	412.2966	418.8191
424.7508	497.5306	526.9501
540.7596	546.4596	554.3514
555.7465	570.2742	584.6773
595.8019	603.0238	609.2870
662.4204	673.8170	728.7679
739.8541	757.5423	805.7121
808.9012	813.2825	822.6340
846.2670	855.5676	892.8034
922.1836	937.4596	954.7374
964.3597	974.2919	1013.7552
1017.7174	1021.5682	1028.3630
1033.8672	1037.3641	1038.4872
1044.7286	1053.6689	1062.1745
1094.1446	1095.3237	1108.5424
1112.4890	1114.4511	1142.8665
1150.5309	1173.4175	1185.5126
1188.5810	1237.6462	1245.2548
1281.5714	1290.4236	1315.1441
1373.8569	1380.1396	1380.7398
1383.6225	1391.6638	1395.6772

H	0.24824	-3.88833	-0.12937	1400.7829	1405.2309	1422.1317
C	1.35065	-2.57669	2.22638	1434.2391	1439.1020	1442.8822
H	0.78134	-3.47605	1.97340	1449.1045	1451.3933	1455.1648
H	2.20894	-2.87887	2.84013	1456.7724	1464.4065	1465.1435
H	0.70378	-1.93843	2.84090	1467.8974	1470.5188	1472.6041
C	2.87138	0.14429	2.25913	1473.7146	1479.2107	1479.3829
H	3.72336	-0.37964	2.71287	1481.9070	1493.1510	1498.4163
H	3.17990	1.17377	2.05938	1509.5894	1511.2054	1517.5923
H	2.06554	0.17641	3.00286	1558.0945	1609.3168	1653.7082
C	-1.27020	-1.28704	-0.35878	1776.2592	1831.0731	2467.4640
N	1.54296	3.25778	1.63838	3033.6430	3034.7111	3037.9569
N	1.17428	3.15553	2.67495	3038.9356	3040.5930	3047.1574
C	0.13274	3.78601	-1.59063	3050.3361	3051.3041	3103.8853
H	0.28430	4.18118	-0.58093	3106.9108	3110.3662	3116.4183
H	0.77755	4.29264	-2.31148	3119.5716	3123.2136	3139.3070
H	-0.91665	3.98483	-1.84395	3142.1934	3144.1420	3147.4214
O	1.10422	1.83272	-2.53075	3148.7482	3149.9123	3159.5697
O	-0.99032	-0.18979	1.56161	3166.1250	3170.7210	3185.3446
C	-3.62045	-2.48088	0.40597	3185.9529	3195.4652	3195.6667
C	-3.11780	-2.68523	-0.87927			
C	-1.91407	-2.08253	-1.28010			
H	-3.37166	-1.49520	2.33530			
H	-4.54930	-2.97092	0.69365			
H	-3.66409	-3.31584	-1.57747			
H	-1.52358	-2.23996	-2.28566			
H	-2.80335	-1.22132	2.48290			
Cl	0.54455	-0.60687	-2.60437			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.448482 Electronic Energy = -1368.83736037
Internal Energy (E)= -1368.35727637 Enthalpy (H)= -1368.35633237
Gibbs Free Energy (G)=-1368.44964337 Gibbs Free Energy of Solvation=-1369.58522495

St.Pt.	General Structure	Ball & Stick model
7TS		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-2.12114	-1.84494	-0.13849
C	-2.20599	-1.03253	1.06843
C	-2.57649	0.30342	0.68798
C	-2.70583	0.32698	-0.75838
C	-2.43237	-1.00270	-1.24499
C	1.55953	-1.39339	-0.76675
Ir	-0.65039	-0.18137	-0.17534
C	2.42581	-2.47470	-1.00876
C	0.82196	0.93563	0.60946
C	0.78331	1.43739	2.00261
C	1.83607	1.55487	-0.30561
C	3.98482	1.39726	-1.23254
H	3.51478	1.26201	-2.21583
H	4.20032	2.46658	-1.11421
C	5.20520	0.53285	-1.06006
H	5.95193	0.76624	-1.82565
H	5.65934	0.68787	-0.07580
H	4.93364	-0.52501	-1.14587
O	3.04375	0.98991	-0.22874
O	1.58691	2.52019	-0.99311
C	-2.85357	1.42661	1.62373
H	-2.66017	2.39687	1.15307
H	-3.89971	1.41184	1.95629
H	-2.21247	1.35888	2.50847
C	-2.01200	-1.52039	2.46095
H	-1.48490	-0.77400	3.06322
H	-2.98088	-1.73892	2.92927
H	-1.41590	-2.43842	2.47775
C	-1.73591	-3.28377	-0.18915
H	-0.93398	-3.50427	0.52479
H	-2.58771	-3.93560	0.04517
H	-1.36577	-3.55777	-1.18281
C	-2.37798	-1.37650	-2.68417
H	-1.69213	-2.21235	-2.85328
H	-3.37011	-1.66365	-3.05530
H	-2.01841	-0.53656	-3.28787
C	-3.18605	1.46080	-1.59516
H	-4.21992	1.28623	-1.92416
H	-3.17125	2.40362	-1.04142
H	-2.56932	1.59355	-2.49098
C	1.24409	-1.09103	0.57744
N	-0.90479	3.82142	-0.19253
N	-1.12546	4.16746	-1.21854
C	1.42189	2.77742	2.25708
H	1.13286	3.51429	1.50108
H	1.15696	3.12467	3.25768
H	2.51253	2.66590	2.19042
O	0.26611	0.80080	2.91014
O	0.92286	-0.65765	-1.64904
C	2.94508	-3.15376	0.08707
C	2.62303	-2.82226	1.41443
C	1.75639	-1.76533	1.67349
H	2.67040	-2.76023	-2.02965
H	3.62889	-3.98286	-0.08978

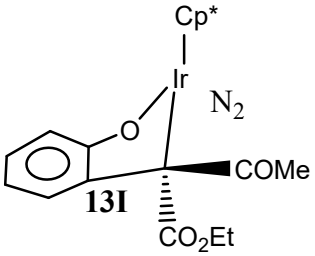
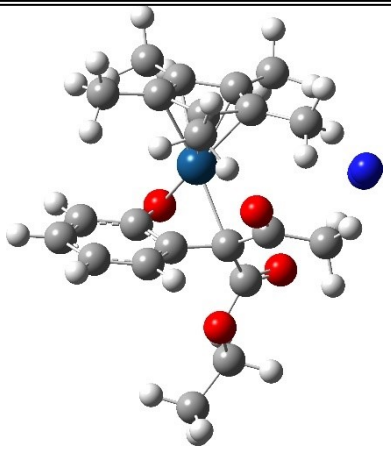
Frequencies

-272.3020	25.8406	34.2379
42.2733	43.8072	49.3255
63.3997	71.2625	73.0353
82.1868	90.5088	94.3628
98.3344	104.9116	116.2240
123.6014	130.1622	134.8603
137.4329	157.2543	159.3936
168.3359	178.5623	185.2080
194.5879	199.7497	217.3044
222.9440	236.5610	242.9745
267.7166	275.6666	281.5028
290.2175	292.5337	299.2639
305.5086	316.7666	327.9961
339.0323	378.2078	397.3012
404.1051	414.9562	425.6193
441.8370	490.1970	505.1128
534.6266	543.3273	544.7374
545.4996	548.5654	556.4270
580.5623	596.7959	601.1265
624.2367	641.8985	712.0110
727.4742	762.5407	791.7988
805.9277	810.5613	816.0651
847.2251	853.1881	890.5528
918.8641	939.7034	952.8937
962.1598	967.7176	970.9512
1003.0042	1019.5967	1028.4463
1030.9599	1037.3208	1040.0013
1041.8721	1044.8475	1051.7437
1091.2461	1095.7947	1108.5329
1108.8401	1113.7806	1140.9707
1145.7538	1172.4667	1183.2426
1187.3572	1226.1294	1251.4649
1284.6015	1314.5080	1344.7559
1368.1222	1371.8605	1379.8560
1381.6927	1388.8206	1391.9882
1397.2591	1399.3046	1427.4904
1431.0854	1435.7786	1441.4264
1444.2543	1446.2669	1446.8208
1451.2213	1455.3908	1460.5346
1462.7599	1465.3630	1468.0562
1473.8987	1476.1594	1482.1237
1489.3743	1494.6989	1498.5519
1500.3369	1501.5660	1511.6619
1538.0625	1600.9604	1627.5125
1776.0086	1832.8115	2465.9274
3032.8579	3033.6535	3037.2041
3038.9770	3042.1397	3043.5304
3044.1307	3045.6250	3097.0697
3110.3908	3114.1646	3121.7486
3123.2656	3126.1709	3133.5608
3136.9121	3137.1483	3141.5638
3148.1542	3148.6934	3155.4046
3165.7176	3168.1653	3176.9267
3183.9241	3189.9551	3198.9087

H	3.06356	-3.38484	2.23381
H	1.49264	-1.45820	2.68450
H	-2.80335	-1.22132	2.48290
Cl	0.54455	-0.60687	-2.60437

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.445445 Electronic Energy = -1368.83438192
Internal Energy (E)= -1368.35584592 Enthalpy (H)= -1368.35490192
Gibbs Free Energy (G)=-1368.45361992 Gibbs Free Energy of Solvation=-1369.58922866

St.Pt.	General Structure	Ball & Stick model
13I		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-2.80050	-0.22233	-0.45897
C	-2.47576	0.36613	0.82332
C	-1.81724	1.62824	0.58132
C	-1.68822	1.79839	-0.84543
C	-2.28541	0.63601	-1.47763
C	0.48993	-1.85208	-0.72363
Ir	-0.59555	0.01596	-0.21623
C	-0.13286	-3.08040	-1.09742
C	1.23382	-0.21277	0.93055

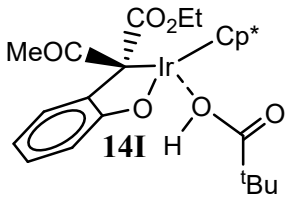
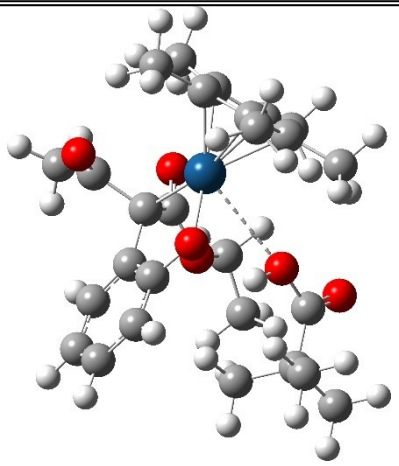
Frequencies

6.5119	18.5839	38.1305
40.9958	57.6035	59.8694
64.5321	73.2296	93.7750
97.7734	102.2845	107.0019
118.0695	126.7949	133.9879
138.8996	145.1331	148.0119
160.2460	168.2447	178.7165
183.4507	193.3212	194.8489
201.8026	230.6677	235.8153
238.0179	258.2993	279.4863
281.9431	288.2545	300.6830
303.2098	312.4339	319.9985
334.2757	345.7815	358.3531

C	1.09142	0.42979	2.26006	369.2298	392.4446	402.0938
C	2.43548	0.17616	0.12123	414.6360	426.2849	441.4712
C	4.32664	-0.62907	-1.00062	483.1896	504.6246	522.6241
H	3.89711	-0.24355	-1.93448	531.4782	541.5582	542.2166
H	4.98706	0.14995	-0.59897	551.2253	561.1410	575.3151
C	5.04446	-1.93742	-1.20141	585.7755	598.2022	601.6261
H	5.87461	-1.81291	-1.90424	657.5841	660.2686	708.3281
H	5.44755	-2.31162	-0.25451	761.7481	775.4711	805.7040
H	4.36175	-2.69281	-1.60366	806.4476	810.9412	822.8600
O	3.25836	-0.86659	-0.07854	834.3107	835.6803	904.0838
O	2.69014	1.29686	-0.26418	926.3892	947.4418	951.8122
C	-1.39619	2.59494	1.63127	969.8076	975.0222	1018.3307
H	-0.56547	3.22150	1.28703	1024.5429	1031.5032	1031.9833
H	-2.23062	3.25405	1.90362	1034.6679	1043.7268	1046.8162
H	-1.06962	2.07225	2.53772	1052.3434	1054.0502	1090.4772
C	-2.81980	-0.20443	2.15389	1093.3520	1109.3901	1118.2935
H	-2.00950	-0.03090	2.86939	1126.5666	1141.1757	1148.4995
H	-3.74519	0.23725	2.54639	1170.2601	1183.0134	1186.2671
H	-2.96461	-1.28833	2.08527	1203.5767	1253.7077	1294.5531
C	-3.46988	-1.53892	-0.64719	1305.2792	1333.8479	1342.6949
H	-2.99775	-2.32071	-0.03644	1358.0471	1377.1673	1379.9688
H	-4.52809	-1.48427	-0.36100	1387.5186	1390.9197	1392.3091
H	-3.42033	-1.86672	-1.69031	1394.5454	1406.6259	1428.7897
C	-2.30619	0.38513	-2.94510	1433.1926	1435.7125	1439.9666
H	-2.21451	-0.68448	-3.16485	1444.0404	1446.4157	1447.5000
H	-3.23353	0.75308	-3.40265	1454.0386	1455.7610	1463.8466
H	-1.46384	0.88642	-3.43273	1465.1783	1466.7474	1475.7086
C	-1.15602	2.98586	-1.56912	1476.5671	1477.6980	1482.9367
H	-1.96271	3.51493	-2.09450	1490.9269	1492.9268	1495.1597
H	-0.68827	3.69262	-0.87842	1495.9401	1508.9955	1513.0286
H	-0.39922	2.70186	-2.30927	1533.2722	1575.3380	1670.4778
C	0.67319	-1.55574	0.69721	1761.5268	1837.3179	2470.1128
N	1.72510	4.07807	-0.10722	3024.5942	3030.7502	3038.0197
N	2.36119	4.19420	-1.00294	3038.2018	3039.7407	3045.2904
C	1.94099	1.63753	2.56149	3049.0454	3055.8723	3097.2694
H	1.81418	2.40933	1.79520	3099.8505	3110.8486	3113.1247
H	1.66049	2.01879	3.54605	3117.5946	3119.3289	3134.6393
H	3.00644	1.37760	2.55903	3139.6630	3141.1359	3141.8362
O	0.28977	0.03212	3.10103	3143.4416	3146.0396	3147.3096
O	0.83360	-0.91386	-1.57458	3175.8599	3179.9350	3188.3489
C	-0.55141	-3.95723	-0.13284	3188.6759	3199.7929	3210.2255
C	-0.39659	-3.66176	1.24685			
C	0.19456	-2.49471	1.65491			
H	-0.24413	-3.28579	-2.15998			
H	-1.01333	-4.89852	-0.42524			
H	-0.74220	-4.37916	1.98744			
H	0.31532	-2.26085	2.70865			
H	-2.80335	-1.22132	2.48290			
Cl	0.54455	-0.60687	-2.60437			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.448616 Electronic Energy = -1368.90206963
Internal Energy (E)= -1368.42060763 Enthalpy (H)= -1368.41966363
Gibbs Free Energy (G)=-1368.51911863 Gibbs Free Energy of Solvation=-1369.65410781

St.Pt.	General Structure	Ball & Stick model
14I		

14I

Cartesian co-ordinate

Atoms	X	Y	Z
C	-2.53661	-1.94958	-0.94046
C	-1.66670	-2.41516	0.07562
C	-1.85147	-1.57718	1.26480
C	-2.88121	-0.62443	0.98426
C	-3.24650	-0.79744	-0.40511
O	1.58553	-1.50045	-0.03629
C	2.81429	-1.76144	0.42891
O	2.91960	-2.27124	1.52119
C	3.98781	-1.38448	-0.47031
C	0.78473	1.16172	-1.84460
H	1.52700	-1.04805	-0.89860
C	-0.72815	-3.56416	-0.00903
H	0.14061	-3.41905	0.63914
H	-1.23992	-4.48607	0.29799
H	-0.35748	-3.70726	-1.02929
C	-1.13276	-1.77076	2.55212
H	-1.59955	-2.57451	3.13706
H	-0.08418	-2.04411	2.37720
H	-1.14542	-0.85176	3.14624
C	-4.25704	0.01353	-1.13220
H	-4.17947	-0.13103	-2.21367
H	-5.26998	-0.27431	-0.82014
H	-4.11752	1.08071	-0.93289
C	-2.64866	-2.46488	-2.33204
H	-1.77331	-3.06303	-2.60306
H	-3.53970	-3.09384	-2.45526
H	-2.71419	-1.64300	-3.05340
C	-3.48345	0.36018	1.92357
H	-4.29570	-0.10397	2.49751
H	-2.73265	0.74879	2.61854
H	-3.90254	1.21173	1.37617
Ir	-1.17318	-0.28965	-0.32623
C	5.27024	-1.92936	0.14673

Frequencies

38.0555	51.6220	53.9234
61.2564	69.0512	74.1904
83.8640	84.5069	90.2815
91.6485	109.7013	114.0258
117.5930	123.0833	128.2933
136.0067	138.4794	145.6267
151.1061	160.5413	167.1956
182.6371	187.1240	198.5684
201.4059	210.5467	215.2863
225.8480	230.6460	244.8831
245.3737	257.5554	264.8170
273.0083	276.1543	287.7022
298.8144	309.4359	312.8823
316.3047	317.8661	327.1053
328.2961	334.4225	343.2223
367.0561	374.1642	387.2435
389.0569	392.6319	401.2026
403.0573	436.7210	451.0828
462.4481	471.2987	524.6209
526.9001	532.3570	537.2864
544.9293	548.3572	575.4638
580.0640	583.5775	594.7176
597.1602	601.4010	636.1479
646.1481	688.7236	693.0573
749.9140	769.8896	777.8006
795.4291	806.2096	810.8985
813.8472	834.3192	851.4203
854.6337	865.3186	886.3846
888.0230	917.1662	935.8696
948.3652	950.6723	958.2637
959.4233	967.1878	975.5446
1003.0856	1023.3586	1027.1284
1029.9425	1035.0493	1036.1141
1039.0858	1045.4433	1053.5813
1056.7820	1064.9295	1092.9114
1099.6016	1103.1424	1109.6508
1122.4267	1140.7179	1141.3042

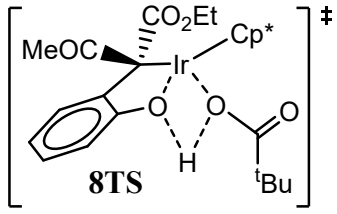
H	5.22769	-3.01847	0.25732	1149.7886	1178.5115	1186.6013
H	6.12476	-1.67631	-0.49273	1189.1524	1206.6599	1219.1860
H	5.44440	-1.50452	1.14063	1228.2726	1237.9586	1257.4377
C	3.79375	-1.98325	-1.86730	1277.3241	1297.1373	1300.8092
H	2.90974	-1.58413	-2.38219	1311.5047	1355.7680	1364.0260
H	4.66293	-1.73812	-2.48980	1366.6987	1371.2681	1381.0774
H	3.70419	-3.07595	-1.82882	1383.0141	1388.6867	1390.9423
C	4.06095	0.14409	-0.57440	1392.1454	1397.4635	1411.9942
H	3.21910	0.56126	-1.13693	1418.4575	1426.8854	1428.9147
H	4.06953	0.62155	0.41245	1430.0992	1433.6707	1442.9963
H	4.98003	0.42648	-1.10325	1447.9134	1449.7771	1451.1084
O	0.11629	-0.01136	-1.85024	1454.4967	1456.0265	1460.2874
C	0.68591	1.99097	-0.72203	1466.5120	1467.4730	1469.1146
C	1.46540	3.14290	-0.65943	1470.9969	1476.0762	1478.8600
C	1.60510	1.51666	-2.91889	1479.0961	1482.0285	1487.2616
C	2.30594	3.49229	-1.71348	1488.5653	1490.4529	1506.4013
C	2.35725	2.68422	-2.84754	1511.2773	1511.5504	1517.3507
H	1.64555	0.86217	-3.78737	1530.9448	1532.5722	1553.1465
H	2.99723	2.96092	-3.68292	1642.0063	1654.4550	1773.8631
H	2.90836	4.39540	-1.65562	1792.2857	1861.7602	3025.5628
H	1.41910	3.77157	0.23062	3026.2661	3036.7735	3037.4848
C	-0.34599	1.59632	0.31172	3038.0696	3039.3286	3039.8455
C	-1.47534	2.61878	0.20129	3045.3068	3046.7548	3050.5579
C	0.13933	1.38020	1.70268	3052.5299	3099.1069	3105.8597
C	1.91059	0.79108	3.11964	3111.6606	3117.6051	3120.5520
H	1.46008	-0.15624	3.44327	3120.6084	3121.4214	3125.3191
H	1.55190	1.57285	3.79898	3128.2973	3130.7703	3133.8232
C	3.41278	0.70725	3.09929	3136.7195	3137.2172	3140.5197
H	3.78987	0.59923	4.12167	3140.8880	3149.6319	3151.8417
H	3.74828	-0.16417	2.52792	3152.4654	3155.4983	3155.7628
H	3.84787	1.61656	2.66910	3160.8321	3172.9222	3173.3158
O	1.44888	1.08709	1.79090	3186.7006	3196.4784	3692.0991
O	-0.57412	1.42361	2.69450			
O	-2.26232	2.58441	-0.72971			
C	-1.55158	3.73917	1.20646			
H	-2.26182	4.48799	0.84914			
H	-1.86619	3.34702	2.17851			
H	-0.56651	4.19674	1.36191			

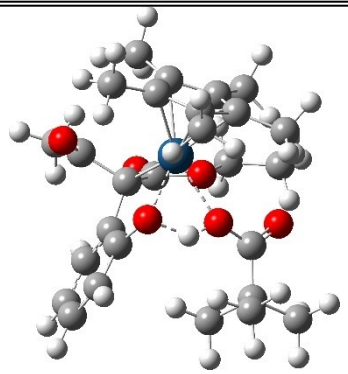
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.592124 Electronic Energy = -1606.27992951
Internal Energy (E)= -1605.65020151 Enthalpy (H)= -1605.64925851
Gibbs Free Energy (G)=-1605.75336851 Gibbs Free Energy of Solvation=-1607.07737895

St.Pt.	General Structure	Ball & Stick model

8TS





Cartesian co-ordinate

Atoms	X	Y	Z
C	-2.49028	-1.66196	-1.14500
C	-1.95951	-2.28960	0.00631
C	-2.15567	-1.39940	1.14832
C	-2.90648	-0.25625	0.69334
C	-3.04260	-0.37021	-0.74033
O	1.07645	-1.22134	-0.50700
C	2.08552	-1.79383	0.15439
O	1.89501	-2.32657	1.22581
C	3.43169	-1.73271	-0.56405
C	0.96041	1.40370	-1.80726
H	1.06438	-0.59886	-1.40602
C	-1.21352	-3.57410	0.06988
H	-0.30917	-3.47034	0.68046
H	-1.83753	-4.35765	0.51894
H	-0.90835	-3.91095	-0.92583
C	-1.76002	-1.70145	2.55118
H	-2.53915	-2.27522	3.07063
H	-0.83174	-2.28450	2.56855
H	-1.57475	-0.77601	3.10678
C	-3.75834	0.54965	-1.66179
H	-3.20472	0.65354	-2.60160
H	-4.75571	0.15115	-1.89321
H	-3.85878	1.55017	-1.23801
C	-2.44334	-2.14423	-2.55221
H	-1.78928	-3.01530	-2.65631
H	-3.44314	-2.42747	-2.90607
H	-2.06091	-1.35972	-3.21569
C	-3.47116	0.80584	1.56664
H	-4.40241	0.44794	2.02462
H	-2.76717	1.06249	2.36625
H	-3.69745	1.71281	0.99842
Ir	-0.95968	-0.31250	-0.25216
C	4.41387	-2.66221	0.13919
H	4.06060	-3.69956	0.12700
H	5.38572	-2.62173	-0.36789
H	4.56034	-2.37584	1.18567
C	3.27044	-2.16878	-2.02387
H	2.64734	-1.47672	-2.60353
H	4.25691	-2.19699	-2.50266
H	2.83182	-3.17189	-2.09893
C	3.94401	-0.28818	-0.51568
H	3.27721	0.40212	-1.04491

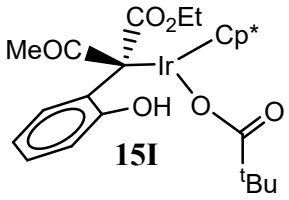
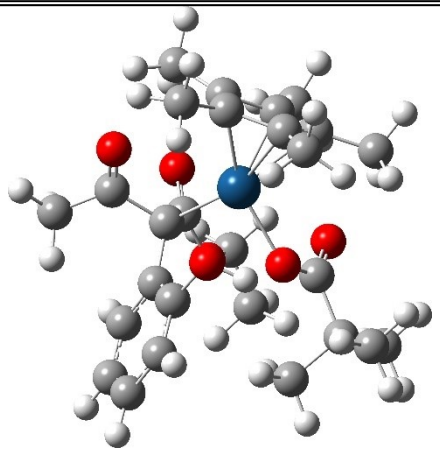
Frequencies

-940.1180	42.9497	54.9025
61.5067	67.7253	71.2197
79.0165	82.6333	94.2995
98.4875	109.8125	113.9507
122.9757	125.4379	133.9375
142.4343	154.8754	164.8022
166.0468	170.9383	172.9168
179.8627	185.2215	189.9136
194.7964	203.5184	209.8650
219.0251	224.3031	229.4321
234.6272	240.4852	247.6467
249.7776	266.8800	275.5560
284.3298	296.2057	299.5467
309.4248	317.1247	322.5545
324.7824	331.6132	347.3532
368.0387	372.8590	379.6292
387.0632	390.2692	400.4760
417.8816	436.6901	449.9856
454.6828	463.7801	485.8491
531.3961	533.8864	539.1313
547.4311	551.6192	565.6069
579.7021	589.1952	595.9019
601.6980	602.4073	607.8115
639.8740	649.3263	692.7356
752.0917	763.2877	771.7930
806.8865	809.4057	810.6278
817.1017	826.4691	846.6381
854.4341	865.1440	884.3692
919.4048	936.5759	940.7306
943.3517	951.3248	957.0878
958.4110	969.9515	983.8347
1007.0729	1026.8334	1029.8146
1034.7413	1036.0191	1042.4932
1042.8886	1051.4557	1053.6630
1057.8615	1062.8286	1093.6282
1096.1539	1103.6289	1111.3573
1124.7099	1139.5384	1150.5310
1178.8712	1182.5050	1190.4624
1202.5682	1209.9984	1218.8540
1227.4594	1241.8583	1258.7996
1283.1502	1284.4348	1301.8042
1306.2373	1338.4258	1353.7088
1373.4349	1376.7285	1378.3230
1379.9349	1386.2296	1390.1867
1394.6680	1400.2354	1407.2470
1415.2808	1417.4095	1434.2972

H	4.04505	0.07023	0.51526	1434.8738	1439.7968	1440.7296
H	4.93038	-0.23954	-0.99403	1444.0728	1444.2966	1450.0365
O	0.23657	0.27237	-2.02348	1455.4612	1457.4795	1458.4685
C	0.95576	1.99065	-0.53430	1460.6515	1462.2332	1463.4086
C	1.84449	3.03489	-0.27475	1467.6662	1468.3045	1471.3915
C	1.80363	1.89051	-2.80790	1476.0319	1477.7359	1480.5655
C	2.70598	3.50781	-1.25944	1488.2188	1491.8804	1503.9991
C	2.66823	2.94361	-2.53250	1505.1126	1507.4203	1514.4840
H	1.78044	1.41128	-3.78464	1520.3944	1521.2269	1556.9169
H	3.32838	3.31560	-3.31329	1635.0424	1655.9468	1770.7055
H	3.39527	4.31878	-1.03766	1813.0380	1834.2776	2113.9686
H	1.87031	3.47445	0.72255	3028.0064	3029.6990	3034.4370
C	-0.12062	1.55738	0.43875	3036.2868	3037.5713	3038.6265
C	-1.15780	2.68002	0.34417	3042.5029	3042.8856	3043.7139
C	0.27303	1.23496	1.83461	3053.6974	3059.2959	3099.5947
C	1.85894	0.29923	3.27976	3111.7624	3114.9610	3116.1401
H	1.20569	-0.55260	3.51186	3117.4622	3120.2054	3122.6336
H	1.64126	1.08770	4.01000	3126.3217	3127.8073	3129.9453
C	3.31064	-0.09475	3.28880	3135.2478	3136.4909	3140.4132
H	3.60956	-0.39407	4.29878	3141.8564	3142.6353	3146.5701
H	3.47879	-0.94351	2.61878	3147.9366	3162.9062	3164.7838
H	3.94575	0.74274	2.97823	3175.8615	3176.3093	3176.3654
O	1.53236	0.77992	1.96628	3177.0819	3190.5561	3200.0243
O	-0.48429	1.31025	2.79258			
O	-1.90294	2.76510	-0.61423			
C	-1.17113	3.75859	1.39955			
H	-1.74600	4.60898	1.02600			
H	-1.62061	3.37323	2.31977			
H	-0.15546	4.07526	1.66332			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.588112 Electronic Energy = -1606.26871473
Internal Energy (E)= -1605.64365573 Enthalpy (H)= -1605.64271173
Gibbs Free Energy (G)=-1605.74461673 Gibbs Free Energy of Solvation=-1607.0571249

St.Pt.	General Structure	Ball & Stick model
15I	 **15I**	

Cartesian co-ordinate

Atoms	X	Y	Z
C	-2.65207	-1.47061	-0.99494
C	-2.03372	-2.16394	0.07122
C	-2.04888	-1.29378	1.24378
C	-2.81694	-0.10595	0.90078
C	-3.11548	-0.17553	-0.49449
O	0.93274	-1.05707	-0.70560
C	1.68133	-1.78274	0.06844
O	1.41090	-2.11408	1.21836
C	2.99171	-2.19242	-0.62296
C	0.92969	1.56475	-1.92139
H	0.37224	-0.18674	-2.38223
C	-1.38481	-3.50089	0.01880
H	-0.46065	-3.50258	0.60567
H	-2.05535	-4.26693	0.42984
H	-1.13597	-3.78764	-1.00874
C	-1.55631	-1.67612	2.59449
H	-2.27291	-2.34323	3.09267
H	-0.58981	-2.18415	2.50593
H	-1.40310	-0.79250	3.22102
C	-3.85634	0.81738	-1.31746
H	-3.36170	0.96442	-2.28469
H	-4.88089	0.46988	-1.50709
H	-3.89340	1.79484	-0.83282
C	-2.81314	-1.92689	-2.40207
H	-2.13732	-2.75425	-2.63944
H	-3.83994	-2.27000	-2.58592
H	-2.61165	-1.11187	-3.10686
C	-3.24886	0.93796	1.86662
H	-4.13394	0.58570	2.41263
H	-2.45862	1.14395	2.59586
H	-3.51441	1.87245	1.36395
Ir	-0.95798	-0.24026	-0.23565
C	3.79041	-3.13230	0.27047
H	3.21035	-4.02896	0.51639
H	4.71231	-3.44140	-0.23935
H	4.06556	-2.65685	1.21782
C	2.66430	-2.90802	-1.93551
H	2.12398	-2.25061	-2.62581
H	3.58889	-3.23570	-2.42876
H	2.04689	-3.79880	-1.75624
C	3.79209	-0.92006	-0.91728
H	3.24831	-0.25788	-1.60292
H	3.98693	-0.34987	0.00056
H	4.75749	-1.17787	-1.37321
O	-0.09341	0.65759	-2.22664
C	1.10011	1.95333	-0.59517
C	2.17018	2.80941	-0.31861
C	1.76324	1.99560	-2.94168
C	3.02934	3.24284	-1.32260
C	2.82344	2.84339	-2.63874
H	1.57640	1.65797	-3.95875
H	3.48746	3.18474	-3.42894
H	3.86159	3.89712	-1.07463
H	2.34864	3.11485	0.71083

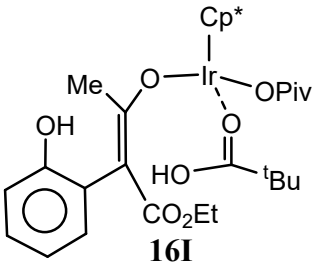
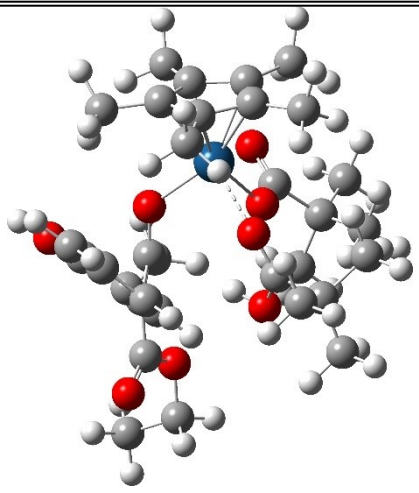
Frequencies

51.0064	59.6567	62.1920
72.6298	78.4958	82.0840
87.4745	103.4911	111.1661
114.5564	124.2630	127.6672
135.6812	143.1516	143.4823
152.5972	157.5905	160.0561
175.6944	177.6496	180.3376
188.8594	190.9945	201.7554
208.9238	215.6937	226.4455
231.0516	237.3253	242.1818
246.7222	252.5334	267.6923
270.8698	280.0774	287.7412
298.3196	306.5143	310.1006
312.1897	318.3356	319.9716
328.3633	347.4412	361.4702
374.4570	383.4507	390.6755
391.5825	402.3232	421.6454
428.2997	439.1639	447.8515
462.0591	464.2585	518.6352
521.8098	524.6776	534.5901
539.4614	548.4061	569.2334
573.3307	583.7322	590.6762
596.3579	602.4719	632.1490
643.5295	674.3929	690.0118
746.6401	764.3133	785.7190
804.7029	805.9244	808.8052
809.9662	816.8436	834.3560
846.2993	863.0413	888.1099
918.4149	919.7498	944.2330
944.7320	948.2771	956.9903
962.5732	976.9609	984.0929
999.5204	1028.4925	1031.8775
1037.2068	1038.5097	1041.6785
1044.3339	1045.1591	1049.5762
1053.6777	1066.0334	1091.4177
1099.8875	1102.4590	1113.9693
1124.6618	1142.4995	1156.5792
1171.0245	1184.9591	1186.8970
1197.1940	1216.3383	1239.5157
1245.2175	1253.8756	1263.2561
1278.7723	1303.3750	1304.4726
1318.8475	1360.9739	1365.3854
1371.2676	1374.4905	1377.9621
1379.3988	1387.9539	1393.6720
1394.7832	1398.6002	1401.1468
1420.2303	1428.8318	1431.7453
1432.0669	1435.3513	1443.3537
1444.0404	1446.0702	1448.7152
1452.6510	1456.7008	1458.8515
1464.7954	1465.1143	1467.9418
1469.9457	1474.7706	1475.0248
1476.8041	1478.8414	1482.0718
1487.9126	1488.7568	1495.3058
1501.1620	1510.5514	1525.4674
1525.8400	1531.0186	1560.5811
1641.3577	1669.0226	1765.7904
1779.9966	1807.9759	3019.7334
3026.1516	3034.9094	3035.6247

C	0.07218	1.54950	0.43791	3036.3237	3037.6659	3038.1835
C	-0.90987	2.72551	0.45681	3039.6506	3046.3445	3049.8882
C	0.57452	1.17942	1.78911	3055.9702	3100.9158	3110.5575
C	2.28017	0.22783	3.07663	3111.0991	3112.5295	3113.9915
H	1.68762	-0.66799	3.29908	3118.4727	3122.9314	3123.3347
H	2.07731	0.97297	3.85500	3127.4363	3128.7109	3131.7560
C	3.74611	-0.08476	2.96013	3136.1280	3139.3489	3141.9633
H	4.13814	-0.42660	3.92353	3144.0440	3147.6237	3154.9049
H	3.90987	-0.87867	2.22484	3157.3765	3159.1612	3171.0962
H	4.31396	0.79982	2.64988	3172.2689	3178.7013	3187.0504
O	1.84378	0.74665	1.81126	3194.5133	3205.0197	3685.0093
O	-0.10924	1.22653	2.80100			
O	-1.70936	2.88299	-0.44753			
C	-0.79379	3.76005	1.54750			
H	-1.39572	4.63000	1.27518			
H	-1.13058	3.34524	2.50181			
H	0.25159	4.05890	1.69343			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.593259 Electronic Energy = -1606.28447461
Internal Energy (E)= -1605.65431361 Enthalpy (H)= -1605.65336961
Gibbs Free Energy (G)=-1605.75435461 Gibbs Free Energy of Solvation=-1607.07078597

St.Pt.	General Structure	Ball & Stick model
16I	 **16I**	

Cartesian co-ordinate

Atoms	X	Y	Z
H	1.45307	1.09820	0.48692
C	-2.20153	-2.25000	-1.06311
C	-2.16893	-2.30390	0.36583
C	-2.96810	-1.19652	0.88458

Frequencies

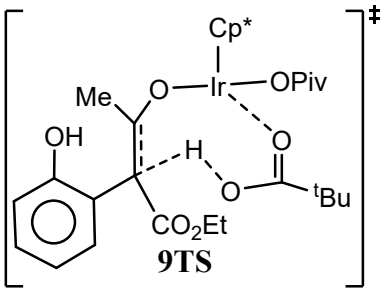
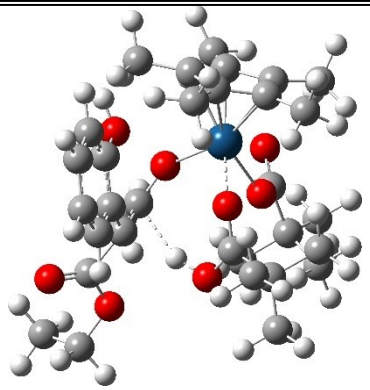
-40.1543	28.1043	36.7020
40.5955	46.0385	48.3227
56.0135	59.7896	66.5274
75.3934	76.6970	81.4357
87.0824	92.7880	101.6178
105.3970	115.6231	122.0308
125.3679	131.5342	135.2603
145.8340	155.1173	161.5640

C	-3.47293	-0.45089	-0.23008	168.6742	172.8418	187.4141
C	-2.95388	-1.06167	-1.44961	188.1787	194.4660	201.4497
C	-1.45944	2.51013	-0.79585	205.8446	215.1230	218.2187
O	-0.84737	1.59025	-0.11030	221.0042	228.3648	232.1473
O	-2.15888	2.31601	-1.78522	238.5497	245.2761	250.6200
C	-1.20771	3.92899	-0.25610	259.2457	265.4115	267.7365
O	0.03347	-0.30856	1.69016	275.6577	281.1198	288.3613
C	0.79030	0.53651	2.15865	295.0555	306.1292	306.8688
O	1.55632	1.32540	1.43763	311.5447	316.4775	319.8241
C	0.91562	0.73626	3.65984	323.1306	327.7759	331.8451
C	-4.36207	0.73846	-0.16521	333.9570	344.6259	351.9154
H	-5.41409	0.42840	-0.21477	364.1572	367.9703	371.8284
H	-4.21896	1.28831	0.77206	375.7129	380.1464	392.4582
H	-4.15094	1.42471	-0.98957	394.7668	399.7522	425.8707
C	-3.21509	-0.60399	-2.83854	432.0778	446.1928	447.4982
H	-4.20821	-0.92314	-3.18135	458.7816	472.9966	482.0504
H	-3.14392	0.48797	-2.88286	499.1321	523.2475	535.1850
H	-2.46405	-1.01474	-3.52115	537.8962	542.4748	548.5490
C	-3.23767	-0.91674	2.31987	560.4818	563.9005	568.2192
H	-2.43331	-1.30263	2.95477	586.8845	594.3451	596.8603
H	-3.31872	0.16070	2.50433	602.9881	606.3800	626.4950
H	-4.17567	-1.38755	2.64201	654.8461	661.5694	721.4654
C	-1.39829	-3.26938	1.19465	744.5156	757.4563	763.9327
H	-1.00160	-2.78039	2.09086	781.5953	783.8606	791.7523
H	-2.02425	-4.11486	1.50743	806.2842	810.0986	814.4389
H	-0.53240	-3.65478	0.64454	818.3242	822.5024	847.9594
C	-1.47867	-3.13908	-2.01200	849.0250	885.6127	899.4809
H	-0.93621	-3.92688	-1.47833	913.6885	939.3510	942.6990
H	-2.18123	-3.61237	-2.70855	943.4006	944.5485	946.9823
H	-0.74161	-2.55996	-2.58391	954.4252	956.8614	959.2881
C	-0.46078	1.17718	4.16542	962.1620	975.7592	1016.2492
H	-0.42280	1.33526	5.25003	1034.7555	1036.1975	1039.1233
H	-0.77700	2.11625	3.69329	1039.8282	1041.3197	1042.5206
H	-1.21579	0.41424	3.94945	1044.3422	1045.5911	1045.8829
C	1.96648	1.78242	4.01290	1052.7318	1056.9599	1057.2005
H	2.02712	1.88409	5.10331	1088.5849	1093.7721	1099.5816
H	2.95633	1.49793	3.63856	1102.1363	1108.7761	1119.9488
H	1.71750	2.76148	3.58886	1137.8541	1164.8555	1182.2501
C	1.28568	-0.61245	4.28322	1184.8349	1186.8544	1190.8820
H	0.56099	-1.38756	4.01005	1231.8930	1239.1690	1240.7736
H	2.27864	-0.94567	3.95519	1241.7907	1245.3756	1261.7251
H	1.30535	-0.51891	5.37585	1268.1029	1299.2849	1313.5764
C	-2.28259	4.86928	-0.78729	1316.6716	1325.6493	1344.4766
H	-3.27869	4.55908	-0.44598	1358.4678	1370.0986	1373.1318
H	-2.10091	5.89192	-0.43145	1374.6326	1375.8893	1378.2937
H	-2.29637	4.87157	-1.88130	1379.2889	1380.9276	1386.1656
C	0.16933	4.38793	-0.74295	1387.3545	1391.3571	1398.6346
H	0.37276	5.40762	-0.38928	1402.9881	1406.4666	1412.1672
H	0.96618	3.73347	-0.36438	1412.4993	1420.0107	1427.9949
H	0.21495	4.39651	-1.83977	1436.2172	1439.8216	1443.7321
C	-1.22559	3.92376	1.27186	1445.1767	1446.5956	1450.3023
H	-1.11356	4.94672	1.65533	1452.8897	1453.3453	1456.0788
H	-2.17183	3.51949	1.65951	1456.9767	1461.1059	1462.5502
H	-0.40724	3.31196	1.66731	1463.9047	1466.8417	1467.7124
Ir	-1.32163	-0.44261	-0.29286	1470.2607	1470.7341	1471.0855
C	2.46792	-0.37275	-0.97441	1473.0947	1474.2485	1477.8179
C	2.42081	-1.71457	-0.34169	1478.3499	1479.9289	1481.7711
C	2.11727	-2.87665	-1.07543	1482.8324	1483.7798	1490.9207
C	2.70034	-1.87928	1.01639	1495.3270	1498.0210	1503.7169
C	2.03235	-4.11876	-0.44195	1510.3813	1518.7159	1534.9924
C	2.63156	-3.11263	1.65538	1547.2226	1586.3792	1652.0632

H	2.98708	-0.99514	1.58716	1666.8042	1766.8932	1774.5376
C	2.28652	-4.23963	0.92003	1820.2416	3018.7362	3023.4551
H	1.79040	-5.00158	-1.03724	3030.4565	3031.6773	3032.2752
H	2.85360	-3.19106	2.71744	3034.8125	3037.0156	3038.7990
H	2.22558	-5.21626	1.39556	3038.9038	3040.5098	3042.7803
O	1.93354	-2.77177	-2.41641	3044.0480	3062.6826	3063.1380
H	1.83709	-3.65686	-2.78323	3098.1673	3108.5460	3112.1413
C	1.36426	0.08584	-1.67118	3114.0174	3115.7873	3118.8540
C	3.72857	0.35760	-0.82828	3119.0563	3119.3667	3120.5618
C	4.79282	2.46490	-0.98907	3121.8048	3125.3822	3126.2238
H	5.40084	2.11421	-0.14766	3128.7283	3132.1002	3137.1882
H	4.45963	3.48829	-0.78567	3137.8966	3138.6344	3141.4105
C	5.56215	2.37908	-2.28660	3142.2036	3144.7888	3145.6267
H	6.44120	3.03230	-2.25946	3147.3106	3149.1491	3150.0537
H	5.90297	1.35317	-2.45696	3150.6601	3153.6027	3164.5695
H	4.93279	2.68490	-3.13014	3172.4472	3174.4454	3178.6594
O	3.59119	1.69493	-1.05322	3195.3789	3625.6224	3891.0190
O	4.78524	-0.12877	-0.47679			
C	1.32057	1.29574	-2.56052			
H	0.53089	1.12963	-3.29992			
H	1.04794	2.18779	-1.98564			
H	2.27399	1.50094	-3.05189			
O	0.25675	-0.60333	-1.64109			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.741454 Electronic Energy = -1953.09789867
Internal Energy (E)= -1952.31035467 Enthalpy (H)= -1952.30941067
Gibbs Free Energy (G)=-1952.43163267 Gibbs Free Energy of Solvation=-1954.04494597

St.Pt.	General Structure	Ball & Stick model
9TS		

Cartesian co-ordinate

Atoms	X	Y	Z
H	1.76232	0.84299	0.71363

Frequencies

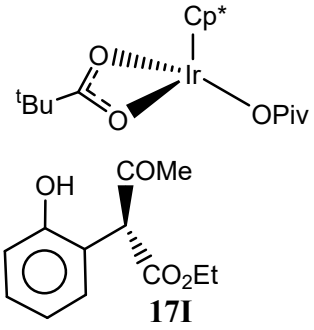
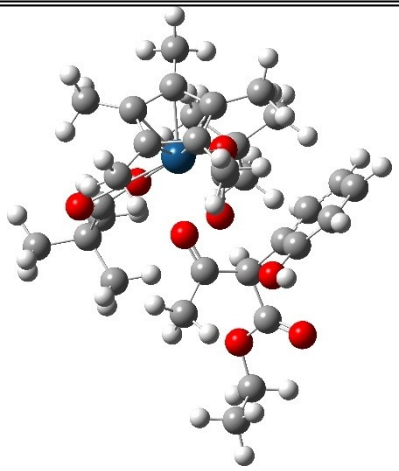
-617.7519	-248.0173	-175.9045
-122.5779	-29.8614	23.4089
39.0279	40.2060	44.9717
50.9106	58.0494	62.6430
69.3452	77.4160	78.4495

C	-1.84458	-2.22942	-1.33963	85.6081	90.6078	95.9589
C	-2.08644	-2.40341	0.05583	96.8050	107.0781	113.9828
C	-3.04931	-1.39161	0.47624	117.3946	128.3879	135.6603
C	-3.41025	-0.61380	-0.68067	138.2592	142.8935	147.3211
C	-2.62261	-1.08754	-1.80291	162.6914	165.5601	178.6325
C	-1.46175	2.49410	-0.90458	184.7129	189.5837	197.0115
O	-1.15713	1.64951	0.03433	202.8163	205.2815	222.3130
O	-2.01021	2.22019	-1.96830	233.6399	235.6240	237.4041
C	-0.99329	3.92637	-0.59507	240.4807	242.7146	249.8008
O	-0.26510	-0.25738	1.66768	266.1489	273.0167	278.5486
C	0.41268	0.62783	2.22130	281.0395	285.5277	288.2125
O	1.43387	1.22388	1.71942	293.3929	297.0475	303.2800
C	0.06343	1.00219	3.65636	308.4830	317.9397	321.1633
C	-4.37342	0.51699	-0.70758	324.9655	328.8857	329.1542
H	-5.36362	0.16227	-1.02117	341.0133	344.8263	347.7154
H	-4.47185	0.97044	0.28441	366.5151	379.7867	385.5997
H	-4.02698	1.29323	-1.39560	395.3516	397.4505	409.0981
C	-2.64088	-0.59627	-3.20773	436.1647	441.7142	453.5032
H	-2.91641	-1.40539	-3.89661	455.1695	461.7436	471.8099
H	-3.33594	0.23608	-3.33014	479.0973	500.7623	537.2445
H	-1.65079	-0.21760	-3.48492	539.2474	543.3690	545.4273
C	-3.59151	-1.26276	1.85413	553.8754	566.2319	569.0932
H	-2.79860	-1.43880	2.59030	577.2750	585.9840	595.5774
H	-3.99545	-0.26096	2.03247	601.6017	604.1691	617.7689
H	-4.39134	-1.99265	2.03535	637.0945	677.2629	722.7370
C	-1.44121	-3.37451	0.98177	754.5301	762.9402	770.3899
H	-0.94462	-2.84298	1.80400	786.2052	792.9288	796.0459
H	-2.18414	-4.05862	1.41097	802.7673	814.1288	817.2314
H	-0.67216	-3.96754	0.47707	824.0751	834.8211	840.8602
C	-0.93461	-3.02628	-2.20071	882.8348	905.3121	914.2630
H	-0.23430	-3.61526	-1.59997	924.4718	931.9370	934.3407
H	-1.51726	-3.71058	-2.83146	943.6969	948.5213	951.2745
H	-0.34178	-2.36936	-2.84536	952.7133	953.8108	956.2984
C	-1.43316	1.32264	3.70592	959.1490	961.7736	964.2462
H	-1.69184	1.73170	4.69046	1014.6029	1032.5538	1034.5857
H	-1.70348	2.06334	2.94117	1037.1752	1040.1488	1040.9200
H	-2.03672	0.42572	3.53365	1041.1483	1043.6461	1044.6880
C	0.86665	2.20145	4.14507	1049.6933	1051.4136	1055.6930
H	0.61818	2.40434	5.19442	1069.1789	1091.6196	1092.6415
H	1.94397	2.02324	4.07097	1100.0544	1106.7594	1117.8165
H	0.63435	3.09997	3.56053	1135.0084	1156.4640	1176.9957
C	0.36966	-0.22292	4.52548	1187.4671	1188.1184	1188.8876
H	-0.14708	-1.11488	4.14910	1223.9253	1237.7335	1240.3606
H	1.44733	-0.43217	4.55057	1248.0360	1250.4263	1264.2733
H	0.04189	-0.03788	5.55623	1270.3495	1281.3246	1296.7931
C	-1.83620	4.92351	-1.38058	1318.0392	1319.8010	1355.9425
H	-2.88447	4.89687	-1.05728	1363.9232	1369.0866	1372.7087
H	-1.45850	5.94321	-1.22777	1373.9400	1375.1002	1375.5883
H	-1.81417	4.69227	-2.44968	1377.4100	1382.5537	1384.9994
C	0.46422	4.00001	-1.06201	1387.9030	1391.7054	1394.6310
H	0.88181	4.99427	-0.85382	1397.4169	1406.6176	1412.7424
H	1.08005	3.25365	-0.54158	1413.4179	1415.1101	1425.5057
H	0.53460	3.81763	-2.14173	1425.6528	1430.8439	1435.2674
C	-1.06089	4.23853	0.89724	1436.1565	1438.9027	1442.0913
H	-0.74298	5.27451	1.07702	1443.0747	1443.3788	1448.7185
H	-2.08350	4.12965	1.28258	1449.4281	1451.0648	1458.2857
H	-0.40530	3.57220	1.47094	1460.3059	1460.8595	1463.2121
Ir	-1.30707	-0.41348	-0.28729	1466.7274	1467.0011	1469.4006
C	2.41130	-0.21566	-0.36540	1470.1618	1472.4316	1474.6046
C	2.21208	-1.61459	0.11988	1476.0442	1479.0437	1485.6891
C	2.18936	-2.66325	-0.81045	1487.5744	1488.3533	1488.8476

C	2.22937	-1.95472	1.47056	1490.7788	1497.2316	1500.8033
C	2.13616	-3.99341	-0.39439	1509.5223	1514.5251	1539.2044
C	2.16559	-3.27623	1.90258	1540.3834	1548.3355	1633.9091
H	2.32274	-1.15604	2.20320	1653.3576	1673.7777	1752.4224
C	2.11837	-4.29976	0.96390	1764.5354	1833.7079	3022.3341
H	2.12889	-4.79016	-1.14033	3023.3281	3024.0403	3030.6497
H	2.17692	-3.50096	2.96666	3031.4958	3032.7272	3036.1150
H	2.08377	-5.33999	1.28025	3037.8100	3038.9582	3040.9693
O	2.22643	-2.32665	-2.12593	3041.4312	3044.6052	3045.9583
H	2.38696	-3.12015	-2.64758	3066.1011	3101.2544	3106.7780
C	1.60125	0.28959	-1.41026	3108.4348	3111.5888	3112.9262
C	3.85012	0.15099	-0.35273	3115.0509	3120.8088	3121.0137
C	5.38011	1.95840	-0.30808	3122.0031	3122.4827	3123.7778
H	5.99188	1.31462	0.33383	3123.9679	3124.7544	3130.0390
H	5.33980	2.96142	0.12851	3135.8015	3136.0863	3137.8733
C	5.92162	1.99205	-1.71885	3141.4864	3146.7526	3146.9372
H	6.95414	2.35793	-1.72268	3148.5436	3148.6465	3150.4040
H	5.91788	0.98772	-2.15444	3152.4339	3154.8271	3155.4058
H	5.32317	2.65517	-2.35390	3169.7020	3176.2867	3181.0792
O	4.02598	1.49673	-0.27452	3187.5629	3197.7247	3892.7106
O	4.78329	-0.62410	-0.34504			
C	2.16680	1.19711	-2.47028			
H	1.36366	1.48131	-3.15440			
H	2.61395	2.09272	-2.03303			
H	2.95743	0.66748	-3.01897			
O	0.37287	0.01412	-1.57020			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.733170 Electronic Energy = -1953.08664842
Internal Energy (E)= -1952.30895742 Enthalpy (H)= -1952.30801342
Gibbs Free Energy (G)=-1952.42757442 Gibbs Free Energy of Solvation=-1954.03459952

St.Pt.	General Structure	Ball & Stick model
17I	 **17I**	

Cartesian co-ordinate

Atoms	X	Y	Z
H	2.07504	0.41640	0.86031
C	-1.53335	-2.08880	-1.64019
C	-2.20188	-2.31338	-0.39885
C	-3.23239	-1.28909	-0.26546
C	-3.22364	-0.48696	-1.48225
C	-2.15050	-0.95038	-2.31263
C	-1.22286	2.60335	-0.93997
O	-1.30885	1.71329	0.00151
O	-1.50599	2.44121	-2.12481
C	-0.60715	3.92324	-0.44987
O	-0.91856	-0.38448	1.66638
C	-0.26430	0.48943	2.36342
O	0.72705	1.12439	2.00451
C	-0.84223	0.67758	3.77393
C	-4.14261	0.64058	-1.78351
H	-5.01088	0.27752	-2.34881
H	-4.50900	1.10797	-0.86353
H	-3.62699	1.41095	-2.36208
C	-1.74759	-0.38971	-3.62954
H	-2.35258	-0.80908	-4.44394
H	-1.84789	0.70004	-3.61532
H	-0.69523	-0.61177	-3.83472
C	-4.18957	-1.18478	0.86653
H	-3.69792	-1.44835	1.80880
H	-4.57713	-0.16640	0.96943
H	-5.04121	-1.86302	0.72427
C	-1.86353	-3.30733	0.65490
H	-1.78558	-2.80601	1.62821
H	-2.62885	-4.09074	0.72438
H	-0.89363	-3.77955	0.46472
C	-0.38868	-2.86307	-2.18608
H	0.07839	-3.48571	-1.41612
H	-0.73103	-3.51471	-3.00073
H	0.38406	-2.19790	-2.58754
C	-2.20220	1.36094	3.60802
H	-2.66770	1.53104	4.58836
H	-2.09202	2.33112	3.10540

Frequencies

28.4347	37.5472	39.1076
47.9320	54.8625	55.7971
63.4266	71.5368	75.3238
78.0821	81.3327	86.1164
95.4740	103.1878	107.9345
113.9770	119.6698	125.8339
132.7015	138.5743	147.5641
151.1382	154.0405	164.5686
169.1156	175.9691	180.5202
187.1747	190.0747	198.2058
201.8261	208.4594	210.8064
218.0193	223.9541	228.5300
230.2701	235.4447	236.1597
245.8013	261.7547	270.6436
273.6148	278.7090	284.3103
297.4155	302.5308	307.3434
308.9108	324.2806	328.5667
332.3135	333.8919	340.4060
344.3107	352.3414	354.5770
359.6783	365.8330	378.4485
388.8669	396.0392	403.7935
412.6488	422.0298	433.0999
436.4173	442.0383	445.7616
455.2709	464.9870	477.1775
495.3190	521.9804	539.0210
541.3143	545.1240	548.2787
560.7543	574.2488	579.1533
582.8656	594.8493	596.3908
608.2763	614.9599	643.9770
655.9289	681.2247	735.6478
759.1174	768.2594	792.5696
795.4376	797.6745	808.6101
814.5800	815.7644	820.6733
823.9902	842.0159	860.2754
880.8375	914.3641	915.9352
919.2316	941.2618	945.1684
945.9124	951.4803	954.4722
956.1747	964.3871	977.8796
980.9893	984.5770	999.3127
1018.5655	1032.2141	1034.4059
1037.2032	1043.7303	1045.2877

H	-2.87580	0.74536	2.99983	1046.4460	1050.1216	1053.1489
C	0.07993	1.54985	4.61454	1059.4083	1060.1837	1073.4344
H	-0.34353	1.68834	5.61845	1083.5470	1097.9394	1103.7766
H	1.07097	1.09161	4.71782	1112.1093	1116.8313	1123.8143
H	0.22176	2.53461	4.15690	1161.9271	1184.5720	1185.4307
C	-1.01740	-0.68502	4.44419	1186.5149	1190.4254	1208.0723
H	-1.68162	-1.33145	3.86087	1234.9134	1241.5593	1245.2605
H	-0.05130	-1.19911	4.55178	1250.3468	1253.9516	1257.6472
H	-1.44164	-0.56335	5.45000	1266.7282	1277.0022	1290.2451
C	-1.08712	5.07566	-1.32329	1316.7565	1318.7279	1332.5578
H	-2.16568	5.23942	-1.20361	1365.0747	1366.7775	1371.7639
H	-0.57100	6.00394	-1.04417	1374.9855	1377.7940	1379.5222
H	-0.89766	4.86650	-2.38063	1380.3686	1381.5515	1382.5007
C	0.90829	3.74111	-0.61545	1383.8726	1390.7438	1391.5865
H	1.43552	4.64640	-0.28534	1394.9968	1406.5979	1408.8657
H	1.26398	2.89708	-0.00699	1411.8294	1417.4522	1422.0559
H	1.15933	3.56323	-1.67030	1426.7040	1435.3420	1437.5276
C	-0.91918	4.19669	1.01849	1443.3767	1448.4364	1453.4370
H	-0.47810	5.15707	1.31903	1454.8811	1455.7335	1456.9694
H	-2.00228	4.25586	1.19008	1460.3716	1460.8227	1462.6156
H	-0.50933	3.40688	1.65816	1464.0764	1466.3851	1468.1352
Ir	-1.38295	-0.31654	-0.38939	1469.8319	1471.8190	1472.5951
C	2.59304	-0.19206	0.08945	1476.0501	1476.6597	1479.8752
C	2.30971	-1.64246	0.38841	1482.5453	1484.3698	1488.3478
C	2.59089	-2.63656	-0.55374	1489.6166	1491.1673	1493.4300
C	1.83565	-2.02980	1.63788	1498.4986	1504.9552	1507.7443
C	2.40568	-3.98196	-0.24762	1522.4107	1539.1590	1542.6359
C	1.63462	-3.37036	1.95353	1547.0855	1661.9183	1675.6240
H	1.63189	-1.25211	2.37110	1740.8575	1758.1927	1779.9607
C	1.92732	-4.34670	1.00800	1871.0926	2930.6384	3018.7048
H	2.63490	-4.74125	-0.99608	3018.8415	3020.5509	3022.1720
H	1.25778	-3.64697	2.93516	3029.4251	3029.9781	3034.1368
H	1.78597	-5.39963	1.24172	3037.5285	3038.8457	3039.8281
O	3.00994	-2.22475	-1.78356	3044.7777	3047.8185	3054.2661
H	3.27749	-2.98889	-2.30502	3074.2449	3094.9099	3100.1043
C	1.92901	0.28486	-1.18846	3104.9936	3105.9622	3108.7710
C	4.07273	0.12184	0.17171	3113.1922	3115.2982	3118.7063
C	5.61492	1.90840	0.27346	3118.7323	3119.7534	3123.1965
H	6.18092	1.24394	0.93493	3125.2965	3126.5867	3129.4877
H	5.55621	2.90155	0.72814	3134.6526	3137.4969	3140.3728
C	6.22481	1.95598	-1.10672	3140.7726	3143.6649	3144.4343
H	7.24165	2.35965	-1.06081	3150.9708	3151.4986	3151.9798
H	6.27661	0.94984	-1.53533	3152.5959	3154.7754	3155.7377
H	5.63468	2.59525	-1.77285	3174.6518	3186.4667	3197.4629
O	4.25359	1.45487	0.21516	3198.7340	3204.7370	3893.3551
O	4.97130	-0.68215	0.22053			
C	2.73277	0.90639	-2.28453			
H	2.09991	1.04036	-3.16461			
H	3.09525	1.88334	-1.94309			
H	3.60697	0.28870	-2.51941			
O	0.71580	0.19143	-1.32641			

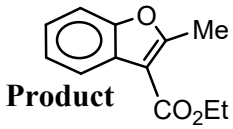
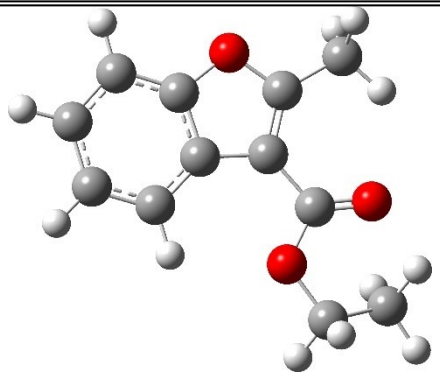
Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm

Zero-point correction= 0.742064 Electronic Energy = -1953.10814983

Internal Energy (E)= -1952.31953483 Enthalpy (H)= -1952.31859083

Gibbs Free Energy (G)=-1952.44165983 Gibbs Free Energy of Solvation=-1954.05312655

St.Pt.	General Structure	Ball & Stick model
Product		

Cartesian co-ordinate

Atoms	X	Y	Z
C	2.10643	0.37921	0.08129
C	0.93272	-0.36659	-0.06256
C	0.46820	1.83820	0.02779
O	1.81563	1.71665	0.13505
C	1.03030	-1.75865	-0.13423
C	3.37389	-0.16938	0.15835
C	2.29130	-2.33337	-0.05884
C	3.44725	-1.55473	0.08456
H	0.13763	-2.36611	-0.24384
H	2.38659	-3.41518	-0.11273
H	4.41773	-2.04126	0.14032
H	4.25347	0.45749	0.26936
C	-0.13130	0.61366	-0.09664
C	-0.05429	3.21647	0.06713
H	0.37389	3.80957	-0.74926
H	-1.14096	3.20148	-0.02276
H	0.23090	3.70452	1.00638

Frequencies

47.7688	52.4134	106.2873
109.2754	129.9871	138.8663
143.8660	220.9719	265.4054
294.2677	311.0205	320.2579
356.5589	396.6532	436.1340
457.9290	501.9082	563.3281
579.2271	631.5223	643.2338
683.0624	745.5742	755.2135
765.8702	782.2616	840.7527
859.0727	868.1286	890.2422
931.4847	961.1485	973.6318
1017.7103	1034.2849	1044.4527
1044.9631	1114.4990	1122.0783
1139.7394	1161.3197	1190.6088
1213.0581	1282.3671	1304.4829
1314.6763	1327.7350	1371.4562
1384.0579	1404.2910	1408.3529
1433.7755	1451.0067	1460.1327
1467.5501	1470.2999	1485.9518
1490.6654	1521.2913	1650.4213
1662.2154	1686.0681	1837.0828

C	-1.57184	0.40603	-0.23107	3044.5773	3051.2367	3071.0762
C	-3.25585	-1.23448	-0.45646	3117.7031	3128.5391	3141.6814
H	-3.26821	-2.21246	-0.94701	3157.2612	3179.5073	3181.0693
H	-3.74136	-0.50289	-1.11072	3193.4061	3212.2378	3217.0639
C	-3.91675	-1.28175	0.89962			
H	-4.95486	-1.61699	0.80506			
H	-3.39058	-1.97633	1.56245			
H	-3.91798	-0.28896	1.35871			
O	-2.41570	1.27890	-0.24892			
O	-1.86327	-0.90562	-0.33985			

Statistical Thermodynamic Analysis

Temperature=298 K Pressure=1 atm
Zero-point correction= 0.216324 Electronic Energy = -689.764148196
Internal Energy (E)= -689.534384196 Enthalpy (H)= -689.533440196
Gibbs Free Energy (G)=-689.588413196 Gibbs Free Energy of Solvation=-690.127187579