Supporting Information

Theoretical study on the mechanism of rearrangement reactions of bicyclic derivatives of cyclopropane to monocyclic derivatives under the catalysis of Pt-salt.

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Contents

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

Basis set used:

LANL2TZf for platinum atom and 6-31G(d,p) basis set for other atoms.

Solvent used for calculation by PCM model:

DiethylEther, Dichloromethane (DCM)

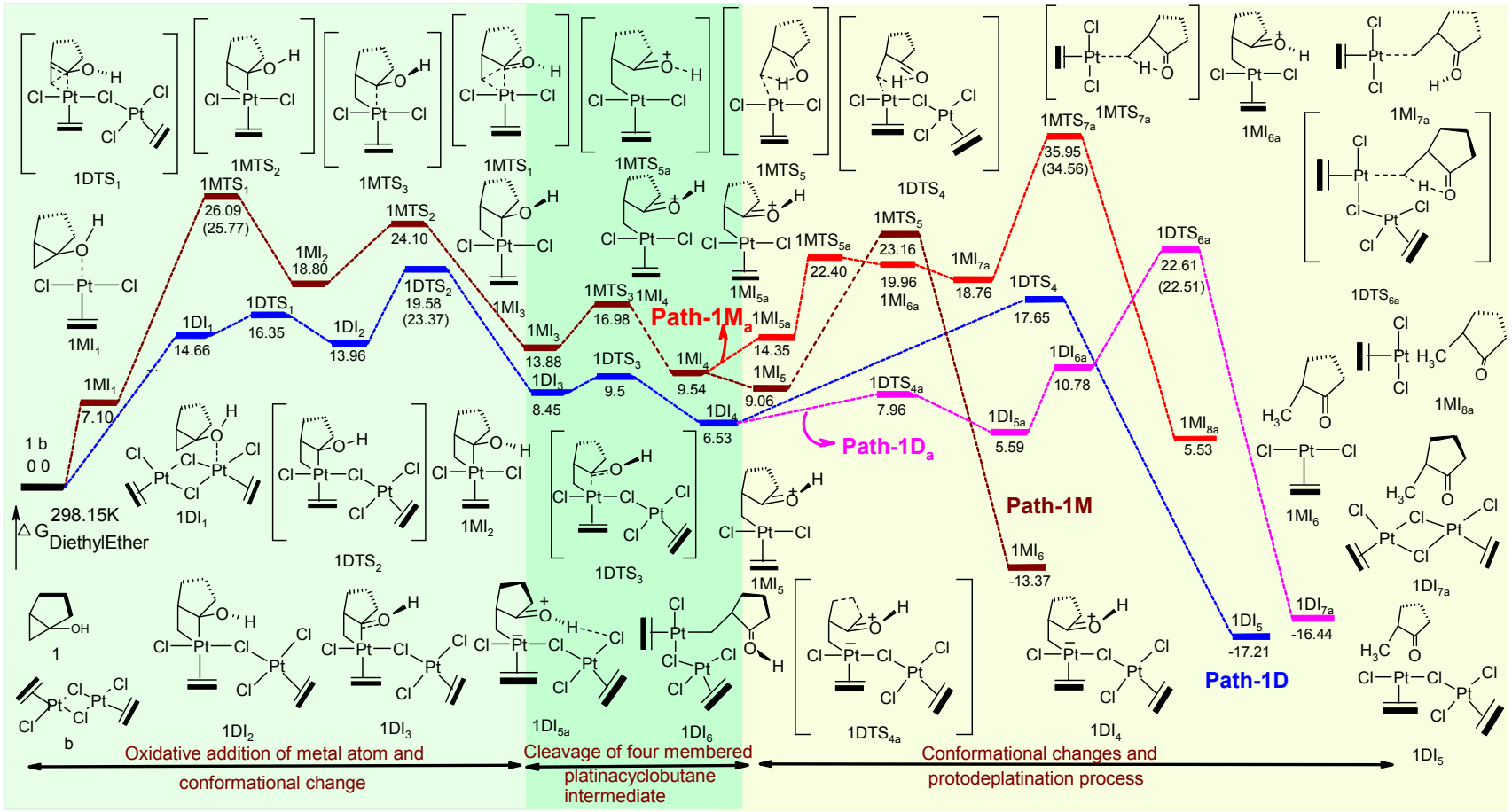
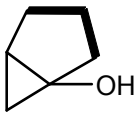
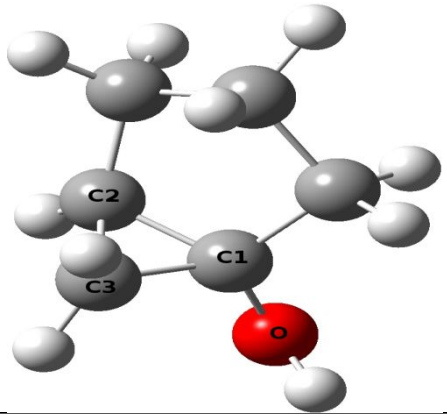


Figure S1. PES along with the thermodynamic parameters and structures of the stationary points of pathway-1M (brown colour), pathway-1M$_a$ (red colour), pathway-1D (blue colour) and pathway-1D$_a$ (magenta colour) under the catalytic condition of monomeric and dimeric form of Pt-salt. Energy values not enclosed in bracket are calculated using M06-2X functional. Values indicated in the round bracket are calculated using M06

functional.

St.Pt.	General Structure	Ball & Stick model
1		

Cartesian co-ordinate

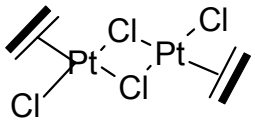
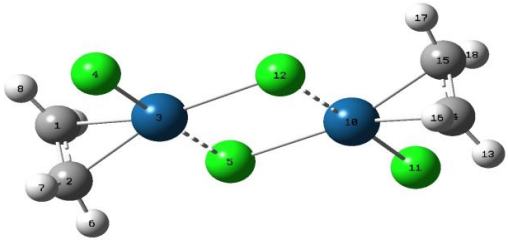
Atoms	X	Y	Z
C	-0.03028	-1.05068	-0.41217
O	2.00227	0.38667	-0.52845
C	0.74672	0.15044	0.02888
C	0.57091	-1.00145	0.97587
H	-0.07826	-0.90477	1.84133
H	1.45155	-1.61605	1.12589
H	2.55325	0.78977	0.15229
C	-0.21550	1.31928	0.14884
H	0.00395	1.98045	0.99447
C	-1.60371	0.66350	0.25353
H	-1.83307	0.43898	1.29968
H	-2.40237	1.31192	-0.11380
C	-1.48666	-0.64650	-0.55506
H	-2.18673	-1.41105	-0.20396
H	-1.70299	-0.45950	-1.61272
H	-0.12787	1.90700	-0.77205
H	0.41549	-1.73776	-1.12287

Frequencies

218.7186	249.7708	346.9290
369.7460	389.5136	457.7402
550.7976	618.5293	712.7037
826.0150	847.4259	898.7741
916.2375	921.1445	967.1094
987.7957	1012.3285	1039.2903
1065.7574	1099.6435	1125.4589
1174.1473	1211.8734	1253.4906
1274.9256	1290.3576	1330.2710
1349.9471	1361.9481	1370.9121
1425.9593	1501.3010	1506.3580
1516.1429	1536.0356	3069.6620
3076.7137	3096.2241	3117.9686
3122.9285	3145.5093	3150.0545
3221.3029	3241.3378	3880.0908

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.152288 Electronic Energy = -309.718741856
Internal Energy (E)= -309.560224856 Enthalpy (H)= -309.559280856
Gibbs Free Energy (G)=-309.595983856 Gibbs Free Energy of Solvation=-309.599133984

St.Pt.	General Structure	Ball & Stick model
b		

Cartesian co-ordinate

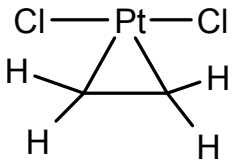
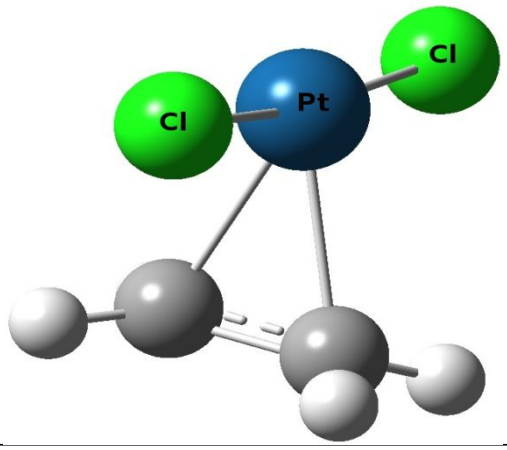
Atoms	X	Y	Z
C	-3.17738	-1.54894	-0.67531
C	-3.15374	-1.54304	0.72645
Pt	-1.80036	-0.07912	-0.00347
Cl	-3.49559	1.48916	0.02492
Cl	0.04341	-1.67277	-0.03359
H	-2.57032	-2.27967	1.27091
H	-3.92403	-1.01455	1.27868
H	-3.96599	-1.02532	-1.20589
H	-2.61278	-2.29059	-1.23260
Pt	1.80031	0.07911	-0.00347
Cl	3.49562	-1.48913	0.02495
Cl	-0.04342	1.67289	-0.03354
H	3.92408	1.01430	1.27865
C	3.15389	1.54294	0.72641
C	3.17757	1.54877	-0.67535
H	2.57058	2.27970	1.27081
H	2.61303	2.29044	-1.23268
H	3.96610	1.02499	-1.20588

Frequencies

2.9387	50.0966	80.5572
87.9864	89.3817	109.7068
124.2386	128.6058	177.8734
178.2620	192.6239	195.6003
237.5322	257.6038	276.6461
281.8348	354.5421	356.1301
404.2840	405.5701	507.5857
507.6732	773.6047	773.9266
847.8907	847.9440	1024.5210
1024.7903	1076.4852	1076.6357
1080.1263	1080.2373	1229.9457
1230.0007	1288.7163	1289.5402
1479.3815	1479.4633	1580.3803
1581.5728	3178.0579	3178.0976
3183.1235	3183.1740	3278.3804
3278.3886	3293.8032	3293.8111

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.117643 Electronic Energy = -2235.96844340
Internal Energy (E)= -2235.8353104 Enthalpy (H)= -2235.8343664
Gibbs Free Energy (G)=-2235.8994584 Gibbs Free Energy of Solvation=-2235.9576833

St.Pt.	General Structure	Ball & Stick model
c		

Cartesian co-ordinate

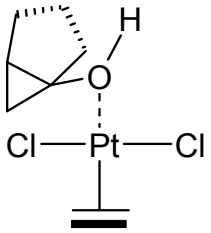
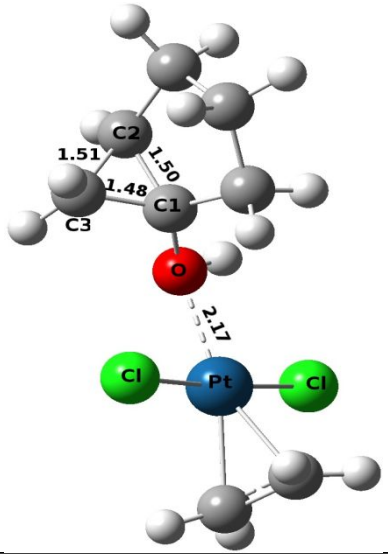
Atoms	X	Y	Z
Pt	-0.00010	-0.20997	-0.00001
Cl	2.31760	-0.35512	0.00004
Cl	-2.31780	-0.35459	0.00001
H	0.92902	1.90430	1.25018
C	0.00057	1.73535	0.71254
C	0.00077	1.73536	-0.71253
H	-0.92785	1.90503	1.24999
H	-0.92750	1.90508	-1.25024
H	0.92937	1.90432	-1.24990
Pt	1.80031	0.07911	-0.00347
Cl	3.49562	-1.48913	0.02495
Cl	-0.04342	1.67289	-0.03354
H	3.92408	1.01430	1.27865
C	3.15389	1.54294	0.72641
C	3.17757	1.54877	-0.67535
H	2.57058	2.27970	1.27081
H	2.61303	2.29044	-1.23268
H	3.96610	1.02499	-1.20588

Frequencies

115.0144	119.7496	137.1477
141.5947	338.9983	353.7419
458.4094	524.4425	811.5035
831.1351	978.9657	1095.1484
1101.7933	1223.8808	1232.6997
1464.1366	1545.3096	3171.1591
3171.6501	3269.9209	3283.7780

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.057798 Electronic Energy = -1117.94345067
Internal Energy (E)= -1117.87862367 Enthalpy (H)= -1117.87767967
Gibbs Free Energy (G)=-1117.91936467 Gibbs Free Energy of Solvation=-1117.96719306

St.Pt.	General Structure	Ball & Stick model
$1MI_1$		

Cartesian co-ordinate

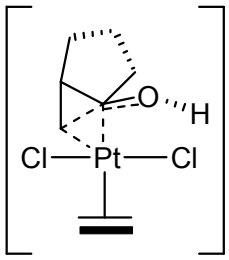
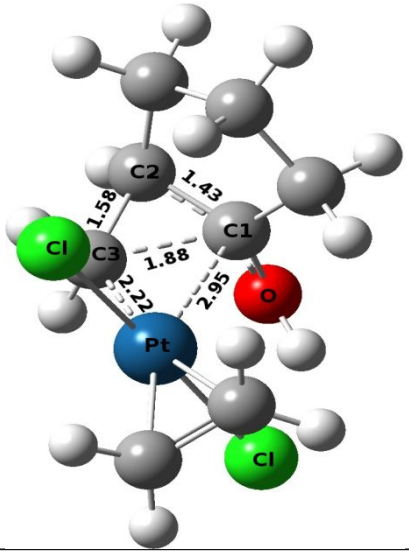
Atoms	X	Y	Z
C	2.57498	-0.54376	1.21860
C	3.00161	-0.65068	-0.11225
Pt	0.99056	-0.01140	-0.07147
Cl	1.57578	2.27367	-0.00114
Cl	0.26419	-2.24293	-0.13946
H	3.01949	-1.62023	-0.59971
H	3.57917	0.14949	-0.56467
H	2.82176	0.33875	1.80011
H	2.26235	-1.43068	1.76051
C	-3.45087	0.49528	-0.93147
O	-0.93170	0.75119	-0.74750
C	-2.14053	0.18566	-0.26675
C	-2.76746	-0.83964	-1.13556
H	-3.16191	-1.74273	-0.68123
H	-2.28418	-0.98417	-2.09497
H	-0.89346	1.70679	-0.56920
C	-2.33305	0.11149	1.23013
H	-1.73176	-0.68185	1.68553
C	-3.84963	-0.10689	1.38511
H	-4.07043	-1.17749	1.35909
H	-4.22989	0.27405	2.33476
C	-4.49416	0.59628	0.16889
H	-5.45254	0.14605	-0.10544
H	-4.67721	1.65316	0.39216
H	-2.02820	1.07099	1.66937
H	-3.48827	1.16858	-1.78134

Frequencies

33.1705	54.9865	69.8338
93.6662	122.2538	132.0655
145.8172	171.2414	175.9543
193.2525	248.7029	294.6753
320.2045	333.0587	368.4720
418.3651	442.3730	493.0247
524.3130	569.1475	617.8736
685.2195	721.3625	790.1960
826.2130	844.2475	851.2342
895.9004	921.7726	953.4159
980.8607	997.6327	1017.1963
1025.8622	1061.5291	1075.1577
1076.1240	1092.0529	1102.4798
1123.2788	1177.7871	1212.8240
1233.9180	1255.2608	1269.5880
1287.5674	1289.2649	1321.5687
1348.0321	1356.3964	1382.9585
1426.6788	1471.3397	1502.1693
1505.4526	1517.7775	1536.2800
1576.2698	3058.1814	3078.7949
3102.7128	3127.9760	3130.3593
3165.9540	3175.8206	3177.3053
3189.9803	3210.4364	3270.1737
3275.8864	3295.1308	3754.6798

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.213120 Electronic Energy = -1427.71546047
Internal Energy (E)= -1427.48799047 Enthalpy (H)= -1427.48704647
Gibbs Free Energy (G)=-1427.54582647 Gibbs Free Energy of Solvation=-1427.57830534

St.Pt.	General Structure	Ball & Stick model
$1MTS_1$		

Cartesian co-ordinate

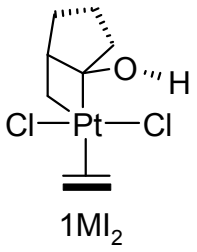
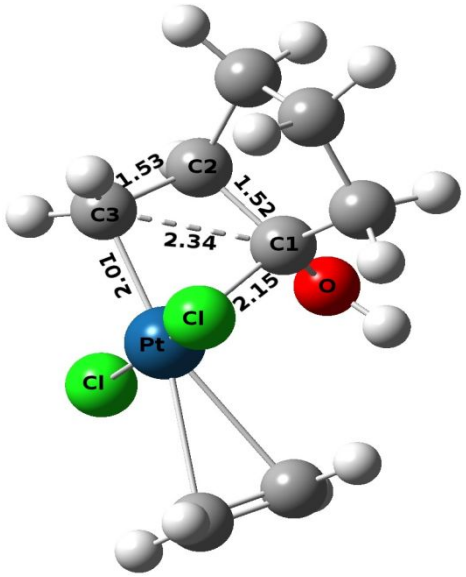
Atoms	X	Y	Z
C	2.85892	-0.16356	0.09587
C	2.27494	-0.19743	1.35235
Pt	0.68675	-0.04666	-0.15229
Cl	0.64416	-2.40995	-0.25683
Cl	0.89403	2.33439	0.01698
H	2.20609	0.70798	1.94682
H	2.10566	-1.14657	1.85018
H	3.15000	-1.08518	-0.39686
H	3.24790	0.76791	-0.30233
C	-2.75752	0.02055	-0.83771
O	-2.01326	2.19035	-0.19026
C	-2.10205	0.90635	0.08116
C	-1.23963	-0.07260	-1.27356
H	-1.08580	-1.11883	-1.53778
H	-1.07373	0.63913	-2.07870
H	-1.17929	2.56192	0.17781
C	-2.04061	0.31705	1.46942
H	-1.10284	0.50393	1.99674
C	-2.38943	-1.16328	1.25365
H	-1.47728	-1.74622	1.11165
H	-2.92800	-1.58324	2.10468
C	-3.23871	-1.18307	-0.03956
H	-3.13033	-2.12022	-0.59116
H	-4.30073	-1.04491	0.18968
H	-2.84405	0.83813	2.00915
H	-3.39269	0.44293	-1.61122

Frequencies

-197.2068	47.4892	70.7521
102.6045	122.0883	136.7096
168.5095	182.1534	191.6588
206.1806	244.2241	287.5761
295.9921	306.9692	331.1574
363.0522	378.2574	419.8832
443.9840	472.5042	584.7263
646.9451	663.1708	696.4807
721.9115	786.1640	840.8074
848.9823	893.8485	900.5265
941.4314	958.7791	1030.1913
1044.4389	1048.7860	1058.8809
1062.9560	1080.6073	1130.9227
1143.7660	1198.1217	1223.8084
1228.5521	1235.7291	1262.5282
1312.7331	1315.5092	1339.0258
1345.6958	1365.2800	1408.7100
1450.3822	1468.8710	1483.1938
1499.3987	1524.3065	1592.8463
1598.0878	3067.1709	3083.9374
3112.5510	3117.7416	3141.6160
3148.3555	3173.9802	3182.8730
3190.7446	3191.3843	3233.1852
3280.2584	3297.7431	3485.6603

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.210539 Electronic Energy = -1427.68971230
Internal Energy (E)= -1427.4652093 Enthalpy (H)= -1427.4642653
Gibbs Free Energy (G)=-1427.5208403 Gibbs Free Energy of Solvation=-1427.54804589

St.Pt.	General Structure	Ball & Stick model
$1MI_2$		

Cartesian co-ordinate

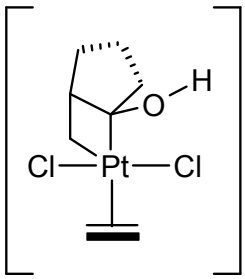
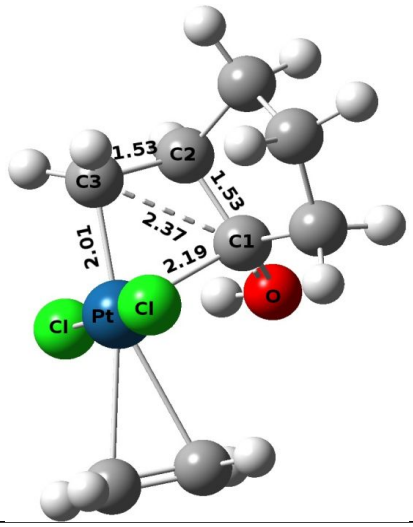
Atoms	X	Y	Z
C	-2.71249	0.96958	0.74923
C	-1.95118	0.62268	1.80315
Pt	-0.52578	0.09434	-0.29261
Cl	0.13537	2.35820	-0.49596
Cl	-1.51283	-2.04969	-0.39390
H	-2.01479	-0.37824	2.22171
H	-1.31222	1.35322	2.29288
H	-2.69420	1.98127	0.35495
H	-3.39477	0.25346	0.30028
C	1.82851	-1.21426	-0.38337
O	0.69437	-1.50956	1.75850
C	1.15406	-0.62664	0.85243
C	0.95735	-0.58283	-1.48403
H	1.42568	0.26451	-1.98723
H	0.53709	-1.30265	-2.18461
H	0.41583	-1.04460	2.55928
C	2.02282	0.51367	1.39102
H	1.46858	1.41538	1.65198
C	3.08789	0.72940	0.30617
H	2.71774	1.44839	-0.42901
H	4.01791	1.12190	0.72221
C	3.25839	-0.66353	-0.32472
H	3.72334	-0.63203	-1.31373
H	3.87534	-1.29926	0.32015
H	2.49174	0.10662	2.29720
H	1.74378	-2.30282	-0.38173

Frequencies

69.4846	77.0695	94.6644
105.1562	123.2676	131.8973
143.5042	160.0065	173.5037
222.1871	244.4469	271.8355
292.4516	297.8729	312.9043
323.9412	365.7933	413.4900
426.8764	516.1204	538.3508
570.8766	635.5568	672.2428
810.6335	851.6005	853.3775
864.8492	883.4888	925.7250
953.8652	1004.7848	1007.4186
1035.6864	1043.6655	1065.2397
1075.5702	1110.9419	1123.3348
1159.3003	1192.9062	1198.5841
1246.5029	1250.6608	1281.0281
1306.5099	1322.0938	1330.5089
1363.6782	1375.3713	1377.8858
1426.3632	1467.8115	1472.8592
1483.9408	1503.0390	1524.0733
1677.3289	3058.1027	3087.4644
3118.9708	3130.3268	3141.5296
3145.0224	3159.1647	3172.4516
3177.2097	3179.5291	3221.9091
3257.0148	3284.5696	3851.5740

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.211275 Electronic Energy = -1427.69492913
Internal Energy (E)= -1427.46878613 Enthalpy (H)= -1427.46784213
Gibbs Free Energy (G)=-1427.52613213 Gibbs Free Energy of Solvation=-1427.55966694

St.Pt.	General Structure	Ball & Stick model
$1MTS_2$		

Cartesian co-ordinate

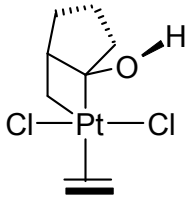
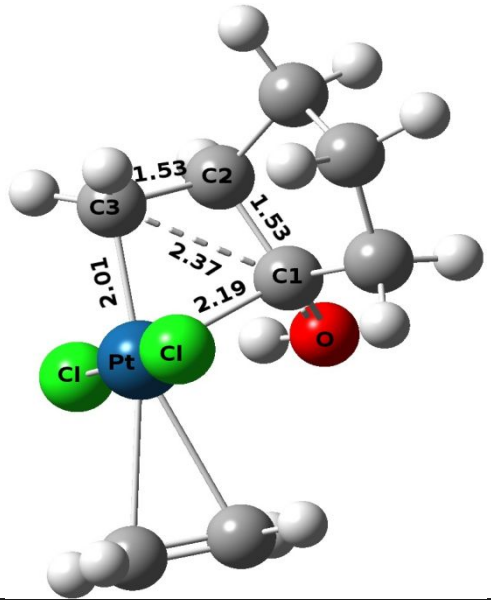
Atoms	X	Y	Z
C	-2.69103	0.95394	0.82034
C	-1.87499	0.63610	1.84238
Pt	-0.51690	0.09817	-0.29887
Cl	0.14613	2.35378	-0.53076
Cl	-1.51037	-2.03483	-0.42060
H	-1.86227	-0.36212	2.26921
H	-1.22675	1.38454	2.29062
H	-2.71942	1.96316	0.41929
H	-3.37479	0.21863	0.40551
C	1.80144	-1.22831	-0.36263
O	0.49734	-1.38596	1.80337
C	1.08236	-0.59050	0.83999
C	0.96550	-0.59714	-1.48830
H	1.44551	0.24778	-1.98374
H	0.53769	-1.31019	-2.19084
H	1.19895	-1.83184	2.29873
C	1.99633	0.50887	1.38918
H	1.47148	1.42214	1.66859
C	3.08382	0.69772	0.32707
H	2.74197	1.41514	-0.42387
H	4.01505	1.07747	0.75246
C	3.23924	-0.70494	-0.28638
H	3.72591	-0.69567	-1.26549
H	3.83570	-1.34305	0.37678
H	2.43666	0.08292	2.30314
H	1.68956	-2.31496	-0.35239

Frequencies

-402.6412	74.8197	92.9946
100.3383	114.4929	125.9228
136.4702	145.1162	168.8999
181.3402	234.7186	254.8791
279.7358	305.6706	309.0655
320.7890	330.0811	377.4367
419.5856	430.8765	548.5055
579.0608	641.9752	665.6772
813.1815	841.3206	846.6041
859.7781	882.5386	923.2232
953.7440	1004.9005	1027.1441
1040.9723	1041.2935	1063.2095
1082.2982	1098.2088	1144.4993
1154.9506	1177.6314	1194.1953
1230.6309	1240.9319	1243.5503
1286.5678	1291.4894	1324.6567
1340.4844	1366.4153	1372.0053
1378.0670	1471.8069	1478.6352
1479.5207	1501.6375	1523.0144
1676.4925	3041.9939	3074.5087
3112.9855	3132.9998	3134.0223
3136.5611	3166.1735	3168.9749
3174.7135	3179.7012	3226.8528
3264.2586	3284.6447	3838.7545

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.209890 Electronic Energy = -1427.68398025
Internal Energy (E)= -1427.45966125 Enthalpy (H)= -1427.45871625
Gibbs Free Energy (G)=-1427.51592725 Gibbs Free Energy of Solvation=-1427.5512149

St.Pt.	General Structure	Ball & Stick model
$1MI_3$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-2.72385	0.82956	0.79456
C	-1.87131	0.63896	1.82018
Pt	-0.53877	0.11804	-0.30466
Cl	0.08299	2.37609	-0.45391
Cl	-1.37644	-2.13422	-0.38004
H	-1.79749	-0.31974	2.32472
H	-1.27309	1.45910	2.20714
H	-2.83040	1.80740	0.33339
H	-3.36592	0.02638	0.44488
C	1.82637	-1.16440	-0.42871
O	0.62969	-1.46579	1.77311
C	1.15642	-0.65170	0.85330
C	0.96517	-0.48255	-1.50806
H	1.44131	0.38607	-1.96496
H	0.56704	-1.17135	-2.25219
C	2.01036	0.45270	1.45112
H	1.43479	1.32600	1.75841
C	3.07521	0.74006	0.38583
H	2.70338	1.49808	-0.30880
H	4.00405	1.11070	0.82344
C	3.25458	-0.61150	-0.32738
H	3.72241	-0.52114	-1.31132
H	3.87043	-1.28170	0.28276
H	2.46029	0.00392	2.34566
H	1.75974	-2.25342	-0.49744
H	0.12089	-2.16985	1.32535

Frequencies

72.4947	77.7677	97.5313
117.8857	126.3536	140.3269
143.6949	173.4011	177.4511
224.1746	234.1874	280.2966
288.6975	293.9028	320.3751
328.4770	364.1429	436.2684
445.1202	517.0384	578.2169
625.1029	669.4198	729.2313
804.5401	834.7244	843.7566
858.1470	875.5440	923.2882
956.5145	1009.2390	1019.4869
1040.4362	1045.7410	1063.6329
1078.7139	1113.1128	1139.2166
1169.6113	1193.2733	1198.2594
1238.4919	1253.4234	1280.6964
1308.9677	1317.4995	1332.5328
1364.8892	1372.6054	1397.4877
1447.6739	1465.3453	1468.6855
1479.7649	1503.7008	1526.0966
1671.7095	3078.3818	3087.5698
3116.1064	3127.2268	3134.5675
3148.7288	3169.4200	3171.5839
3181.0082	3182.0379	3214.5960
3265.4078	3286.2741	3663.3101

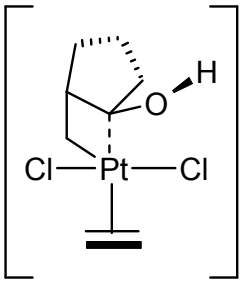
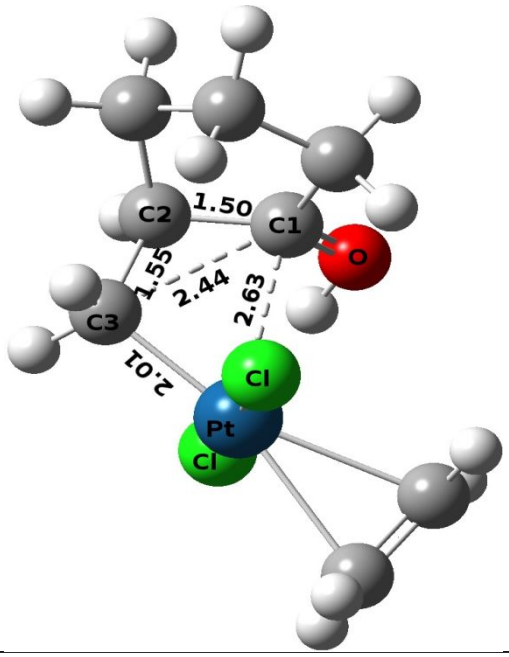
Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm

Zero-point correction= 0.211607 Electronic Energy = -1427.70866046

Internal Energy (E)= -1427.48240046 Enthalpy (H)= -1427.48145646

Gibbs Free Energy (G)=-1427.53919446 Gibbs Free Energy of Solvation=-1427.56750827

St.Pt.	General Structure	Ball & Stick model
$IMTS_3$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	2.85637	-0.58577	0.59946
C	2.06028	-0.39265	1.67879
Pt	0.65457	-0.12456	-0.27971
Cl	0.09668	-2.40543	-0.18622
Cl	1.10946	2.26959	-0.30990
H	1.97534	0.58569	2.14269
H	1.57438	-1.23066	2.16865
H	3.02055	-1.58219	0.20093
H	3.42577	0.23409	0.17190
C	-1.97496	0.99202	-0.57283
O	-0.96875	1.57505	1.63223
C	-1.55918	0.74213	0.85413
C	-0.93706	0.25437	-1.45925
H	-1.34706	-0.68193	-1.84113
H	-0.61348	0.89915	-2.27797
C	-2.29717	-0.41371	1.45088
H	-1.60403	-1.16037	1.84724
C	-3.18803	-0.91316	0.30322
H	-2.66279	-1.70828	-0.23214
H	-4.13853	-1.31024	0.66209
C	-3.36284	0.32481	-0.59685
H	-3.65888	0.07465	-1.61808
H	-4.11813	0.99856	-0.17608
H	-2.87542	-0.00516	2.29047
H	-1.97525	2.06460	-0.78385
H	-0.39769	2.19873	1.09338

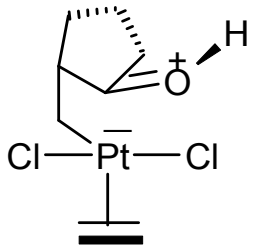
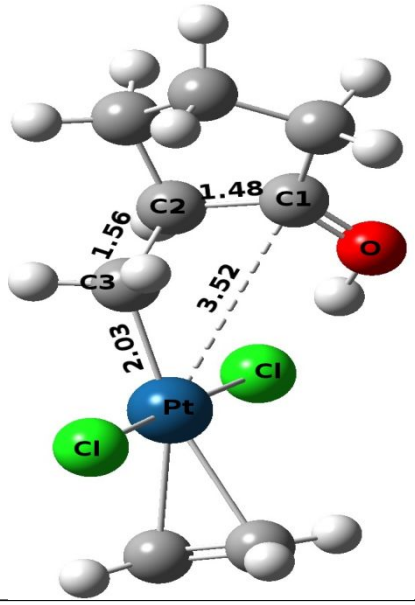
Frequencies

-138.1756	77.3860	91.7579
100.0824	117.4208	131.0062
144.4863	155.7848	168.0061
185.8670	205.9501	250.3130
281.0420	287.9897	319.8491
330.9600	348.0334	439.5908
468.1303	519.4780	585.1767
617.6934	664.5841	790.6940
821.4747	837.7719	839.2657
864.0530	893.3953	917.7511
958.4854	1006.2371	1019.7535
1027.7172	1050.0608	1056.7054
1072.8845	1094.2681	1156.3651
1179.5655	1206.6210	1214.4458
1239.7168	1256.9111	1293.3349
1294.7622	1319.8312	1338.0496
1361.8910	1365.6857	1434.9671
1458.1537	1470.2025	1486.7626
1503.8775	1521.7012	1609.8247
1656.7184	3072.2909	3080.3974
3114.1226	3125.9569	3128.6365
3154.4842	3155.5072	3156.9964
3177.6153	3183.1416	3189.3129
3193.6125	3272.5367	3292.0165

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm

Zero-point correction= 0.210519	Electronic Energy = -1427.70458879
Internal Energy (E)= -1427.47996179	Enthalpy (H)= -1427.47901779
Gibbs Free Energy (G)=-1427.53571679	Gibbs Free Energy of Solvation=-1427.56256105

St.Pt.	General Structure	Ball & Stick model
$1MI_4$		

Cartesian co-ordinate

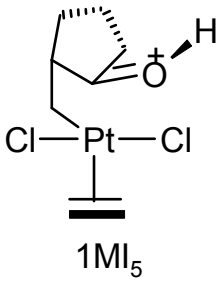
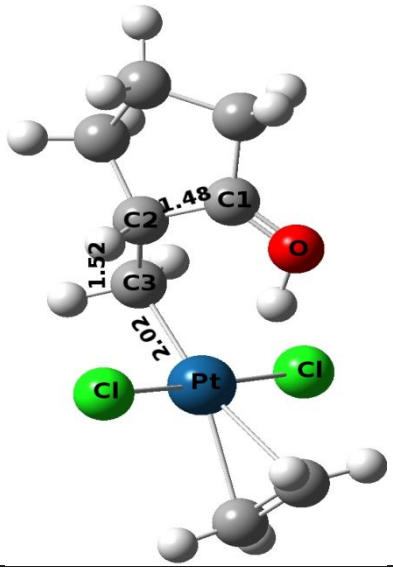
Atoms	X	Y	Z
C	3.12699	0.54239	-0.24125
C	2.77357	0.65267	1.06912
Pt	0.87154	-0.07879	-0.09759
Cl	1.48514	-2.29975	0.32333
Cl	0.25408	2.27348	-0.47352
H	2.46302	1.60678	1.48321
H	2.92811	-0.17080	1.75845
H	3.57038	-0.37212	-0.62187
H	3.10817	1.40576	-0.89878
C	-2.16636	0.13539	-0.78389
O	-1.91228	1.56194	1.19009
C	-2.51299	0.65980	0.55737
C	-0.95471	-0.83187	-0.58369
H	-1.20839	-1.60439	0.15012
H	-0.83001	-1.34618	-1.54380
C	-3.70103	-0.02737	1.14565
H	-3.51939	-0.31693	2.18361
C	-4.00534	-1.15821	0.15115
H	-3.47567	-2.06697	0.44597
H	-5.06964	-1.39125	0.10441
C	-3.44959	-0.62253	-1.18142
H	-3.23650	-1.41554	-1.90047
H	-4.16893	0.06613	-1.63899
H	-4.50403	0.72380	1.15622
H	-1.87145	0.93457	-1.46856
H	-1.09738	1.94221	0.63690

Frequencies

35.3350	70.0342	92.1634
106.5057	123.2822	129.7933
146.9156	153.0937	162.8720
181.5463	213.6835	226.4268
262.7326	286.4428	306.9132
326.7837	392.2480	500.9893
512.8295	580.3164	598.5675
618.4923	681.2451	706.9250
830.4850	834.5975	853.2780
870.5078	923.0155	946.6754
992.3497	1021.7487	1027.2064
1030.2236	1064.5818	1066.7859
1079.0382	1103.4828	1145.9267
1199.0006	1215.3837	1218.1147
1236.7029	1260.3171	1284.8712
1315.8979	1322.8372	1345.4257
1352.6986	1365.1555	1438.6986
1453.5844	1468.3333	1485.1859
1504.0518	1518.7724	1641.0518
1718.5302	2318.9606	3064.4856
3076.8315	3087.9122	3116.1986
3127.8807	3138.4874	3149.8850
3157.9814	3173.4197	3178.3753
3188.5256	3271.1318	3289.9807

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.209342 Electronic Energy = -1427.70934541
Internal Energy (E)= -1427.48513941 Enthalpy (H)= -1427.48419541
Gibbs Free Energy (G)=-1427.54363841 Gibbs Free Energy of Solvation=-1427.57442864

St.Pt.	General Structure	Ball & Stick model
$1MI_5$	 $1MI_5$	

Cartesian co-ordinate

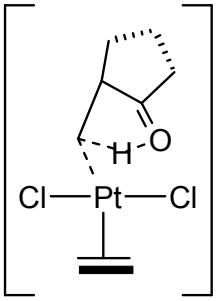
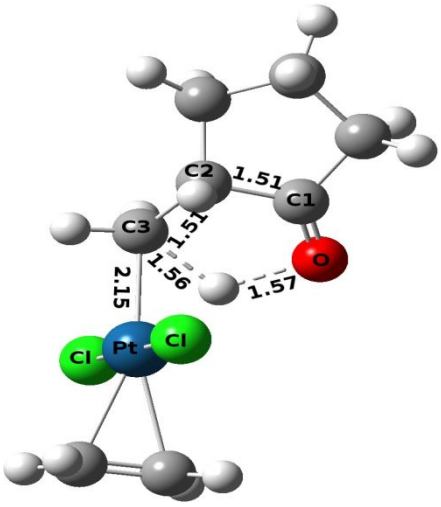
Atoms	X	Y	Z
C	-3.17462	0.44850	0.35867
C	-2.54108	0.24555	1.53878
Pt	-0.86537	0.03009	-0.20296
Cl	-0.38450	2.35368	-0.02861
Cl	-1.26561	-2.29166	-0.27860
H	-2.50645	-0.74214	1.98760
H	-2.14659	1.08197	2.10743
H	-3.29641	1.45015	-0.04212
H	-3.65598	-0.37342	-0.16220
C	2.09976	0.24782	-0.51118
O	1.36034	-0.57704	1.66442
C	2.27938	-0.29146	0.86084
C	0.85289	-0.22617	-1.25290
H	1.97584	1.33272	-0.31200
H	0.74616	0.37621	-2.16032
H	0.95888	-1.27860	-1.53101
C	3.48717	0.01612	-1.14072
C	4.46134	0.17770	0.03906
C	3.71541	-0.48277	1.21059
H	0.42480	-0.42325	1.19140
H	3.68195	0.71191	-1.95741
H	3.87043	-1.57171	1.21360
H	3.94471	-0.12144	2.21545
H	5.43615	-0.27681	-0.13977
H	4.61744	1.23922	0.25303
H	3.53533	-1.00164	-1.54490

Frequencies

27.2547	62.8911	69.0469
101.6269	106.1223	119.2245
138.5268	146.8085	174.7270
187.4775	202.8376	235.9484
255.4671	303.1680	305.0058
319.4264	341.3260	464.0952
528.1147	532.8850	589.6351
627.4702	659.0666	729.8961
808.9482	840.8075	856.1165
909.1980	932.5675	942.8883
998.5301	1020.1122	1024.4254
1037.1275	1062.5034	1064.7485
1073.7255	1114.8585	1157.8466
1182.7634	1196.7660	1224.1078
1242.3597	1249.0395	1263.8464
1317.9675	1329.3950	1337.6499
1353.5997	1362.5839	1435.6921
1460.8468	1468.1914	1479.9313
1507.2908	1519.8560	1654.5929
1700.4605	2265.0968	2970.3687
3058.6526	3084.2336	3086.6986
3103.6347	3152.4270	3152.4674
3166.0662	3172.4670	3176.7214
3191.7180	3269.5847	3294.7091

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.208462 Electronic Energy = -1427.70544006
Internal Energy (E)= -1427.48187806 Enthalpy (H)= -1427.48093406
Gibbs Free Energy (G)=-1427.54141406 Gibbs Free Energy of Solvation=-1427.57518482

St.Pt.	General Structure	Ball & Stick model
$1MTS_5$		

Cartesian co-ordinate

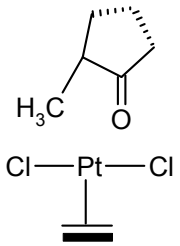
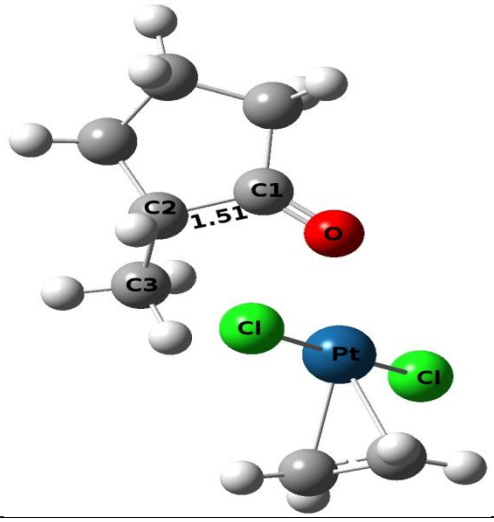
Atoms	X	Y	Z
C	-3.08198	-0.79470	0.16994
C	-2.70392	-0.75151	-1.14526
Pt	-0.92960	-0.00411	0.11253
Cl	-0.15018	-2.23112	0.33518
Cl	-1.74607	2.19440	-0.08006
H	-2.93534	0.11268	-1.75981
H	-2.29379	-1.63084	-1.63219
H	-2.98450	-1.71333	0.74037
H	-3.62490	0.03456	0.61332
C	2.24594	0.06746	0.60076
O	1.65613	0.20210	-1.70405
C	2.53670	0.02292	-0.88292
C	0.94061	0.80041	0.81507
H	2.14850	-0.97642	0.93329
H	0.57829	0.68377	1.84271
H	1.01186	1.86683	0.58921
C	3.55569	0.65499	1.14625
C	4.62987	-0.04172	0.28206
C	4.02113	-0.09833	-1.13245
H	0.51568	0.40914	-0.63492
H	3.68949	0.47630	2.21426
H	4.31977	0.75264	-1.75370
H	4.24961	-1.00659	-1.69556
H	5.58787	0.47971	0.30361
H	4.79482	-1.05584	0.65802
H	3.57437	1.73876	0.97843

Frequencies

-797.8640	37.6732	61.3710
74.2994	93.7218	117.9403
122.9703	139.8294	149.1610
164.6739	169.0789	208.9362
246.9510	259.3560	314.6470
316.2879	331.3267	394.7891
458.8111	563.9340	574.0099
601.2474	607.2156	617.9457
739.3761	793.3962	831.4634
853.0058	901.8242	926.6706
968.3645	970.7779	1019.2615
1034.0027	1050.3920	1056.4726
1061.9244	1092.4447	1150.5355
1178.9820	1188.5168	1199.7497
1213.6986	1235.7513	1239.4969
1297.2575	1315.3759	1325.2248
1338.9645	1347.9983	1382.7758
1392.2271	1454.3502	1461.9568
1472.2297	1505.2211	1518.7852
1620.1984	1876.7809	3066.4682
3077.9152	3087.6682	3098.0556
3102.2443	3150.9150	3157.2547
3163.1034	3164.6624	3177.1748
3186.7400	3276.9018	3295.9441

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.204230 Electronic Energy = -1427.67847823
Internal Energy (E)= -1427.45930323 Enthalpy (H)= -1427.45835823
Gibbs Free Energy (G)=-1427.51830023 Gibbs Free Energy of Solvation=-1427.55271722

St.Pt.	General Structure	Ball & Stick model
$1MI_6$		

Cartesian co-ordinate

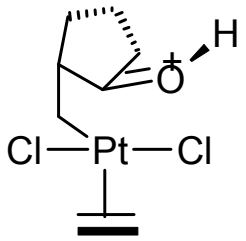
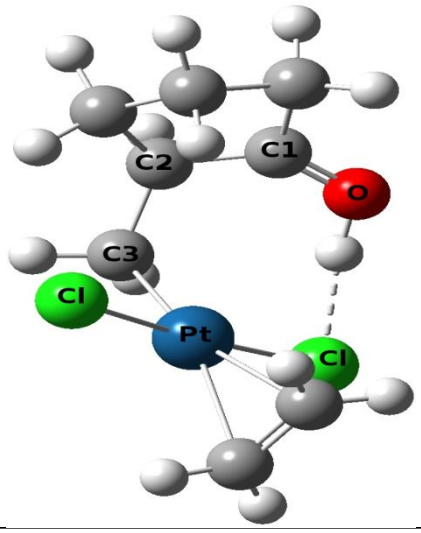
Atoms	X	Y	Z
C	2.54011	0.51562	1.14850
C	2.97692	0.57889	-0.18173
Pt	0.93946	0.02723	-0.13795
Cl	0.25908	2.29279	-0.21269
Cl	1.50884	-2.24772	-0.02023
H	3.52129	-0.25416	-0.61453
H	3.03539	1.53649	-0.68916
H	2.26561	1.42597	1.67183
H	2.75072	-0.36563	1.74584
C	-2.45961	0.20005	0.87102
O	-0.98665	-0.51372	-0.95798
C	-2.10810	-0.31359	-0.50831
C	-1.65875	-0.42812	2.00880
H	-2.23624	1.27792	0.81866
H	-0.60785	-0.12832	1.98278
H	-2.07266	-0.10210	2.96617
C	-3.98082	-0.01160	0.94266
C	-4.45958	0.13711	-0.50997
C	-3.35906	-0.56457	-1.31444
H	-1.70274	-1.52012	1.96503
H	-4.46329	0.68657	1.62920
H	-3.51058	-1.65252	-1.31986
H	-3.23047	-0.24425	-2.34966
H	-5.44821	-0.29138	-0.68077
H	-4.50053	1.19637	-0.78304
H	-4.18621	-1.02790	1.30183

Frequencies

-29.1370	39.5378	59.8395
64.1790	102.7749	122.6731
140.0231	154.1497	158.0115
169.1246	190.8933	211.6602
232.3615	287.2370	315.4800
332.7439	356.8316	418.7252
508.3569	526.2287	559.5001
567.8855	641.7342	744.7820
788.5839	838.8024	842.8045
867.8801	916.1053	955.2972
975.4025	993.8789	1025.5958
1033.1121	1073.6559	1085.6280
1087.3798	1164.3012	1195.5036
1205.7517	1216.0815	1230.0987
1248.9099	1287.7451	1300.4817
1320.3627	1332.4741	1355.3398
1375.7051	1422.1715	1451.1740
1465.2762	1494.7728	1505.3169
1509.7263	1521.2891	1572.1556
1826.2424	3048.5768	3067.7680
3073.7803	3077.0698	3103.6375
3153.4866	3158.1993	3159.9605
3161.7996	3170.8148	3179.1905
3181.7342	3275.3827	3290.0219

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.210710 Electronic Energy = -1427.74422573
Internal Energy (E)= -1427.51893773 Enthalpy (H)= -1427.51799373
Gibbs Free Energy (G)=-1427.57712473 Gibbs Free Energy of Solvation=-1427.61092709

St.Pt.	General Structure	Ball & Stick model
$1MI_{5a}$		

Cartesian co-ordinate

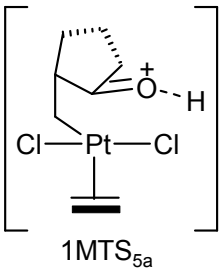
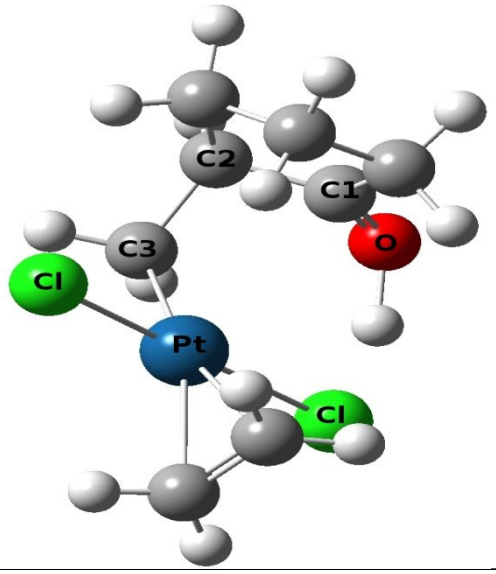
Atoms	X	Y	Z
C	2.88457	-0.51067	0.78965
C	2.02255	-0.30722	1.81884
Pt	0.75537	-0.10999	-0.19098
Cl	0.23591	-2.40128	-0.09824
Cl	1.11420	2.31068	-0.25897
H	1.90900	0.67571	2.26546
H	1.52499	-1.14338	2.29932
H	3.09013	-1.51217	0.42525
H	3.47932	0.30393	0.38759
C	-2.12240	0.34014	-0.94328
O	-1.52818	2.08521	0.70417
C	-2.19832	1.08608	0.35314
C	-0.71440	0.18469	-1.55450
H	-0.75092	-0.66838	-2.23609
H	-0.45935	1.07727	-2.13212
C	-3.18839	0.47285	1.28151
H	-2.98712	0.73716	2.32014
C	-3.06472	-1.01163	0.89351
H	-2.16330	-1.44013	1.34366
H	-3.92692	-1.59602	1.21706
C	-2.89048	-0.97268	-0.63559
H	-2.32483	-1.83564	-0.98812
H	-3.86477	-0.96223	-1.13307
H	-4.18135	0.85549	1.00427
H	-2.72180	0.97146	-1.62425
H	-0.63836	2.28523	0.16712

Frequencies

46.3161	58.0919	81.2575
105.1335	115.5536	130.0877
138.2714	147.7221	166.8671
185.5868	195.7427	228.2991
265.8332	309.7091	317.2220
362.2554	402.8128	471.4490
524.6697	550.3868	579.7887
592.5484	678.5435	761.3410
816.4302	838.2530	845.4328
871.8516	927.5047	968.0200
988.2373	1015.9249	1021.2740
1027.6464	1066.7993	1069.7843
1087.1663	1109.1879	1179.5362
1187.1133	1214.9764	1222.9578
1239.3939	1275.0096	1282.2413
1292.3643	1317.5734	1336.9627
1356.7830	1358.0563	1415.2693
1456.2694	1471.1756	1483.4089
1498.3132	1516.9489	1649.3235
1723.9903	2273.4687	2997.2006
3058.9830	3092.7784	3101.0606
3104.1853	3162.4751	3173.4692
3173.6832	3180.2360	3181.6322
3195.0752	3268.4365	3295.3175

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.209146 Electronic Energy = -1427.70406074
Internal Energy (E)= -1427.48003274 Enthalpy (H)= -1427.47908874
Gibbs Free Energy (G)=-1427.53848074 Gibbs Free Energy of Solvation=-1427.56675139

St.Pt.	General Structure	Ball & Stick model
$1MTS_{5a}$	 $1MTS_{5a}$	

Cartesian co-ordinate

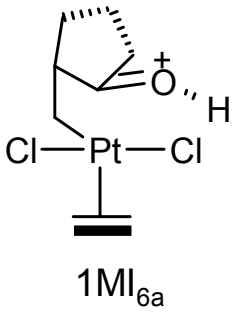
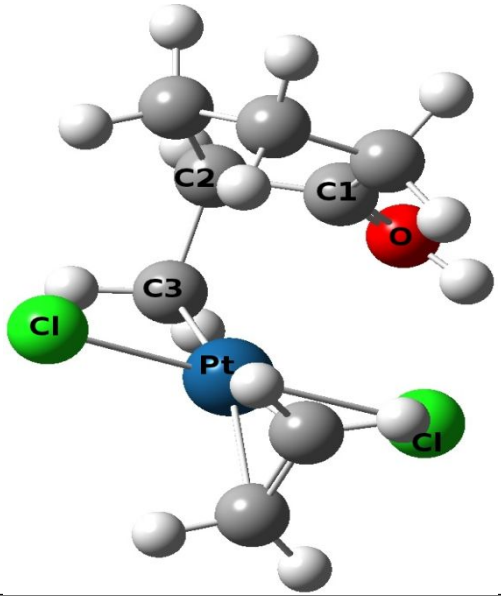
Atoms	X	Y	Z
C	2.88560	0.19404	0.66937
C	2.06046	0.06048	1.73886
Pt	0.67017	-0.01280	-0.21492
Cl	0.88123	-2.33316	-0.25922
Cl	0.44055	2.47088	-0.10831
H	1.69350	0.93111	2.27444
H	1.85440	-0.91746	2.16226
H	3.35228	-0.67358	0.21407
H	3.20061	1.17298	0.32078
C	-2.30084	-0.32590	-0.87501
O	-2.22419	1.97369	-0.14374
C	-2.33805	0.76339	0.14533
C	-0.88740	-0.18649	-1.51683
H	-0.71368	-1.06757	-2.13853
H	-0.88970	0.71067	-2.14423
C	-2.43909	0.22006	1.53558
H	-1.79127	0.76763	2.22612
C	-2.17777	-1.28570	1.38778
H	-1.11810	-1.49922	1.54514
H	-2.75146	-1.87497	2.10514
C	-2.56397	-1.61046	-0.07348
H	-1.98771	-2.45403	-0.45850
H	-3.62776	-1.86324	-0.13286
H	-3.47798	0.42176	1.84110
H	-3.04444	-0.14305	-1.65975
H	-1.08259	2.37993	-0.06316

Frequencies

-228.3143	56.8211	63.4434
107.3943	115.3834	125.0329
136.4426	150.7856	154.3228
171.9573	184.4205	206.3989
278.9067	303.6023	343.0649
355.6540	382.6201	468.7482
476.4130	531.8867	552.5539
573.0397	595.4944	642.8830
690.6896	797.0889	828.8714
830.2099	836.3599	867.2701
912.7198	950.7331	1012.1998
1015.9904	1027.5101	1028.5393
1068.8925	1070.4361	1099.5694
1156.5226	1172.0638	1196.7676
1213.7860	1236.4921	1238.8063
1259.1554	1289.4637	1314.2806
1330.5144	1357.8865	1358.5091
1363.4319	1428.9971	1461.6931
1469.8590	1497.8307	1518.3858
1649.7822	1763.8548	3045.4477
3082.2102	3090.2985	3097.1854
3111.2248	3133.1662	3159.1886
3165.8163	3166.7402	3172.3813
3182.1300	3265.8392	3284.2039

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.203323 Electronic Energy = -1427.69076721
Internal Energy (E)= -1427.47293121 Enthalpy (H)= -1427.47198721
Gibbs Free Energy (G)=-1427.52994421 Gibbs Free Energy of Solvation=-1427.5539267

St.Pt.	General Structure	Ball & Stick model
$1MI_{6a}$	 $1MI_{6a}$	

Cartesian co-ordinate

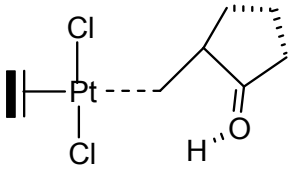
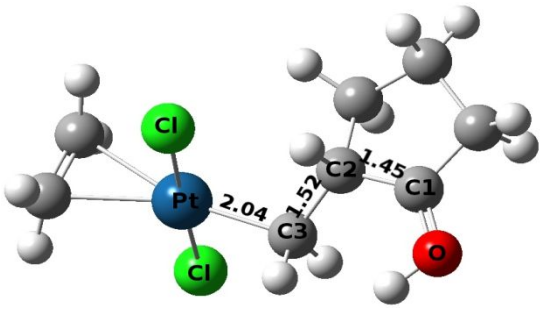
Atoms	X	Y	Z
C	2.83406	0.55566	0.44288
C	2.12263	0.33583	1.58418
Pt	0.65390	0.04208	-0.21860
Cl	1.18387	-2.25400	-0.23577
Cl	0.13457	2.42398	-0.02936
H	1.68232	1.16526	2.12896
H	2.11246	-0.64474	2.04962
H	3.39781	-0.24677	-0.02202
H	2.96741	1.56051	0.05501
C	-2.35401	-0.69630	-0.77736
O	-2.60186	1.65467	-0.49532
C	-2.40521	0.51248	0.03678
C	-0.93824	-0.41766	-1.43438
H	-0.67798	-1.34892	-1.94365
H	-1.07588	0.39350	-2.15409
C	-2.18592	0.25374	1.48494
H	-1.45773	0.94089	1.92517
C	-1.85752	-1.24805	1.56440
H	-0.77865	-1.39208	1.64344
H	-2.32813	-1.71301	2.43203
C	-2.37383	-1.84921	0.23412
H	-1.74283	-2.67677	-0.09608
H	-3.39897	-2.21532	0.34862
H	-3.16829	0.47344	1.93511
H	-3.10735	-0.73947	-1.56770
H	-2.07869	2.35569	-0.02758

Frequencies

62.2638	68.0955	98.3742
108.5722	128.7002	133.2442
155.2726	157.4305	168.0044
202.5734	220.1382	223.2459
258.9219	291.4215	312.8209
361.1278	397.8299	438.3275
496.2105	531.1245	577.4102
591.1497	631.6473	664.1714
770.5561	800.4364	831.3921
837.3267	872.7351	901.5774
924.3879	986.8199	1016.7075
1028.2465	1039.7394	1047.6299
1059.6746	1078.0374	1135.7966
1171.6777	1183.5215	1218.9488
1237.8552	1248.6627	1267.9483
1309.2205	1324.3897	1342.3603
1348.8456	1358.2248	1430.7820
1438.6244	1464.8126	1466.1382
1497.3253	1515.6595	1636.6877
1660.4969	3036.8373	3085.1715
3089.1941	3121.1423	3130.6975
3147.6487	3162.0745	3165.1851
3171.1606	3177.7891	3189.0678
3267.3719	3291.1846	3424.5736

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.210025 Electronic Energy = -1427.69556099
Internal Energy (E)= -1427.47062099 Enthalpy (H)= -1427.46967699
Gibbs Free Energy (G)=-1427.52829399 Gibbs Free Energy of Solvation=-1427.55781609

St.Pt.	General Structure	Ball & Stick model
$1MI_{7a}$		

Cartesian co-ordinate

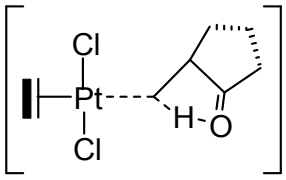
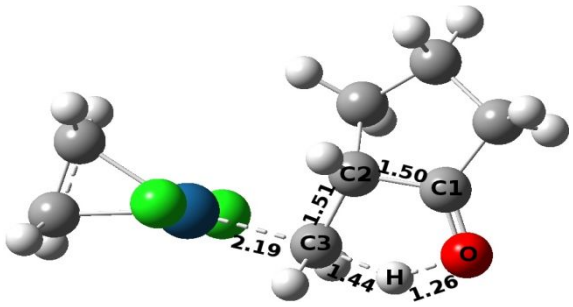
Atoms	X	Y	Z
C	2.69999	0.86154	1.11428
C	3.13553	0.72555	-0.17471
Pt	0.96836	-0.02202	-0.10698
Cl	0.15292	2.18755	-0.62886
Cl	1.68843	-2.20551	0.43054
H	3.68321	-0.15919	-0.48274
H	3.08853	1.56042	-0.86659
H	2.30194	1.80795	1.46621
H	2.89465	0.08788	1.84954
C	-1.99613	0.02529	-0.11505
O	-3.59986	-1.00710	-1.59607
C	-3.32857	-0.39933	-0.50403
C	-0.83932	-0.79931	-0.66707
H	-1.90696	1.04964	-0.56312
H	-0.91529	-1.84199	-0.34189
H	-0.82450	-0.75879	-1.76985
C	-2.14230	0.25422	1.40126
C	-3.60034	0.72451	1.55232
C	-4.36770	-0.12038	0.51553
H	-2.76283	-1.17744	-2.08153
H	-1.40918	0.98563	1.74341
H	-4.63664	-1.10424	0.93068
H	-5.27846	0.30598	0.08708
H	-3.99842	0.59635	2.55895
H	-3.67635	1.78378	1.28932
H	-1.96297	-0.68886	1.93011

Frequencies

18.7146	47.6735	66.4184
97.2149	111.1922	130.5137
136.1153	151.1706	154.1974
189.1507	198.3445	221.1984
238.5499	276.6774	309.4807
326.4782	417.3772	459.8293
503.2757	549.4735	606.2106
620.3829	671.1632	730.0856
769.4102	817.2391	842.5807
871.0286	895.6651	938.8001
960.3170	1001.2755	1022.4664
1025.2304	1031.7413	1061.5110
1066.1000	1129.0313	1146.7643
1181.5142	1193.1579	1204.7461
1240.3737	1244.5072	1251.5368
1276.3138	1311.6448	1330.3329
1344.7159	1347.3842	1428.0034
1463.8977	1470.6905	1488.8231
1504.8861	1516.4839	1630.6234
1633.9444	2820.8571	3001.1174
3052.3745	3090.2160	3107.3604
3122.8504	3145.0563	3176.1745
3180.1348	3180.9332	3193.3860
3276.2213	3296.1331	3601.6623

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.209860 Electronic Energy = -1427.68249314
Internal Energy (E)= -1427.45741714 Enthalpy (H)= -1427.45647314
Gibbs Free Energy (G)=-1427.51783114 Gibbs Free Energy of Solvation=-1427.55972315

St.Pt.	General Structure	Ball & Stick model
$1MTS_{7a}$		

Cartesian co-ordinate

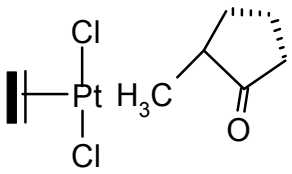
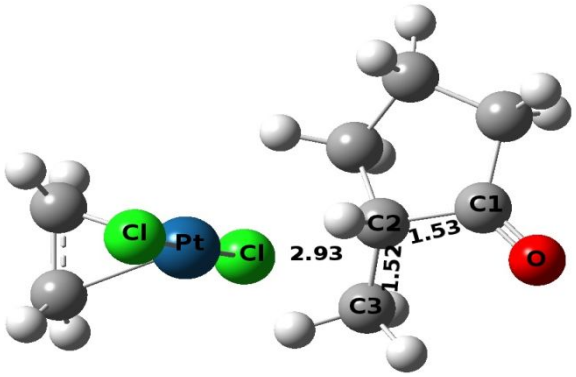
Atoms	X	Y	Z
C	2.46357	0.04768	-1.43508
C	3.10390	-0.08193	-0.21016
Pt	0.95800	-0.01744	0.13075
Cl	0.79632	-2.37745	-0.08806
Cl	1.01460	2.34255	0.29783
H	3.50567	0.79244	0.29150
H	3.42605	-1.05737	0.13989
H	2.28362	-0.82745	-2.05125
H	2.36750	1.02361	-1.89956
C	-1.93138	-0.30404	-0.01665
O	-3.42321	-0.19552	1.77178
C	-3.32376	-0.22542	0.54131
C	-0.99120	-0.03379	1.14180
H	-1.77362	-1.33183	-0.38337
H	-0.91925	0.98286	1.53052
H	-0.64819	-0.87396	1.75251
C	-2.07289	0.63207	-1.23137
C	-3.48760	0.29728	-1.76276
C	-4.35479	0.04011	-0.50395
H	-2.17699	-0.16712	1.95748
H	-1.28949	0.46400	-1.97226
H	-4.92960	0.91798	-0.19059
H	-5.06008	-0.79094	-0.59380
H	-3.90158	1.09030	-2.38632
H	-3.44312	-0.61203	-2.36872
H	-1.99970	1.67537	-0.90384

Frequencies

-1405.8522	21.8381	45.7827
62.5720	99.2291	111.2835
130.4345	143.9811	150.1312
159.6972	179.4596	207.5513
247.5685	307.4176	314.1918
317.1965	354.6911	450.4855
486.3209	571.4795	600.2062
645.2274	707.5958	727.3212
762.8792	825.3333	834.9348
842.9906	846.3035	916.0816
930.4353	958.0936	967.0625
1018.5901	1033.1942	1052.0976
1057.4621	1057.9591	1148.0478
1184.2377	1188.1242	1215.9248
1229.1901	1235.0594	1262.5486
1286.8459	1305.0273	1309.0237
1312.2033	1345.9428	1363.5857
1437.0698	1446.6106	1464.8720
1502.5318	1515.5132	1590.2663
1684.3176	1841.1316	3042.3160
3091.8728	3095.4282	3100.2648
3106.5648	3146.1155	3164.1126
3171.0354	3177.6638	3185.3572
3213.5744	3274.4523	3292.1492

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.205204 Electronic Energy = -1427.65881601
Internal Energy (E)= -1427.43888301 Enthalpy (H)= -1427.43793901
Gibbs Free Energy (G)=-1427.49826901 Gibbs Free Energy of Solvation=-1427.53233945

St.Pt.	General Structure	Ball & Stick model
$1MI_{8a}$		

Cartesian co-ordinate

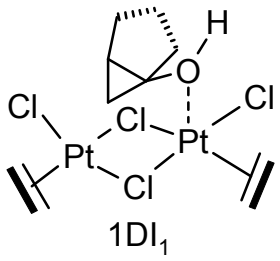
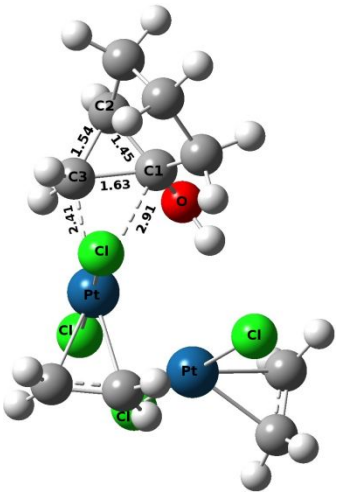
Atoms	X	Y	Z
C	2.78133	0.11595	1.02153
C	3.05539	0.10198	-0.37333
Pt	1.00384	0.00523	-0.04662
Cl	0.81629	2.33957	-0.09176
Cl	1.06116	-2.33146	-0.00053
H	3.37027	-0.82115	-0.85042
H	3.27332	1.03275	-0.88813
H	2.79782	1.05731	1.56232
H	2.89250	-0.79711	1.59851
C	-2.18881	0.29166	-0.39273
O	-4.34328	-0.01964	-1.47268
C	-3.69903	0.03992	-0.45643
C	-1.46745	-0.30531	-1.59285
H	-2.06803	1.38625	-0.40161
H	-1.36361	-1.39009	-1.50777
H	-0.46536	0.13472	-1.76678
C	-1.81413	-0.22124	1.00402
C	-3.03537	0.14770	1.87056
C	-4.23061	-0.15547	0.96035
H	-2.02756	-0.07440	-2.50381
H	-0.89896	0.23349	1.41900
H	-4.53948	-1.20432	1.04408
H	-5.11598	0.45963	1.13348
H	-3.05959	-0.40378	2.81163
H	-3.00221	1.21580	2.10804
H	-1.67119	-1.30862	0.98198

Frequencies

17.8160	45.9072	49.5990
75.7747	85.6544	93.4035
108.2373	120.8175	141.8218
165.0550	181.7967	214.5073
237.9538	322.4030	336.0688
344.2245	354.4602	451.7713
466.7801	534.5200	546.3191
560.9740	616.2962	715.8883
809.8983	828.4086	831.5237
874.0652	909.4465	953.6124
969.4688	993.2582	998.3660
1040.9270	1064.6883	1084.0273
1094.4830	1155.4581	1187.0539
1191.3923	1213.4853	1222.6474
1242.8367	1247.3811	1306.6570
1315.2663	1323.4200	1357.6175
1383.0081	1419.5690	1458.0905
1463.2724	1466.4210	1487.0233
1513.9944	1522.2234	1547.3878
1910.4292	2959.2955	3002.1204
3046.1687	3081.1735	3091.7923
3103.2406	3111.8853	3149.8059
3158.7814	3170.8055	3173.9739
3176.7991	3272.4381	3286.5882

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.209500 Electronic Energy = -1427.71207201
Internal Energy (E)= -1427.48689901 Enthalpy (H)= -1427.48595501
Gibbs Free Energy (G)=-1427.54924701 Gibbs Free Energy of Solvation=-1427.58081817

St.Pt.	General Structure	Ball & Stick model
$1DI_1$	 $1DI_1$	

Cartesian co-ordinate

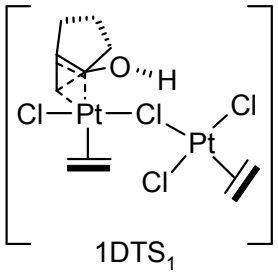
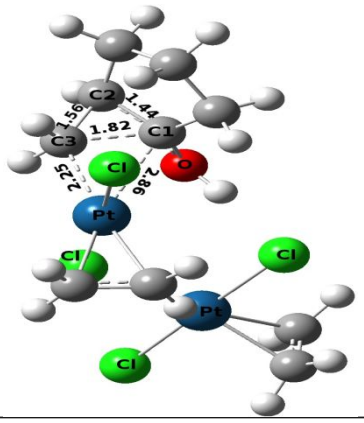
Atoms	X	Y	Z
C	-1.22019	-3.02450	-0.16943
C	-0.65249	-2.45932	0.98089
Pt	-1.52464	-0.91854	-0.21186
Cl	-3.55260	-1.26527	0.88435
Cl	0.55176	-0.67028	-1.40945
H	0.41340	-2.26324	1.03242
H	-1.19509	-2.46404	1.92090
H	-2.20525	-3.47755	-0.12441
H	-0.59332	-3.27565	-1.01957
Pt	2.34374	0.17397	0.09852
Cl	3.82610	-0.00797	-1.68928
Cl	0.84942	0.36737	1.96789
H	4.79860	-0.33694	0.95022
C	3.98769	0.19427	1.43791
C	3.68261	1.50898	1.05630
H	3.63292	-0.19170	2.38822
H	3.09010	2.14106	1.70998
H	4.25540	1.99409	0.27260
C	-2.63883	2.53266	-1.27034
O	-0.48831	2.21761	-0.19831
C	-1.82980	1.97746	-0.19334
C	-2.42138	1.00137	-1.36061
H	-3.35663	0.44897	-1.29658
H	-1.76325	0.77317	-2.19332
H	-0.07798	1.73758	0.54240
C	-2.62232	2.05190	1.10332
H	-2.47904	1.19857	1.77029
C	-4.07777	2.23173	0.64305
H	-4.54060	1.25119	0.50684
H	-4.67771	2.77604	1.37460
C	-3.97446	2.97623	-0.70381
H	-4.81506	2.76530	-1.37045
H	-3.93476	4.05947	-0.54561
H	-2.25546	2.95285	1.61011
H	-2.14697	3.09698	-2.05489

Frequencies

14.1999	37.8597	49.8787
63.7793	75.8017	91.7218
93.0926	103.2254	104.1376
112.3150	121.9928	147.8602
157.7615	169.7678	173.1685
179.9131	184.2203	202.1569
213.6465	238.9002	268.7777
276.4455	287.5229	300.5991
338.2751	343.9166	355.6391
388.1225	392.9039	409.1460
443.1523	500.7035	512.8275
553.5350	588.1055	642.3610
652.0215	733.8710	774.6988
791.2711	830.9361	833.8208
844.7469	879.9197	894.9935
918.2523	948.0375	959.9919
1021.9869	1028.0299	1029.8397
1038.7053	1082.9692	1084.4174
1086.4897	1087.0776	1089.6363
1110.1251	1140.9360	1183.0774
1218.1706	1223.9829	1229.2213
1235.0570	1260.1824	1284.5002
1285.5452	1292.1088	1331.6291
1340.7039	1360.0012	1403.8625
1429.6433	1467.6612	1471.7756
1490.8179	1503.5628	1526.9123
1537.5034	1570.9875	1573.9237
3077.0122	3080.3249	3116.4683
3133.3901	3135.9033	3144.5370
3168.5774	3183.4763	3185.8364
3192.5117	3198.3523	3227.3755
3250.0821	3278.8890	3290.1377
3293.4532	3306.2720	3699.5711

Statistical Thermodynamic Analysis

Temperature=298.15 K	Pressure=1 atm
Zero-point correction= 0.271519	Electronic Energy = -2545.69413625
Internal Energy (E)= -2545.39958725	Enthalpy (H)= -2545.39864325
Gibbs Free Energy (G)=-2545.47816425	Gibbs Free Energy of Solvation=-2545.53345763

St.Pt.	General Structure	Ball & Stick model
$1DTS_1$	 $1DTS_1$	

Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.95185	-2.95982	0.14909
C	-0.50600	-2.21526	1.23188
Pt	-1.53977	-0.88682	-0.17267
Cl	-3.53363	-1.36576	0.95057
Cl	0.52499	-0.53849	-1.38978
H	0.52163	-1.87170	1.28323
H	-1.08743	-2.16627	2.14675
H	-1.88582	-3.50920	0.20669
H	-0.27301	-3.20803	-0.66110
Pt	2.38560	0.21397	0.06868
Cl	3.84894	-0.37904	-1.64214
Cl	0.91704	0.84325	1.86699
H	4.73371	-0.53164	1.04640
C	4.00282	0.16446	1.44483
C	3.89401	1.45299	0.90421
H	3.58470	-0.05110	2.42312
H	3.39116	2.23680	1.46165
H	4.53869	1.75337	0.08469
C	-2.84538	2.22230	-1.36841
O	-0.66925	2.23171	-0.37083
C	-1.95962	1.94836	-0.26653
C	-2.58131	0.67721	-1.42375
H	-3.53309	0.15102	-1.37239
H	-1.97688	0.48557	-2.30682
H	-0.17309	1.87049	0.39535
C	-2.71710	1.99688	1.04604
H	-2.46394	1.19858	1.74603
C	-4.19532	2.01291	0.62206
H	-4.57626	0.99063	0.60407
H	-4.81262	2.58559	1.31609
C	-4.19692	2.61617	-0.79782
H	-5.03125	2.26075	-1.40804
H	-4.24882	3.70955	-0.75887
H	-2.41942	2.95502	1.49244
H	-2.44424	2.75319	-2.22632

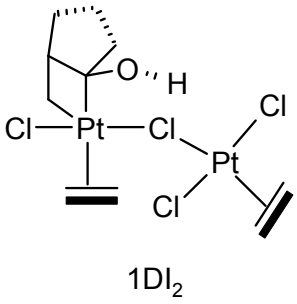
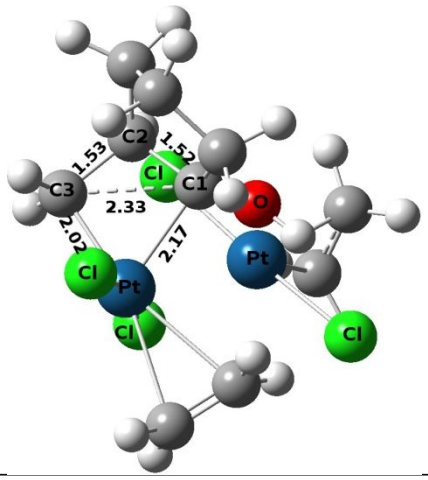
Frequencies

-192.3843	22.3346	38.6039
52.9152	69.7467	77.5234
93.4949	102.6346	109.4501
120.0926	130.6907	144.1220
146.4252	162.4307	165.9614
178.4067	193.4434	201.8476
211.9803	240.7249	246.8615
267.0421	282.5430	295.2592
323.6542	332.6721	338.1070
344.2120	388.1438	407.4027
422.8987	453.3485	468.8454
513.7866	585.9258	653.7244
719.8592	728.0540	765.5684
781.6452	792.3507	826.8587
844.3864	845.2722	895.8410
907.9167	945.6876	960.2650
1025.0802	1040.3713	1042.8909
1045.8774	1063.3802	1073.0504
1079.3049	1083.6530	1095.3272
1127.0525	1149.1674	1190.4358
1222.7285	1224.1981	1233.0396
1234.3408	1262.4974	1286.5381
1310.6304	1312.9466	1335.7087
1343.2254	1361.5325	1410.6253
1442.2624	1465.5552	1471.3918
1483.3493	1501.6275	1528.9749
1575.0962	1577.9906	1588.9065
3071.2956	3085.9394	3121.1816
3123.1978	3140.4048	3157.1723
3175.8342	3178.3330	3187.5135
3190.1386	3192.0191	3197.6871
3237.7627	3274.6543	3284.3174
3295.4718	3299.2427	3509.8121

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm

Zero-point correction= 0.270445	Electronic Energy = -2545.69303228
Internal Energy (E)= -2545.40008728	Enthalpy (H)= -2545.39914228
Gibbs Free Energy (G)=-2545.47679528	Gibbs Free Energy of Solvation=-2545.53076601

St.Pt.	General Structure	Ball & Stick model
$1DI_2$	 $1DI_2$	

Cartesian co-ordinate

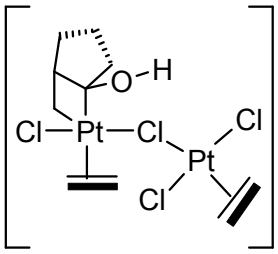
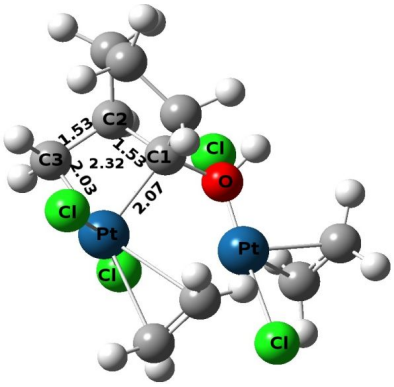
Atoms	X	Y	Z
C	-2.05531	-2.96767	-0.18282
C	-1.62418	-2.54022	1.01970
Pt	-1.87122	-0.41971	-0.46476
Cl	-4.13746	-0.30393	0.09970
Cl	0.29256	-0.79747	-1.45320
H	-0.56090	-2.51331	1.25117
H	-2.33543	-2.28727	1.80212
H	-3.11599	-3.06596	-0.39712
H	-1.34776	-3.28661	-0.94350
Pt	2.30334	-0.03946	-0.00777
Cl	2.52302	1.82902	-1.40535
Cl	1.99509	-1.83644	1.52967
H	4.77296	0.12654	-0.92040
C	4.37850	-0.28933	0.00133
C	3.99594	0.57027	1.05761
H	4.58737	-1.33569	0.20235
H	3.92894	0.18091	2.06851
H	4.10780	1.64346	0.94150
C	-1.09096	2.15888	-0.05272
O	0.12033	0.59500	1.33875
C	-1.09587	1.02606	0.96327
C	-1.86191	1.47489	-1.19363
H	-2.89321	1.81389	-1.29910
H	-1.32404	1.46169	-2.14125
H	0.11042	-0.15452	1.96125
C	-2.11212	1.33151	2.06161
H	-2.74331	0.48728	2.33987
C	-2.88325	2.54905	1.52905
H	-3.73386	2.21046	0.93295
H	-3.26611	3.17015	2.34119
C	-1.85750	3.28603	0.64968
H	-2.32003	3.97070	-0.06560
H	-1.16729	3.86436	1.27341
H	-1.50393	1.61796	2.92958
H	-0.06783	2.40461	-0.35221

Frequencies

32.7419	37.2026	48.0353
62.1567	69.2983	85.3025
88.1205	102.3930	108.6207
123.9936	133.8866	141.9075
150.6144	159.3043	162.8473
178.1113	187.2464	198.8159
206.1177	229.5601	239.4274
264.5817	282.5712	295.6897
301.9252	302.4466	329.5451
332.8456	365.6470	429.6822
436.3821	449.6718	524.8973
538.6821	552.8057	584.0474
638.2010	658.4234	805.4758
809.4653	842.0289	847.7711
849.2446	858.9552	875.1430
922.9609	954.0366	1008.1626
1009.1768	1032.6420	1042.2860
1045.8363	1071.6648	1074.5991
1087.5855	1090.8468	1099.8684
1116.3306	1162.1575	1186.7475
1199.7996	1231.0309	1246.2646
1248.3375	1257.0268	1280.2391
1301.0242	1313.7180	1331.8596
1352.8404	1368.1799	1378.8927
1412.1874	1470.6840	1471.0922
1472.6631	1478.6987	1499.1482
1521.0693	1560.7209	1672.4835
3078.0012	3085.7822	3114.5784
3122.2040	3133.1719	3147.8507
3153.9866	3169.4905	3170.4496
3178.9864	3180.3268	3188.6415
3209.5912	3252.3059	3273.2305
3278.3353	3294.6916	3724.3033

Statistical Thermodynamic Analysis

Temperature=298.15 K	Pressure=1 atm
Zero-point correction= 0.270306	Electronic Energy = -2545.69496250
Internal Energy (E)= -2545.4012175	Enthalpy (H)= -2545.4002725
Gibbs Free Energy (G)=-2545.4799805	Gibbs Free Energy of Solvation=-2545.5345693

St.Pt.	General Structure	Ball & Stick model
$1DTS_2$	 $1DTS_2$	

Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.26360	-2.95380	0.24144
C	-1.22798	-2.28490	1.41054
Pt	-1.81701	-0.52526	-0.42212
Cl	-4.02104	-0.73929	0.32359
Cl	0.26550	-0.48630	-1.61673
H	-0.28511	-1.90475	1.79429
H	-2.12592	-2.16109	2.00986
H	-2.18770	-3.39906	-0.12145
H	-0.34799	-3.12316	-0.31932
Pt	2.25837	0.03506	0.00865
Cl	2.29134	2.31511	-0.60728
Cl	2.20770	-2.20722	0.73419
H	4.64396	0.65817	-0.91140
C	4.32852	-0.07661	-0.17692
C	3.98648	0.34067	1.13440
H	4.60041	-1.11112	-0.36162
H	4.00828	-0.37972	1.94597
H	4.06060	1.39166	1.39523
C	-1.38679	2.10837	-0.34912
O	0.04034	0.68417	1.20655
C	-1.22123	1.06853	0.77134
C	-2.20444	1.25178	-1.32955
H	-3.27898	1.43281	-1.30419
H	-1.80761	1.21293	-2.34281
H	0.37705	1.34740	1.82847
C	-2.17803	1.44212	1.90321
H	-2.69529	0.58887	2.34201
C	-3.09271	2.52012	1.31224
H	-3.94412	2.04826	0.81377
H	-3.48592	3.18926	2.08007
C	-2.18983	3.24184	0.29680
H	-2.74904	3.82050	-0.44301
H	-1.50866	3.92754	0.81398
H	-1.54614	1.88558	2.68744
H	-0.41858	2.39046	-0.76959

Frequencies

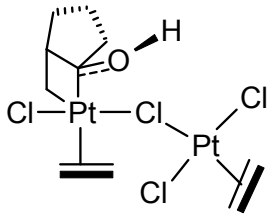
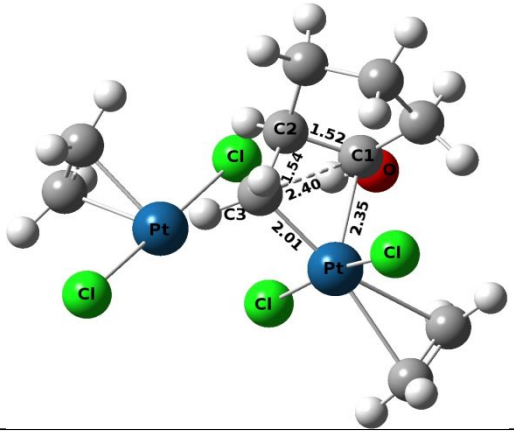
-358.7387	35.8009	48.9132
67.3340	69.0321	79.6023
83.2518	97.6036	115.2278
120.6326	134.8289	145.6047
148.7588	161.4644	169.0473
183.8466	189.9204	192.1121
200.5220	212.4404	243.3884
252.5174	287.2336	296.3569
308.6857	317.7946	320.3881
322.8485	337.0599	375.4164
440.2786	441.1816	449.1314
547.4628	558.1195	579.3145
637.5640	660.1935	811.6389
812.5030	834.7584	842.2162
847.1177	856.0994	881.1574
924.4432	953.5784	1001.6233
1004.8996	1035.5529	1039.2736
1053.9742	1065.7764	1067.1403
1087.8502	1090.9592	1096.6964
1140.2663	1147.5820	1177.2783
1197.2058	1227.9593	1236.5550
1245.8264	1249.2821	1249.9413
1280.7832	1293.2715	1330.6462
1337.3780	1366.2242	1370.2114
1374.6231	1462.3549	1467.0857
1474.5588	1478.4078	1501.1219
1521.5714	1553.1226	1668.9401
3040.7640	3076.3379	3114.5382
3127.2861	3139.9303	3151.2732
3162.6024	3165.8032	3171.7388
3172.2119	3178.2303	3179.4694
3214.6518	3263.8666	3269.7229
3285.5785	3290.1856	3821.3738

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm

Zero-point correction= 0.269543 Electronic Energy = -2545.68239038

Internal Energy (E)= -2545.39010338	Enthalpy (H)= -2545.38915938
Gibbs Free Energy (G)=-2545.46650538	Gibbs Free Energy of Solvation=-2545.52561891

St.Pt.	General Structure	Ball & Stick model
$1DI_3$	 $1DI_3$	

Cartesian co-ordinate

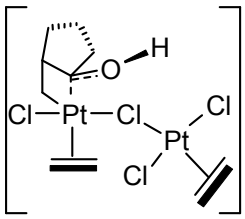
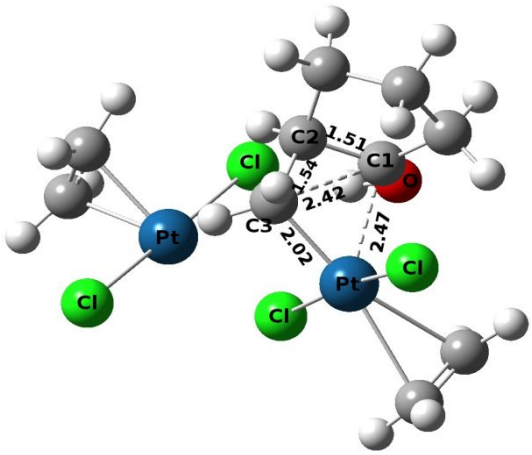
Atoms	X	Y	Z
C	-0.71505	-2.80373	0.62254
C	-0.56611	-1.88451	1.59942
Pt	-1.68607	-0.68646	-0.32310
Cl	-3.77477	-1.38194	0.43860
Cl	0.40306	-0.25838	-1.53444
H	0.37116	-1.34425	1.71104
H	-1.33733	-1.72979	2.34873
H	-1.61515	-3.40884	0.56022
H	0.10071	-3.00878	-0.06605
Pt	2.37387	0.13714	-0.08953
Cl	1.96444	2.47890	-0.31794
Cl	2.76048	-2.15465	0.14853
H	4.65487	1.48247	0.08513
C	4.37359	0.52904	0.52151
C	3.54674	0.48938	1.65070
H	4.96028	-0.34180	0.24734
H	3.49492	-0.41213	2.25274
H	3.18564	1.41254	2.09319
C	-2.10519	2.01519	-0.60360
O	-0.47102	1.49403	1.21982
C	-1.67375	1.38110	0.71360
C	-2.50510	0.78421	-1.44325
H	-3.58472	0.64549	-1.50869
H	-2.04347	0.77491	-2.43120
H	0.20305	1.81097	0.56793
C	-2.80678	1.45525	1.72174
H	-3.02515	0.50848	2.21439
C	-3.97978	2.04607	0.92653
H	-4.57376	1.23764	0.49328
H	-4.63658	2.64626	1.55871
C	-3.30236	2.87862	-0.17761
H	-3.96254	3.09164	-1.02213
H	-2.94780	3.83273	0.22797
H	-2.44763	2.16267	2.47923
H	-1.27833	2.56401	-1.06537

Frequencies

27.2805	40.8075	46.5614
58.6234	72.0327	72.5835
95.2827	109.5124	115.5668
132.0479	138.3835	145.1323
154.1445	162.8365	168.3403
169.0544	176.3071	182.0627
196.7581	225.0324	227.6343
271.7922	276.0456	289.1718
294.3053	299.6424	335.5579
336.7987	356.6818	401.7329
451.9410	463.7767	506.9022
511.6666	571.9206	622.9500
665.4347	774.0454	777.6626
805.3250	839.4318	840.2883
841.2820	855.4730	875.0018
916.8485	952.9365	1008.5420
1021.2028	1028.7354	1037.6732
1046.0114	1059.6756	1075.7923
1079.2945	1082.2341	1098.4625
1144.0163	1176.8958	1181.8724
1201.4132	1234.5719	1243.2631
1248.9255	1288.4025	1288.8853
1310.3504	1321.6165	1327.8337
1357.6750	1368.0173	1392.3396
1460.8659	1464.5711	1468.2703
1472.8634	1499.4367	1509.9330
1521.4372	1575.7834	1662.7329
3086.2317	3088.2219	3117.5803
3120.7411	3123.0082	3147.8659
3169.0347	3174.3664	3175.0553
3183.0280	3185.0577	3187.7623
3198.6349	3265.4715	3282.6416
3282.8952	3297.4917	3363.2400

Statistical Thermodynamic Analysis

Temperature=298.15 K	Pressure=1 atm
Zero-point correction= 0.270096	Electronic Energy = -2545.70540644
Internal Energy (E)= -2545.41185844	Enthalpy (H)= -2545.41091344
Gibbs Free Energy (G)=-2545.49080944	Gibbs Free Energy of Solvation=-2545.54334678

St.Pt.	General Structure	Ball & Stick model
$1DTS_3$	 $1DTS_3$	

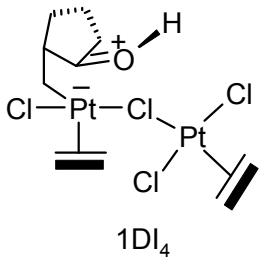
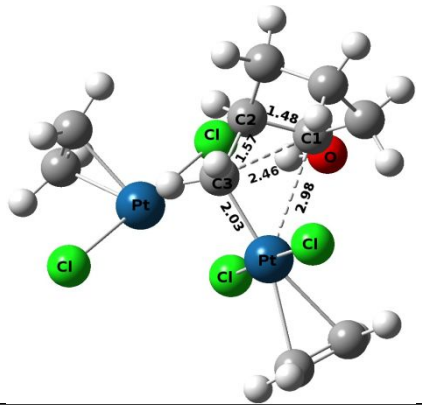
Cartesian co-ordinate

Atoms	X	Y	Z
C	-2.80132	-2.50136	1.18695
C	-2.95052	-1.40513	1.96348
Pt	-1.78206	-0.62958	-0.09090
Cl	-3.83541	-0.30071	-1.14493
Cl	0.32965	-1.25846	0.98807
H	-2.22237	-1.15031	2.72861
H	-3.85171	-0.80192	1.90471
H	-3.57429	-2.79457	0.48285
H	-1.94781	-3.16306	1.30435
Pt	2.33478	-0.15467	0.04795
Cl	2.44793	-1.71851	-1.67476
Cl	2.16763	1.49685	1.77550
H	4.84934	-0.56156	-0.67247
C	4.38199	0.32763	-0.26175
C	3.59016	1.14284	-1.07972
H	4.76423	0.70687	0.68080
H	3.36203	2.15916	-0.77362
H	3.44636	0.88706	-2.12461
C	-0.58837	1.87305	-0.63419
O	-0.90717	1.56058	1.82317
C	-1.39704	1.70934	0.63807
C	-0.84869	0.56765	-1.42469
H	-1.50666	0.74007	-2.27833
H	0.07528	0.07788	-1.74427
C	-2.73111	2.40610	0.52402
H	-3.57638	1.75778	0.75806
C	-2.73806	2.96827	-0.90580
H	-3.22760	2.25629	-1.57324
H	-3.27422	3.91681	-0.96573
C	-1.24735	3.11184	-1.26416
H	-1.06803	3.14947	-2.34132
H	-0.83213	4.02196	-0.81670
H	-2.69350	3.20480	1.27594
H	0.47274	2.00523	-0.40411
H	0.06482	1.34828	1.82531

Frequencies

-67.8656	35.7369	38.4701
52.7568	70.3917	76.4108
82.1049	88.7704	94.7636
114.8626	119.0450	129.9149
147.2559	149.3793	161.7668
167.9194	174.3566	190.0630
195.6389	217.5723	230.0964
259.9620	274.2177	293.8592
303.9526	316.2292	335.1103
342.3888	358.5795	400.9604
459.3745	477.0248	496.5772
508.4639	578.8391	623.2204
661.5333	773.1055	793.0392
812.3810	825.3895	835.4325
838.5229	859.2453	870.5036
920.0310	956.5347	1008.7668
1021.0963	1025.3383	1030.5390
1048.9973	1066.4663	1072.3710
1074.8763	1078.2270	1100.3456
1156.0989	1176.8185	1190.6824
1209.7011	1231.8658	1232.3775
1250.1379	1288.0467	1290.0923
1305.1985	1318.9714	1337.6496
1365.8995	1366.7616	1428.5834
1460.7251	1465.9493	1468.0380
1488.6983	1500.9048	1523.6828
1573.0477	1575.5526	1661.0531
3077.6375	3080.9375	3102.6668
3120.5733	3127.7562	3142.6430
3167.9834	3171.2853	3177.4391
3177.7884	3178.5899	3180.2896
3187.2126	3260.4460	3277.1901
3280.0350	3294.9491	3297.1111

Statistical Thermodynamic Analysis	
Temperature=298.15 K	Pressure=1 atm
Zero-point correction= 0.269753	Electronic Energy = -2545.70506011
Internal Energy (E)= -2545.41249811	Enthalpy (H)= -2545.41155311
Gibbs Free Energy (G)=-2545.48994011	Gibbs Free Energy of Solvation=-2545.5416783

St.Pt.	General Structure	Ball & Stick model
$1DI_4$	 $1DI_4$	

Cartesian co-ordinate

Atoms	X	Y	Z
C	0.05949	-3.28163	0.19417
C	-0.17807	-2.72482	-1.01929
Pt	1.37278	-1.26941	0.14744
Cl	3.00893	-2.16894	-1.24458
Cl	-0.27920	-0.18935	1.69441
H	-1.06756	-2.12327	-1.18111
H	0.43559	-2.96814	-1.87988
H	0.86156	-4.00022	0.33267
H	-0.63240	-3.12247	1.01705
Pt	-2.01249	0.39416	-0.02854
Cl	-3.16896	-1.53491	0.61088
Cl	-0.90249	2.39501	-0.72952
H	-3.35870	-0.61278	-2.07813
C	-3.08068	0.41364	-1.85933
C	-3.79571	1.14112	-0.89603
H	-2.46175	0.93317	-2.58382
H	-3.72959	2.22414	-0.87437
H	-4.62170	0.67485	-0.36890
C	2.38078	1.53259	-0.07245
O	1.03706	2.43130	1.77663
C	1.78089	2.59209	0.77183
C	2.69030	0.19620	0.62034
H	1.60854	1.39885	-0.85313
H	3.68362	-0.12555	0.30141
H	2.71941	0.31881	1.71152
C	3.54733	2.29111	-0.74424
C	2.99350	3.71105	-0.93302
C	2.21940	3.95620	0.37211
H	0.69378	1.48190	1.86700
H	3.84379	1.80410	-1.67403
H	2.88624	4.31066	1.17168
H	1.36708	4.63856	0.32667
H	3.76622	4.46070	-1.10570
H	2.29863	3.73281	-1.77793
H	4.41430	2.29617	-0.07305

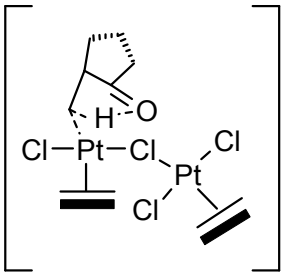
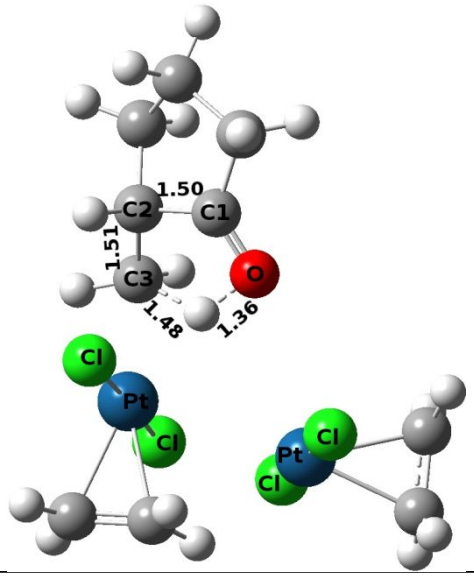
Frequencies

17.5183	37.7144	48.5161
52.8436	62.5449	68.8070
73.1864	84.7506	105.6271
122.3969	125.3039	127.1672
148.5519	158.3970	168.1529
172.8117	180.6389	201.8183
208.0486	213.5039	220.1704
223.6114	235.9264	288.5213
296.5464	323.0921	330.8407
337.2835	347.5168	410.1440
447.0843	514.3956	522.6044
538.0067	566.4261	607.9706
661.6145	724.8851	782.6627
785.9336	833.5361	837.9928
861.6684	894.3245	903.3691
939.0015	967.9864	1017.2791
1023.1994	1026.2123	1029.2810
1037.2655	1075.9537	1080.2946
1084.5497	1091.2240	1121.7217
1160.2342	1189.0444	1200.3950
1214.7505	1229.0421	1238.2836
1246.8189	1277.0079	1283.5676
1315.4174	1319.0171	1336.4344
1351.6992	1360.0583	1431.1307
1464.1529	1466.7923	1474.5105
1483.9367	1505.9483	1517.1865
1570.2703	1649.5683	1705.8727
2963.1536	2999.3629	3059.0837
3060.1542	3081.2471	3102.3863
3150.1501	3150.4734	3165.7436
3171.0129	3177.8758	3181.4180
3187.3171	3188.7794	3268.0028
3279.7652	3292.1593	3295.6777

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm

Zero-point correction= 0.269127	Electronic Energy = -2545.70389177
Internal Energy (E)= -2545.41104877	Enthalpy (H)= -2545.41010377
Gibbs Free Energy (G)=-2545.49175577	Gibbs Free Energy of Solvation=-2545.54640911

St.Pt.	General Structure	Ball & Stick model
$1DTS_4$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	2.34110	-2.46102	-0.84544
C	3.07286	-1.56929	-1.58180
Pt	1.81726	-0.34546	-0.07041
Cl	3.58284	-0.45517	1.43417
Cl	-0.01266	-0.23714	-1.66749
H	2.71606	-1.21626	-2.54491
H	4.08625	-1.30811	-1.29411
H	2.76162	-2.92118	0.04393
H	1.38294	-2.83243	-1.19592
Pt	-1.88282	-0.71116	-0.08591
Cl	-0.61501	-2.43677	0.91735
Cl	-3.11178	1.06937	-1.01568
H	-3.48293	-2.58271	0.88650
C	-3.65158	-1.51827	0.75757
C	-3.08717	-0.60441	1.65843
H	-4.47411	-1.21230	0.11885
H	-3.47711	0.40673	1.71677
H	-2.48135	-0.96169	2.48527
C	0.05810	2.27784	0.56930
O	1.94203	2.76609	-0.80401
C	0.87970	3.15041	-0.34903
C	0.94507	1.20820	1.16556
H	1.68690	1.61157	1.85856
H	0.37018	0.43173	1.68468
C	0.25563	4.52078	-0.46503
H	1.00147	5.24866	-0.12690
C	-0.96236	4.44244	0.47572
H	-1.17184	5.39280	0.96869
H	-1.85121	4.15030	-0.09154
C	-0.61722	3.31672	1.47444
H	0.08642	3.67282	2.23685
H	-1.49960	2.91821	1.97911
H	0.01907	4.75610	-1.50551
H	-0.73086	1.84168	-0.06139

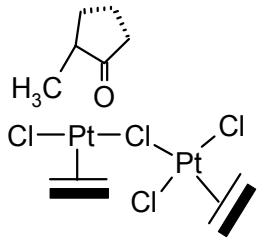
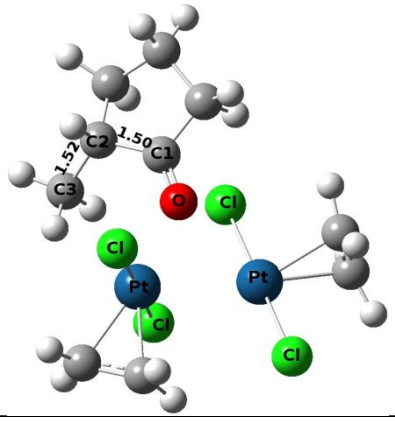
Frequencies

-793.7604	28.3556	37.0034
42.1350	49.6506	63.6878
69.4230	82.4842	88.3510
94.3940	105.8807	123.9774
134.7343	143.6240	154.7607
160.7516	163.5006	178.5452
180.9965	197.8958	218.7525
239.0954	253.9025	266.0449
274.9795	314.6099	321.0270
329.4854	349.2995	384.4322
407.2274	453.3989	513.3408
564.7049	577.6558	595.4301
606.9996	616.3973	741.0109
781.2614	805.9799	840.2968
846.1301	860.8634	903.9238
926.2817	964.2152	969.8427
1019.8008	1020.8517	1037.9845
1052.6183	1060.2277	1065.7803
1076.4447	1080.8639	1093.2082
1156.6118	1181.9053	1192.4830
1202.5929	1214.0977	1234.2763
1237.4830	1238.6268	1285.2551
1307.1518	1317.6398	1324.9510
1346.7292	1358.4419	1396.3039
1415.0050	1456.6544	1467.6920
1478.0910	1479.2989	1504.2802
1520.6219	1572.2076	1631.3316
1872.1365	3073.8093	3085.3853
3094.4260	3097.1681	3106.1375
3148.6662	3159.3575	3168.6368
3169.4083	3176.2872	3181.1854
3184.1145	3193.6326	3273.6242
3283.0866	3289.1760	3300.3617

H	1.89311	1.32598	-0.05458	

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.264064 Electronic Energy = -2545.67887661
Internal Energy (E)= -2545.39125461 Enthalpy (H)= -2545.39031061
Gibbs Free Energy (G)=-2545.47145361 Gibbs Free Energy of Solvation=-2545.52868976

St.Pt.	General Structure	Ball & Stick model
$1DI_5$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	3.36873	-0.66258	-1.65596
C	3.09047	0.70211	-1.50220
Pt	1.90964	-0.42649	-0.13060
Cl	3.58798	-0.25009	1.44373
Cl	0.05200	-0.60909	-1.71233
H	2.39481	1.21506	-2.15763
H	3.73966	1.32917	-0.89961
H	4.24268	-1.10073	-1.18452
H	2.90412	-1.22908	-2.45795
Pt	-1.64803	-0.83586	0.06013
Cl	0.22287	-1.09391	1.59149
Cl	-3.37686	-0.52841	-1.44667
H	-2.38028	-2.42363	2.05623
C	-2.97735	-1.76507	1.43257
C	-2.97961	-0.38251	1.65989
H	-3.76948	-2.22019	0.84654
H	-3.77904	0.22917	1.25379
H	-2.38676	0.04397	2.46442
C	-0.34377	2.59745	0.92918
O	0.98352	2.64073	-1.10383
C	-0.10075	2.70549	-0.56921
C	0.85977	2.98324	1.77101
H	1.12453	4.03167	1.60258
H	0.65460	2.84414	2.83520
C	-1.42623	2.95574	-1.27690
H	-1.33332	3.89108	-1.83961
C	-2.46441	3.04502	-0.14802
H	-3.25115	3.77433	-0.35018
H	-2.94722	2.06968	-0.02471
C	-1.64336	3.38849	1.11093
H	-1.41341	4.46162	1.13408
H	-2.16426	3.14524	2.04110
H	-1.62066	2.15628	-1.99948
H	-0.57688	1.53224	1.09745
H	1.72572	2.36898	1.50606

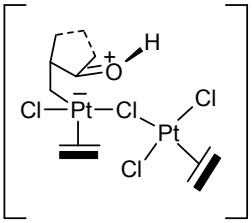
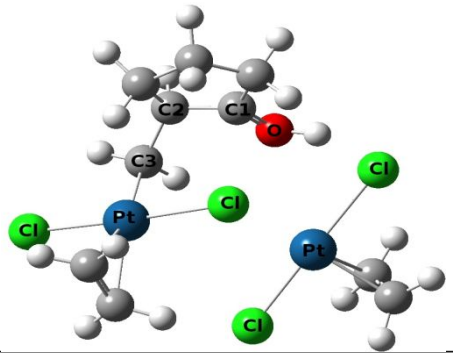
Frequencies

27.4072	32.9149	37.0080
38.1777	50.7678	60.6081
70.9746	81.8184	88.1960
89.5255	93.2913	117.6007
123.4300	130.4140	146.5982
156.0459	164.8349	187.7051
196.6297	198.3021	202.0695
231.3722	256.2310	259.7065
272.2284	279.1214	342.8784
353.3500	355.6382	402.4951
404.3849	457.7823	503.8406
509.6969	559.7590	577.4180
601.6924	724.3190	770.5040
773.7596	824.1151	827.1831
835.5759	868.8783	912.0299
952.0005	963.5444	994.5833
1018.6142	1032.5407	1039.4511
1071.7338	1073.2528	1077.7904
1083.1666	1096.2677	1167.6362
1188.9664	1192.3781	1210.9189
1220.4638	1226.3711	1243.6191
1287.0880	1291.0537	1303.8003
1307.1962	1326.6443	1347.1080
1381.5164	1426.0918	1452.7119
1467.9238	1477.7642	1501.4865
1505.3832	1508.4635	1517.5052
1572.8711	1577.1663	1880.6480
3032.4037	3067.3644	3071.5037
3083.9342	3100.5010	3127.1436
3134.5982	3152.3049	3156.3748
3159.4074	3169.5297	3177.8803
3186.8874	3199.9951	3268.0164
3276.4761	3290.9576	3305.0673

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm

Zero-point correction= 0.269153	Electronic Energy = -2545.73792317
Internal Energy (E)= -2545.44428817	Enthalpy (H)= -2545.44334417
Gibbs Free Energy (G)=-2545.52758717	Gibbs Free Energy of Solvation=-2545.58349943

St.Pt.	General Structure	Ball & Stick model
$1DTS_{4a}$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.93372	-2.44142	1.26768
C	-2.69305	-1.54735	1.95329
Pt	-1.97696	-0.42701	-0.01529
Cl	-3.94037	-1.11628	-1.05840
Cl	0.05985	0.40151	1.15305
H	-2.26411	-0.95100	2.75355
H	-3.76841	-1.50224	1.81559
H	-2.38510	-3.12571	0.55602
H	-0.87985	-2.57835	1.48773
Pt	2.12661	-0.44747	0.07231
Cl	1.17713	-2.53673	-0.26547
Cl	3.16095	1.73660	0.33457
H	3.95868	-2.36207	0.16346
C	4.05194	-1.32600	-0.14570
C	3.58482	-0.92597	-1.40401
H	4.75047	-0.70142	0.40263
H	3.92500	0.00996	-1.83579
H	3.13048	-1.65049	-2.07194
C	-1.46984	2.40599	-0.99306
O	0.88071	2.22271	-1.37676
C	-0.05796	2.66171	-0.64709
C	-1.77264	0.97593	-1.48375
H	-2.70296	1.00184	-2.05333
H	-0.97542	0.65164	-2.16380
C	0.12584	3.58859	0.50265
H	0.88930	3.20080	1.18315
C	-1.27945	3.74434	1.11524
H	-1.28516	3.34912	2.13196
H	-1.55419	4.79873	1.17331
C	-2.26425	2.94309	0.21687
H	-2.67840	2.09186	0.76150
H	-3.10486	3.55670	-0.11063
H	0.52358	4.52461	0.08561
H	-1.61103	3.08399	-1.85800
H	1.78519	2.30953	-0.93096

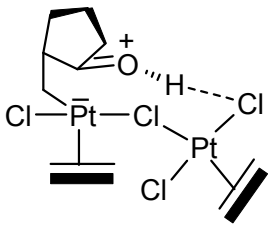
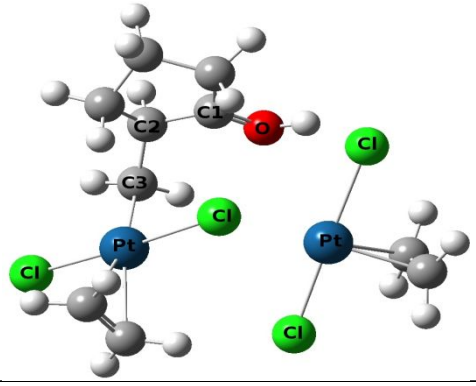
Frequencies

-117.2928	25.3793	33.3701
47.9983	60.2084	74.2542
82.5586	93.8506	95.6552
105.8186	117.7096	125.2675
145.5959	152.2678	158.2237
163.7517	173.8007	182.7117
190.6582	207.9768	213.6151
226.8244	261.2836	272.5029
289.0656	330.3291	346.2228
361.4698	371.1003	400.2225
464.8137	506.6079	534.0063
546.3871	580.6832	618.6090
652.9657	737.4174	757.3497
771.6109	801.0197	827.1176
832.6825	901.2778	907.4793
935.5554	972.3224	1008.9887
1017.5964	1023.7722	1031.9825
1053.8064	1067.0639	1072.5541
1078.9246	1082.8637	1116.1225
1166.7081	1179.2558	1222.5236
1227.2660	1232.5872	1244.0485
1255.6039	1279.6172	1287.9360
1296.7786	1323.3357	1344.1290
1349.9120	1357.7641	1435.8708
1463.7113	1468.0273	1471.6731
1480.8733	1502.1416	1526.7585
1574.0751	1647.3168	1671.7736
2966.2470	2984.5028	3070.3679
3079.1434	3112.4061	3118.9483
3143.7581	3157.0516	3158.8572
3172.0999	3173.4587	3176.9582
3187.7753	3190.3456	3267.4769
3274.4213	3291.0689	3293.1371

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.268913 Electronic Energy = -2545.70148089
Internal Energy (E)= -2545.40961489 Enthalpy (H)= -2545.40866989

Gibbs Free Energy (G)=-2545.48810589 Gibbs Free Energy of Solvation=-2545.54412782

St.Pt.	General Structure	Ball & Stick model
$1DI_{5a}$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.90517	-2.57993	1.10027
C	-2.60095	-1.73823	1.90975
Pt	-2.01268	-0.48810	-0.01976
Cl	-4.03746	-1.09762	-0.98882
Cl	0.07115	0.25826	1.13549
H	-2.10513	-1.20391	2.71498
H	-3.68363	-1.68326	1.86315
H	-2.41974	-3.21169	0.38293
H	-0.83769	-2.73266	1.22461
Pt	2.19293	-0.41342	0.06319
Cl	1.41060	-2.57010	-0.27707
Cl	3.06091	1.84270	0.36290
H	4.17416	-2.17597	0.14764
C	4.18429	-1.13471	-0.15777
C	3.68646	-0.76866	-1.41395
H	4.83073	-0.45836	0.39292
H	3.95011	0.19257	-1.84389
H	3.28873	-1.52407	-2.08369
C	-1.58028	2.38819	-0.89498
O	0.77033	2.25693	-1.31191
C	-0.16792	2.68855	-0.58282
C	-1.86652	0.98048	-1.43052
H	-2.80465	1.00716	-1.98680
H	-1.07259	0.69269	-2.13076
C	-0.01053	3.60592	0.58278
H	0.36925	2.99287	1.41058
C	-1.45352	4.08051	0.84271
H	-1.61828	4.32690	1.89186
H	-1.66077	4.97720	0.24972
C	-2.31566	2.90274	0.35729
H	-2.33576	2.10253	1.10449
H	-3.34738	3.17977	0.13678
H	0.73385	4.38345	0.38863
H	-1.77400	3.11667	-1.71129
H	1.68057	2.36693	-0.87338

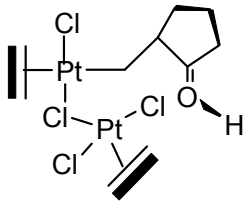
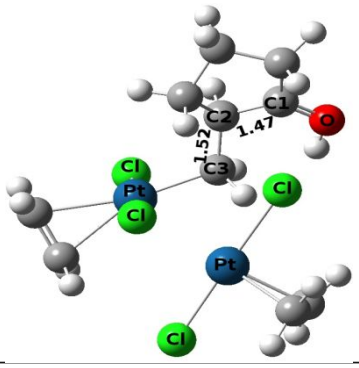
Frequencies

19.1137	39.4063	53.4183
60.6934	70.7892	83.4752
94.0404	103.6269	115.7979
119.3291	122.2955	136.6402
148.2167	150.7528	163.8484
173.2759	180.4917	196.4661
204.0977	211.4046	224.5734
238.1106	264.8683	275.4748
296.9225	331.4117	346.8146
366.5088	374.6913	398.0592
473.8562	505.9493	518.8756
556.7506	580.3540	595.2705
631.6916	718.6452	773.0326
780.5519	832.7790	834.6550
856.5943	889.1463	914.9689
936.1236	973.4312	1010.2290
1024.1186	1025.1987	1027.1652
1031.9897	1072.0273	1077.2893
1078.8568	1080.7982	1111.3846
1154.5958	1189.6144	1198.4928
1226.0137	1230.3942	1238.1656
1249.3685	1264.0400	1289.1446
1315.5810	1324.4131	1332.7355
1349.3284	1359.6549	1427.8720
1464.4486	1467.5385	1477.1796
1480.9049	1504.8676	1518.0357
1574.1943	1646.4511	1684.9311
2915.2514	2955.6051	3077.4475
3083.9908	3094.8991	3104.0327
3145.0191	3157.9606	3168.7010
3175.3579	3180.4506	3183.0469
3187.6271	3190.1222	3276.5951
3278.5261	3294.8448	3294.9356

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm

Zero-point correction= 0.269299	Electronic Energy = -2545.70485773
Internal Energy (E)= -2545.41211573	Enthalpy (H)= -2545.41117173
Gibbs Free Energy (G)=-2545.49150373	Gibbs Free Energy of Solvation=-2545.54791094

St.Pt.	General Structure	Ball & Stick model
$1DI_{6a}$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	1.88269	-3.04628	-0.37916
C	2.67380	-2.44035	-1.30995
Pt	1.74885	-0.76333	0.04119
Cl	3.61562	-0.80603	1.44535
Cl	-0.12432	-0.61771	-1.55076
H	2.29079	-2.20734	-2.29895
H	3.73858	-2.31769	-1.14016
H	2.30520	-3.41596	0.54988
H	0.84657	-3.29627	-0.59309
Pt	-2.06761	-0.30303	-0.07798
Cl	-2.22497	-2.61940	0.15576
Cl	-1.90981	2.09906	-0.25438
H	-4.59462	-1.03475	0.24401
C	-4.09837	-0.11103	0.52374
C	-3.27670	-0.07259	1.65637
H	-4.47042	0.81136	0.08907
H	-3.01868	0.88223	2.10326
H	-3.13623	-0.96504	2.25763
C	1.57134	2.22849	0.18854
O	0.34719	3.58213	1.78751
C	0.83001	3.42624	0.62005
C	1.18411	0.96421	0.95693
C	0.68965	4.45168	-0.43542
H	-0.37624	4.42049	-0.70749
C	1.56084	3.88470	-1.57344
H	1.19385	4.18714	-2.55411
H	2.58920	4.24567	-1.46888
C	1.49427	2.36324	-1.35023
H	0.54180	1.95904	-1.69904
H	2.30271	1.81139	-1.83178
H	0.91245	5.45922	-0.07481
H	2.61643	2.48867	0.46056
H	0.45155	2.74884	2.29607
H	0.09614	0.93087	1.07869
H	1.66639	0.97055	1.94219

Frequencies

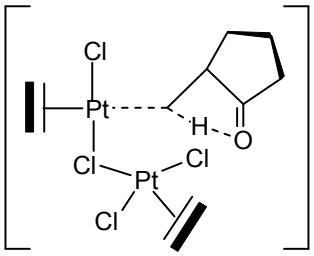
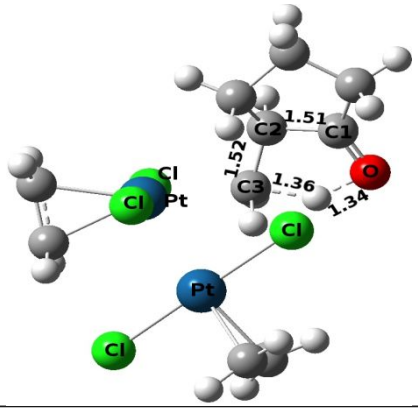
23.6962	26.9290	52.5752
57.1750	61.6105	67.4456
81.3128	84.7311	96.7828
124.8826	130.6202	132.1924
145.9952	148.3005	156.2125
165.4216	171.8090	178.2755
198.6326	205.9021	222.9058
232.9122	262.3470	274.6829
295.7665	326.7431	337.6843
343.1241	397.2779	399.0131
454.1488	500.5717	510.1677
537.6954	593.5783	606.3508
677.9148	720.5922	766.4827
781.5832	822.3429	832.3238
837.9191	864.4457	904.3849
932.4406	954.4268	1011.8122
1018.7919	1019.1813	1023.7887
1055.9630	1058.9128	1070.5425
1075.1628	1077.0517	1135.7153
1139.3255	1181.9221	1211.9596
1219.7674	1229.0295	1234.8214
1237.4356	1267.6235	1287.8835
1290.9225	1312.7131	1326.1855
1350.4842	1352.2708	1418.5974
1463.8098	1477.1044	1479.8765
1486.1250	1508.5621	1518.2673
1572.4219	1640.1865	1654.1938
2964.2360	3061.2305	3066.4162
3091.3408	3133.6098	3137.9839
3146.0536	3169.4751	3172.7425
3174.8427	3183.1559	3188.0381
3199.7969	3269.9875	3270.7373
3288.9534	3290.7949	3615.3994

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm

Zero-point correction= 0.270039 Electronic Energy = -2545.69152678

Internal Energy (E)= -2545.39773178	Enthalpy (H)= -2545.39678778
Gibbs Free Energy (G)=-2545.47850578	Gibbs Free Energy of Solvation=-2545.53963123

St.Pt.	General Structure	Ball & Stick model
$1DTS_{6a}$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	1.24356	-3.08271	-0.38693
C	2.18809	-2.61138	-1.28726
Pt	1.57807	-0.95433	0.00764
Cl	3.31401	-1.48545	1.47086
Cl	-0.15826	-0.43458	-1.62255
H	1.89359	-2.33140	-2.29402
H	3.24654	-2.75726	-1.09817
H	1.56000	-3.58760	0.52040
H	0.19259	-3.15405	-0.65627
Pt	-2.06289	-0.07086	-0.08013
Cl	-2.40684	-2.38790	0.03831
Cl	-1.70179	2.28342	-0.15380
H	-4.62408	-0.60737	0.32529
C	-4.03957	0.25700	0.62397
C	-3.16997	0.16976	1.71841
H	-4.34831	1.22833	0.25075
H	-2.80942	1.07561	2.19559
H	-3.08122	-0.76160	2.26842
C	1.97897	2.08906	0.16334
O	0.91289	3.33925	1.83529
C	1.43854	3.38453	0.72587
C	1.37056	0.99690	1.03084
C	1.48048	4.49306	-0.27382
H	0.43553	4.78101	-0.44336
C	2.09337	3.80581	-1.51363
H	1.70342	4.21715	-2.44514
H	3.17959	3.94455	-1.51528
C	1.75004	2.30836	-1.34253
H	0.70149	2.12778	-1.58918
H	2.36850	1.65423	-1.96040
H	2.01191	5.37330	0.09570
H	3.06662	2.10623	0.34023
H	0.97626	1.99657	1.87051
H	0.28117	0.87285	1.02385
H	1.95289	0.62723	1.87610

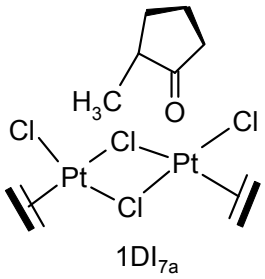
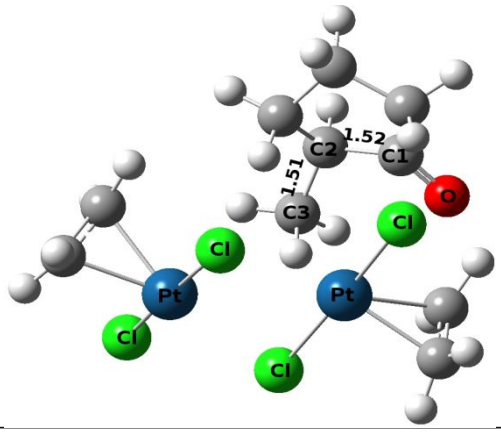
Frequencies

-1259.8304	14.0806	26.9348
32.4722	53.5467	64.2757
72.4401	81.6826	82.6795
100.1948	123.2117	128.9600
132.4672	152.7435	159.2747
166.6422	171.7530	182.2188
193.0845	198.1745	218.2020
242.7179	255.8062	263.9333
301.8965	323.1014	329.7258
335.7262	342.5690	406.6861
454.7441	471.7932	513.7405
557.5097	585.2525	644.9697
671.5963	718.0643	754.5340
776.7037	793.4018	830.0940
837.2950	842.7493	859.7002
925.0965	957.2747	961.7091
970.5841	1018.1751	1021.7107
1040.6463	1046.5545	1055.4977
1073.7630	1081.5861	1085.3703
1151.4444	1172.6194	1192.7415
1208.2482	1227.9117	1230.0160
1233.5800	1244.8297	1288.0847
1299.3449	1307.5286	1310.8124
1316.1247	1352.2799	1370.8660
1424.0805	1440.7271	1466.2316
1471.7204	1501.9609	1516.8527
1573.5369	1593.2905	1648.6235
1840.3775	3037.7079	3071.1015
3085.8142	3091.7587	3122.2434
3150.2274	3175.1642	3175.2055
3176.6903	3180.4931	3185.1707
3187.1721	3197.1252	3271.4929
3276.0304	3286.3220	3294.3422

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm

Zero-point correction= 0.264393	Electronic Energy = -2545.65876030
Internal Energy (E)= -2545.3710623	Enthalpy (H)= -2545.3701183
Gibbs Free Energy (G)=-2545.4516603	Gibbs Free Energy of Solvation=--2545.52078592

St.Pt.	General Structure	Ball & Stick model
$1DI_{7a}$	 $1DI_{7a}$	

Cartesian co-ordinate

Atoms	X	Y	Z
C	3.48897	0.04962	-1.62713
C	2.85296	1.27161	-1.36647
Pt	2.00072	-0.23985	-0.14110
Cl	3.56411	0.21890	1.49673
Cl	0.28456	-0.74381	-1.79611
H	2.07102	1.63299	-2.02802
H	3.31283	1.99462	-0.70009
H	4.44337	-0.17602	-1.16209
H	3.20680	-0.54232	-2.49261
Pt	-1.42223	-1.04629	-0.00338
Cl	0.48699	-1.37413	1.46863
Cl	-3.17631	-0.77756	-1.48551
H	-2.13814	-2.62228	2.01062
C	-2.73776	-1.95398	1.39946
C	-2.71809	-0.57297	1.63181
H	-3.54709	-2.39909	0.82914
H	-3.50102	0.07096	1.24444
H	-2.09463	-0.14127	2.40955
C	-0.60631	3.22280	0.69122
O	-2.55032	2.33590	1.85160
C	-2.05428	2.76452	0.83385
C	0.33078	2.51718	1.65604
C	-2.74683	2.85286	-0.51980
H	-3.02528	1.83094	-0.80725
C	-1.68527	3.42570	-1.46840
H	-1.78052	3.04138	-2.48562
H	-1.76181	4.51752	-1.51395
C	-0.35287	3.02859	-0.80735
H	-0.15210	1.96531	-1.00087
H	0.50043	3.60730	-1.17339
H	-3.67014	3.43300	-0.44811
H	-0.61642	4.30532	0.89768
H	0.05601	2.73350	2.69090
H	0.26758	1.43189	1.52393
H	1.37217	2.81377	1.49976

Frequencies

5.3789	22.0991	29.4019
40.0211	62.6325	63.1175
79.6455	84.1542	91.2118
93.1962	113.2529	123.4007
126.7849	141.3928	144.5896
158.1682	175.3622	184.2382
187.6569	192.6064	211.3716
227.4715	251.6117	257.8250
275.7383	278.1754	351.3334
352.6112	355.3612	401.4199
403.9531	462.9400	500.3184
508.1231	560.2997	569.0524
612.1466	725.6522	768.8571
769.4848	815.1928	831.5567
847.5748	868.7868	915.9051
951.1841	965.2164	997.1863
1020.9014	1024.3812	1036.5775
1069.3522	1073.0435	1082.0372
1083.3738	1101.7586	1162.7532
1182.5445	1191.7859	1211.9909
1216.8002	1230.8784	1247.4795
1286.0306	1287.1724	1306.4572
1317.9682	1327.0624	1349.3366
1380.0177	1416.0546	1460.3171
1462.6500	1476.5732	1493.6436
1503.7527	1504.4973	1519.4239
1569.8378	1577.6681	1884.0749
3028.1817	3063.2510	3072.8731
3085.5206	3088.5767	3125.7710
3145.0077	3147.8932	3154.0391
3167.3492	3176.4633	3183.0419
3185.0530	3186.3146	3275.5859
3276.0186	3290.6588	3292.1610

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm

Zero-point correction= 0.269181	Electronic Energy = -2545.73526445
Internal Energy (E)= -2545.44165645	Enthalpy (H)= -2545.44071245
Gibbs Free Energy (G)=-2545.52632145	Gibbs Free Energy of Solvation=-2545.58301802

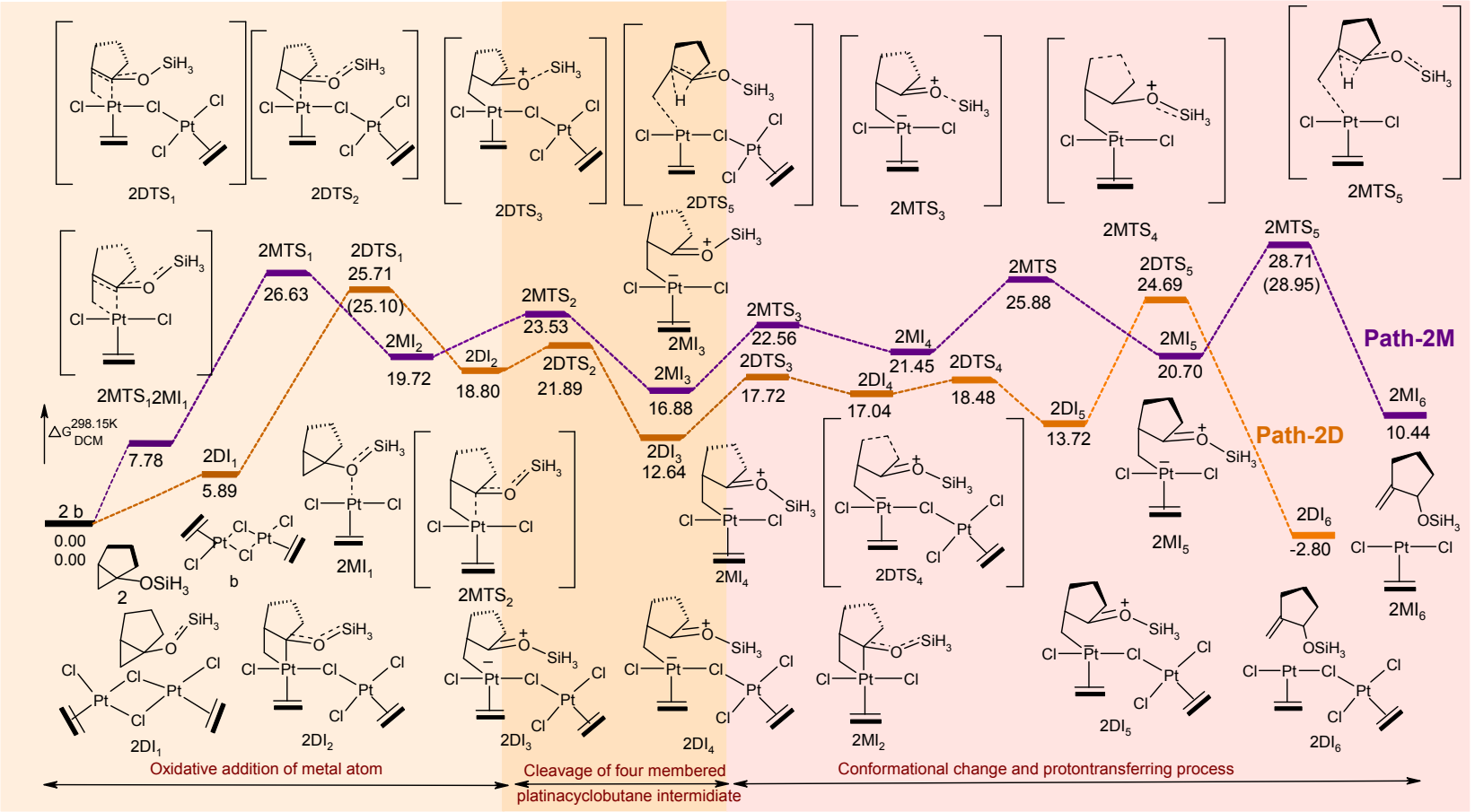
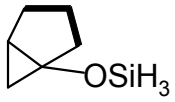
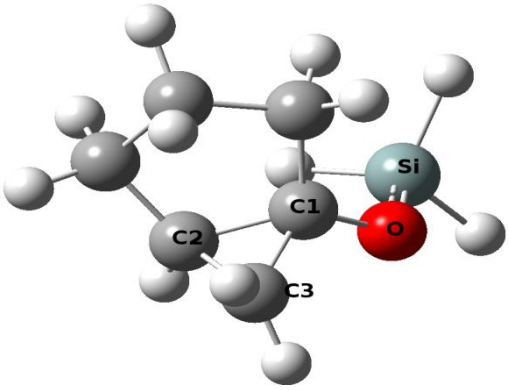


Figure S2. PES along with the thermodynamic parameters and structures of the stationary points of pathway-2M (violet colour) and pathway-2D (orange colour) under the catalytic condition of monomeric and dimeric form of Pt-salt. Energy values not enclosed in bracket are calculated using M06-2X functional. Values indicated in the round bracket are calculated using M06 functional.

St.Pt.	General Structure	Ball & Stick model
2		

Cartesian co-ordinate

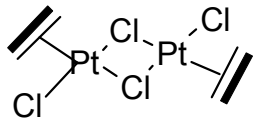
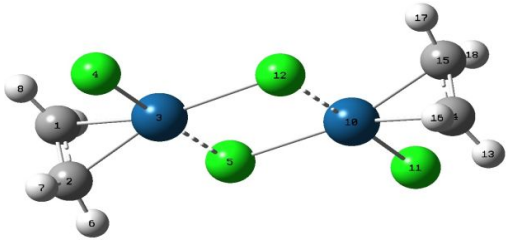
Atoms	X	Y	Z
C	-0.82387	0.80406	0.78579
O	1.29653	0.53614	-0.59065
C	-0.08031	0.34785	-0.44333
C	-0.93806	1.56537	-0.51870
H	-1.86685	1.54693	-1.08105
H	-0.39233	2.50072	-0.56261
C	-0.67963	-0.97251	-0.89477
H	-0.72335	-1.07012	-1.98352
C	-2.06462	-1.00980	-0.22626
H	-2.79922	-0.51298	-0.86677
H	-2.42288	-2.02861	-0.06342
C	-1.89683	-0.22419	1.09259
H	-2.84006	0.21609	1.43070
H	-1.53818	-0.88915	1.88701
H	-0.05079	-1.78840	-0.51358
H	-0.28956	1.28703	1.59732
H	3.66826	0.37054	0.23624
H	1.91830	-0.43706	1.72063
H	2.55476	-1.72213	-0.21136
Si	2.37926	-0.34476	0.31169

Frequencies

50.5800	108.4467	135.7920
235.1995	243.7345	357.1364
398.2266	458.8385	516.8303
613.6786	671.2735	721.3358
761.8710	820.9888	826.5272
870.7087	895.2086	919.7705
956.9564	979.9959	985.1784
991.1530	997.6362	1009.1378
1020.0213	1055.5780	1072.0578
1119.2736	1129.0063	1188.4395
1214.6074	1267.2868	1278.6625
1302.3936	1347.3555	1356.5718
1368.9609	1416.2538	1497.3544
1502.2798	1508.6772	1530.3504
2239.2261	2242.6140	2289.2514
3053.5143	3068.6937	3090.8192
3120.0301	3126.5413	3145.0497
3159.0805	3216.2177	3254.5058

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.167917 Electronic Energy = -600.400552085
Internal Energy (E)= -600.224173085 Enthalpy (H)= -600.223229085
Gibbs Free Energy (G)=-600.266249085 Gibbs Free Energy of Solvation=-600.268488721

St.Pt.	General Structure	Ball & Stick model
b		

Cartesian co-ordinate

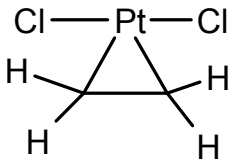
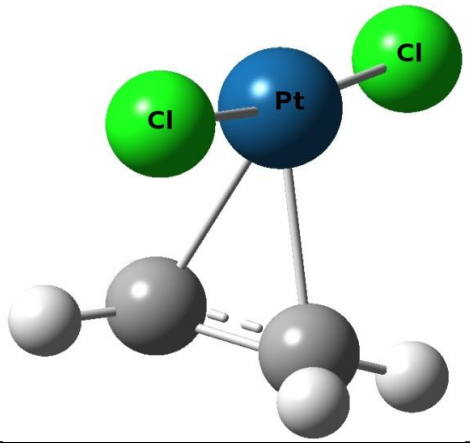
Atoms	X	Y	Z
C	-3.17738	-1.54894	-0.67531
C	-3.15374	-1.54304	0.72645
Pt	-1.80036	-0.07912	-0.00347
Cl	-3.49559	1.48916	0.02492
Cl	0.04341	-1.67277	-0.03359
H	-2.57032	-2.27967	1.27091
H	-3.92403	-1.01455	1.27868
H	-3.96599	-1.02532	-1.20589
H	-2.61278	-2.29059	-1.23260
Pt	1.80031	0.07911	-0.00347
Cl	3.49562	-1.48913	0.02495
Cl	-0.04342	1.67289	-0.03354
H	3.92408	1.01430	1.27865
C	3.15389	1.54294	0.72641
C	3.17757	1.54877	-0.67535
H	2.57058	2.27970	1.27081
H	2.61303	2.29044	-1.23268
H	3.96610	1.02499	-1.20588
H	2.55476	-1.72213	-0.21136
Si	2.37926	-0.34476	0.31169

Frequencies

2.9387	50.0966	80.5572
87.9864	89.3817	109.7068
124.2386	128.6058	177.8734
178.2620	192.6239	195.6003
237.5322	257.6038	276.6461
281.8348	354.5421	356.1301
404.2840	405.5701	507.5857
507.6732	773.6047	773.9266
847.8907	847.9440	1024.5210
1024.7903	1076.4852	1076.6357
1080.1263	1080.2373	1229.9457
1230.0007	1288.7163	1289.5402
1479.3815	1479.4633	1580.3803
1581.5728	3178.0579	3178.0976
3183.1235	3183.1740	3278.3804
3278.3886	3293.8032	3293.8111

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.117643 Electronic Energy = -2235.96844340
Internal Energy (E)= -2235.8353104 Enthalpy (H)= -2235.8343664
Gibbs Free Energy (G)=-2235.8994584 Gibbs Free Energy of Solvation=-2235.96255236

St.Pt.	General Structure	Ball & Stick model
c		

Cartesian co-ordinate

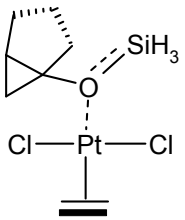
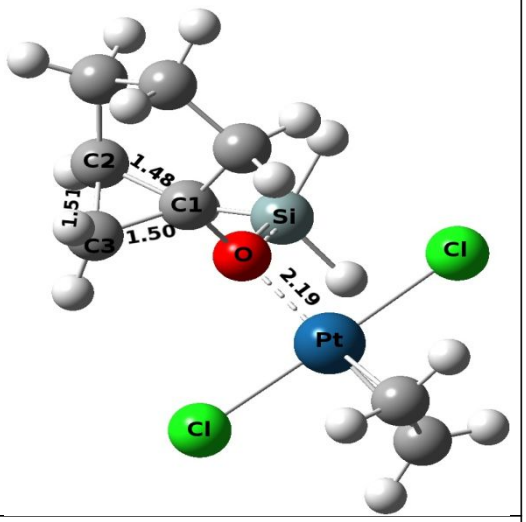
Atoms	X	Y	Z
Pt	-0.00010	-0.20997	-0.00001
Cl	2.31760	-0.35512	0.00004
Cl	-2.31780	-0.35459	0.00001
H	0.92902	1.90430	1.25018
C	0.00057	1.73535	0.71254
C	0.00077	1.73536	-0.71253
H	-0.92785	1.90503	1.24999
H	-0.92750	1.90508	-1.25024
H	0.92937	1.90432	-1.24990
Pt	1.80031	0.07911	-0.00347
Cl	3.49562	-1.48913	0.02495
Cl	-0.04342	1.67289	-0.03354
H	3.92408	1.01430	1.27865
C	3.15389	1.54294	0.72641
C	3.17757	1.54877	-0.67535
H	2.57058	2.27970	1.27081
H	2.61303	2.29044	-1.23268
H	3.96610	1.02499	-1.20588
H	2.55476	-1.72213	-0.21136
Si	2.37926	-0.34476	0.31169

Frequencies

115.0144	119.7496	137.1477
141.5947	338.9983	353.7419
458.4094	524.4425	811.5035
831.1351	978.9657	1095.1484
1101.7933	1223.8808	1232.6997
1464.1366	1545.3096	3171.1591
3171.6501	3269.9209	3283.7780

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.057798 Electronic Energy = -1117.94345067
Internal Energy (E)= -1117.87862367 Enthalpy (H)= -1117.87767967
Gibbs Free Energy (G)=-1117.91936467 Gibbs Free Energy of Solvation=-1117.97494035

St.Pt.	General Structure	Ball & Stick model
$2MI_1$		

Cartesian co-ordinate

Atoms	X	Y	Z
Pt	1.06321	0.03935	-0.01058
Cl	1.15196	2.29960	0.61631
Cl	0.91080	-2.24341	-0.59546
H	2.55864	1.38471	-1.72196
C	2.60843	0.34335	-1.42023
C	3.16957	0.00022	-0.18319
H	2.48769	-0.41145	-2.19072
H	3.48027	-1.02243	0.00650
H	3.55632	0.77428	0.47180
C	-3.31729	0.75032	0.49401
O	-0.95038	-0.15091	0.84732
C	-1.97241	0.31773	-0.02445
C	-2.29697	1.76724	0.02654
H	-2.44546	2.30754	-0.90339
H	-1.78564	2.32185	0.80456
C	-2.15441	-0.42819	-1.33005
H	-1.36768	-0.19809	-2.05670
C	-3.55762	0.00003	-1.79832
H	-3.48841	0.91554	-2.39267
H	-4.03052	-0.75490	-2.42929
C	-4.35710	0.27161	-0.50524
H	-5.16347	0.99368	-0.66289
H	-4.80803	-0.65548	-0.13369
H	-2.10938	-1.50534	-1.13306
H	-3.53799	0.73123	1.55613
H	-1.94081	-2.55833	1.12930
H	-0.01744	-1.83636	2.48675
H	-2.24266	-0.95784	2.91170
Si	-1.30521	-1.46284	1.88536

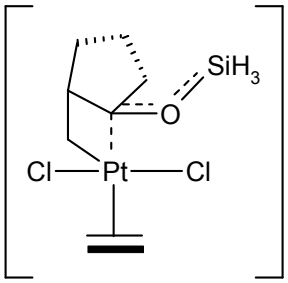
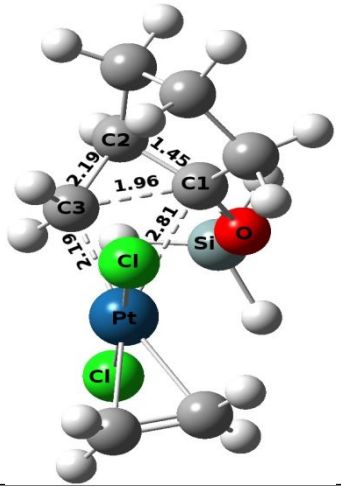
Frequencies

27.1306	50.5511	62.2921
86.9796	93.5489	114.8591
128.1213	139.1293	150.7967
166.2276	174.8112	190.4614
204.2583	255.2275	272.3733
317.6669	330.9051	369.4035
411.5408	437.6016	453.3701
518.0030	537.0375	616.1421
660.1493	712.9688	766.0175
786.8476	804.1516	826.5418
839.0961	865.8636	891.4545
919.8605	943.1841	965.2260
975.5311	983.9132	999.0939
1013.5995	1017.1930	1025.7494
1054.5919	1079.3823	1080.4243
1086.1478	1103.1703	1129.4579
1190.1871	1210.1370	1233.3574
1254.2342	1268.3725	1288.5254
1298.6376	1347.3308	1355.6351
1369.5203	1416.5865	1469.8885
1494.2130	1506.3395	1508.5473
1531.3151	1574.4213	2271.6238
2282.9697	2332.7806	3077.9865
3079.9622	3098.7859	3125.5122
3130.8431	3153.5314	3169.0885
3180.0658	3190.7442	3213.2251
3273.5939	3278.6468	3297.0893

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.228071 Electronic Energy = -1718.39068277
Internal Energy (E)= -1718.14583877 Enthalpy (H)= -1718.14489477

Gibbs Free Energy (G)=-1718.20911177 Gibbs Free Energy of Solvation=-1718.24369707

St.Pt.	General Structure	Ball & Stick model
$2MTS_1$		

Cartesian co-ordinate

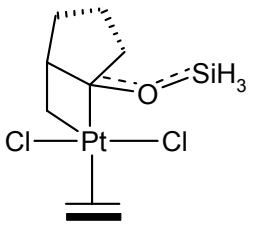
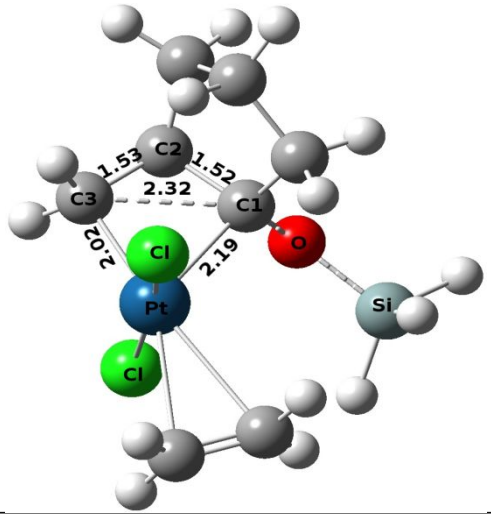
Atoms	X	Y	Z
C	3.03549	0.48739	0.10069
C	2.42759	0.53655	1.34331
Pt	0.90321	0.02770	-0.15643
Cl	1.41713	-2.26251	0.15282
Cl	0.50402	2.34538	-0.52185
H	2.10631	1.48578	1.75977
H	2.47045	-0.32059	2.00733
H	3.55975	-0.40814	-0.21636
H	3.19962	1.39892	-0.46482
C	-2.40810	-0.60669	-0.86454
O	-1.83620	0.91260	1.00040
C	-1.83811	-0.26640	0.42546
C	-0.91057	-0.46597	-1.29918
H	-0.56639	-1.41404	-1.71078
H	-0.84259	0.38126	-1.97896
C	-1.69603	-1.49825	1.28560
H	-0.73287	-1.57889	1.78972
C	-2.01182	-2.66403	0.33859
H	-1.07813	-3.04399	-0.07985
H	-2.50869	-3.48732	0.85418
C	-2.89518	-2.04658	-0.76430
H	-2.81131	-2.57237	-1.71877
H	-3.94984	-2.04528	-0.46804
H	-2.47859	-1.37116	2.04656
H	-3.06146	0.11366	-1.35388
H	-1.90645	3.46070	1.13282
H	-2.45115	2.43966	-1.05616
H	-3.97305	2.24338	0.79249
Si	-2.54395	2.35656	0.41017

Frequencies

-197.8503	37.0003	70.3168
105.2710	113.5130	124.4636
130.9453	141.6791	156.1813
166.0930	176.8732	195.8448
225.5524	231.5137	258.0296
298.2498	308.3981	316.6671
328.3845	387.5667	421.7400
459.5212	468.6236	536.9912
634.5494	698.8403	704.1945
715.1974	743.3147	767.6438
805.7074	838.2430	842.0402
896.0124	909.4000	938.6672
944.6571	975.4176	978.2155
991.9130	1035.7050	1041.1901
1046.5764	1048.6418	1053.9572
1094.6178	1133.0784	1169.8546
1197.5859	1233.6302	1237.9301
1254.5182	1282.4154	1316.4661
1322.0903	1338.2434	1365.9787
1378.4256	1417.7631	1463.0563
1466.6235	1503.8997	1528.3757
1560.6894	1598.0056	2240.0135
2298.0502	2330.8042	3068.5902
3090.7468	3122.7015	3132.9797
3145.8062	3166.6315	3177.2297
3178.6121	3186.6600	3187.4441
3233.6944	3275.5572	3293.0795

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.226134 Electronic Energy = -1718.36402544
Internal Energy (E)= -1718.12153044 Enthalpy (H)= -1718.12058644
Gibbs Free Energy (G)=-1718.18249344 Gibbs Free Energy of Solvation=-1718.2136653

St.Pt.	General Structure	Ball & Stick model
$2MI_2$		

Cartesian co-ordinate

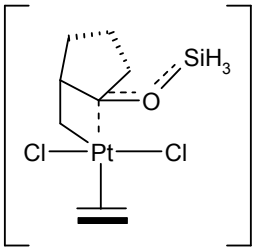
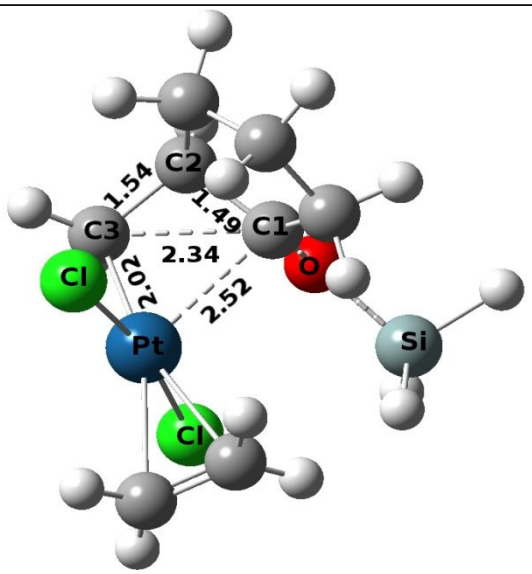
Atoms	X	Y	Z
C	-2.90894	-0.60489	-0.80754
C	-2.30881	0.31183	-1.58577
Pt	-0.52407	-0.47223	0.24405
Cl	0.00396	-2.27577	-1.19564
Cl	-1.38458	1.08954	1.79002
H	-2.40831	1.37049	-1.36546
H	-1.76082	0.02139	-2.47782
H	-2.86008	-1.66250	-1.05126
H	-3.48754	-0.30475	0.06156
C	1.95135	0.19547	1.19724
O	0.93960	2.04814	-0.00024
C	1.27083	0.75172	-0.04955
C	0.96528	-0.92766	1.53475
H	1.32618	-1.92810	1.29089
H	0.54739	-0.86722	2.53875
C	2.04312	0.27383	-1.28540
H	1.41667	-0.10468	-2.09276
C	3.04437	-0.75391	-0.73896
H	2.58747	-1.74625	-0.74360
H	3.94996	-0.79782	-1.34763
C	3.31894	-0.28384	0.69987
H	3.73263	-1.07103	1.33593
H	4.02406	0.55498	0.69754
H	2.57558	1.16562	-1.64388
H	1.98212	0.95514	1.98049
H	-1.22914	3.30981	-0.57969
H	0.89751	4.18543	-1.35270
H	-0.03817	2.19314	-2.38256
Si	0.09420	2.96902	-1.12814

Frequencies

31.1032	55.4465	79.1620
101.9688	108.8744	127.6573
138.4704	146.0286	149.6722
161.3553	169.9935	176.5583
223.2145	224.9806	237.5770
278.4614	285.4718	308.1337
325.2787	353.2832	399.1671
424.3460	496.9685	556.6153
606.2626	661.2455	710.9695
747.2248	800.5094	835.0174
846.6937	848.2885	865.6118
883.1155	922.3848	959.6896
970.5160	981.1573	987.1010
1015.8584	1019.6757	1043.7473
1045.6419	1074.1605	1079.0523
1112.2233	1156.4622	1183.9608
1203.6329	1216.2632	1247.0520
1249.1584	1281.3509	1304.4811
1326.1340	1340.5314	1360.3634
1377.4384	1406.9785	1467.8351
1468.8594	1474.3321	1496.8139
1522.3513	1680.4345	2262.8504
2292.7526	2311.6992	3061.8119
3074.4260	3114.8174	3123.2148
3135.6488	3145.3871	3169.0105
3173.8822	3174.4045	3186.3831
3211.9481	3270.3647	3290.4163

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.226312 Electronic Energy = -1718.37303675
Internal Energy (E)= -1718.12939175 Enthalpy (H)= -1718.12844775
Gibbs Free Energy (G)=-1718.19292675 Gibbs Free Energy of Solvation=-1718.2246734

St.Pt.	General Structure	Ball & Stick model
$2MTS_2$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.43126	-2.38048	1.14059
C	-0.71544	-1.62754	2.00147
Pt	-0.59122	-0.47226	-0.24382
Cl	-2.57103	0.68148	0.34283
Cl	1.13221	-1.94840	-0.95665
H	0.32960	-1.84949	2.19718
H	-1.19047	-0.84080	2.58072
H	-2.49551	-2.21083	1.00652
H	-0.97331	-3.21069	0.61191
C	0.51213	1.98217	-1.12881
O	2.34531	0.66620	-0.32177
C	1.23099	1.25581	-0.03168
C	-0.29232	0.83001	-1.76144
H	-1.26131	1.16086	-2.13860
H	0.29542	0.31942	-2.52531
C	0.94526	1.81518	1.33626
H	0.74928	1.04607	2.08845
C	-0.19636	2.82247	1.12948
H	-1.13342	2.40284	1.49001
H	0.00014	3.74314	1.68222
C	-0.28494	3.08555	-0.39945
H	-1.32727	3.09175	-0.72390
H	0.14914	4.05857	-0.64355
H	1.88282	2.31752	1.62263
H	1.24102	2.39298	-1.83658
H	2.44036	-1.00480	1.68841
H	4.09198	-1.20111	-0.15530
H	4.17452	0.64506	1.41679
Si	3.30221	-0.32250	0.71051

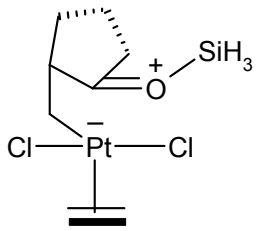
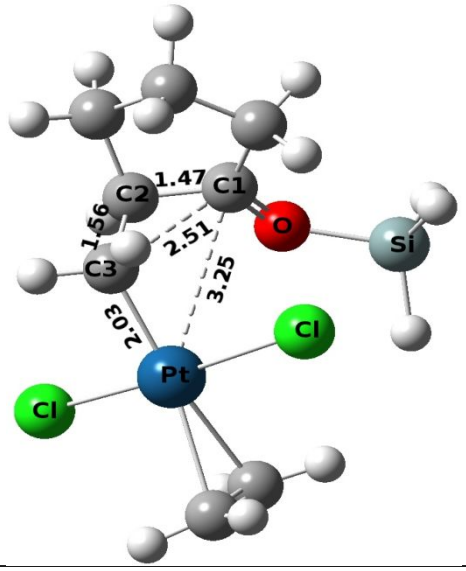
Frequencies

-82.6136	33.9188	77.0550
94.0740	104.5569	115.9650
124.9101	134.4338	142.3566
157.7860	164.1815	165.8643
175.1962	208.3655	214.4141
278.6981	291.3944	301.4750
308.0553	348.8108	432.4903
452.0346	461.6754	541.9901
631.3634	644.4807	696.6994
712.7612	775.9764	800.0252
822.2567	834.5051	843.9545
860.4099	920.4449	927.6051
958.3073	965.3376	985.3594
1012.4371	1028.1135	1030.7963
1047.5968	1071.5201	1092.7283
1126.4650	1155.6292	1197.2683
1229.4230	1243.0801	1246.2725
1254.9507	1292.9265	1313.3402
1322.4787	1353.6019	1367.4496
1368.4922	1453.5196	1456.6932
1466.3250	1502.4273	1526.8093
1553.1302	1666.1376	2248.2240
2313.5996	2338.9491	3035.6727
3092.6526	3104.5875	3113.9996
3122.1914	3136.1937	3168.3528
3174.7492	3184.9468	3197.7764
3199.9976	3269.7221	3290.2227

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm

Zero-point correction= 0.225722	Electronic Energy = -1718.36831894
Internal Energy (E)= -1718.12575994	Enthalpy (H)= -1718.12481494
Gibbs Free Energy (G)=-1718.18803094	Gibbs Free Energy of Solvation=-1718.21860162

St.Pt.	General Structure	Ball & Stick model
$2MI_3$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-2.99555	1.06174	-0.52980
C	-2.41833	1.57016	0.59188
Pt	-1.00656	-0.14305	-0.21105
Cl	0.30286	1.48500	-1.46063
Cl	-2.12724	-1.73053	1.11743
H	-2.68269	1.19313	1.57447
H	-1.78968	2.45329	0.53656
H	-2.83456	1.52359	-1.49893
H	-3.73239	0.26773	-0.46310
C	1.60128	-1.50181	0.58496
O	1.73656	0.79817	1.24255
C	2.16457	-0.14995	0.52751
C	0.46128	-1.50312	-0.50096
H	0.90095	-1.35363	-1.49220
H	0.03841	-2.51045	-0.44119
C	3.30850	-0.05575	-0.42996
H	3.05275	0.65057	-1.22798
C	3.53282	-1.50899	-0.89285
H	3.09836	-1.64962	-1.88396
H	4.59355	-1.75402	-0.95915
C	2.79203	-2.37591	0.15011
H	2.45431	-3.32877	-0.26159
H	3.44353	-2.58773	1.00510
H	4.16681	0.35576	0.11823
H	1.14701	-1.72602	1.55276
H	2.73554	2.84558	-0.09024
H	0.58805	3.09995	1.15726
H	2.69641	2.81943	2.33191
Si	1.93413	2.53071	1.09947

Frequencies

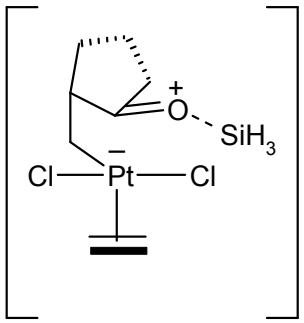
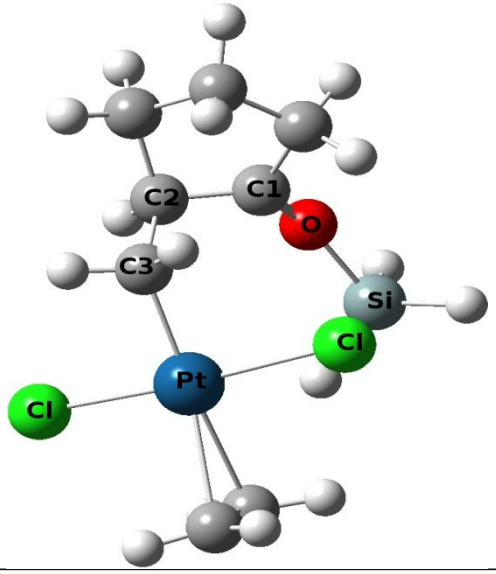
35.5293	44.8336	72.2914
89.2141	99.9989	110.5947
127.2750	139.2697	141.6932
157.9739	175.9172	182.7554
207.7324	224.9582	234.0387
261.9622	270.7509	292.4501
312.8710	387.2471	396.2858
507.5150	534.6674	565.5554
614.1517	683.4123	693.2159
712.0327	727.9705	790.7121
821.1983	831.7841	848.5712
890.7433	907.3117	930.1783
933.6186	960.0146	984.4370
995.2647	1008.6010	1028.4263
1047.7558	1062.0211	1062.9489
1081.8397	1155.4983	1202.4350
1219.5491	1238.7130	1242.5690
1272.7281	1273.0954	1316.6769
1319.0963	1352.1690	1357.8117
1374.7172	1429.7260	1466.5285
1467.3442	1506.1304	1524.3167
1642.5265	1686.5173	2292.5842
2314.3375	2384.4100	3064.7903
3086.4384	3089.1236	3125.0632
3129.2766	3144.4328	3160.3320
3162.2284	3178.0293	3182.2608
3189.4717	3271.5210	3292.1193

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm

Zero-point correction= 0.226232 Electronic Energy = -1718.36985935

Internal Energy (E)= -1718.12611535	Enthalpy (H)= -1718.12517035
Gibbs Free Energy (G)=-1718.19058735	Gibbs Free Energy of Solvation=-1718.22919461

St.Pt.	General Structure	Ball & Stick model
$2MTS_3$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-3.08768	0.55654	-0.77366
C	-2.68100	1.34177	0.25659
Pt	-0.93945	-0.24328	-0.21742
Cl	0.21499	1.39213	-1.58216
Cl	-1.89769	-1.80003	1.26936
H	-2.92754	1.09016	1.28346
H	-2.21565	2.30255	0.06086
H	-2.94958	0.87390	-1.80269
H	-3.67051	-0.34103	-0.59351
C	1.82987	-1.16481	0.66490
O	1.97805	1.22749	1.02868
C	2.33826	0.19250	0.41559
C	0.67688	-1.43353	-0.36274
H	1.07167	-1.35849	-1.38083
H	0.37618	-2.46704	-0.16703
C	3.46904	0.20500	-0.55862
H	3.18004	0.81292	-1.42325
C	3.74048	-1.28321	-0.84293
H	3.27886	-1.57297	-1.78858
H	4.80730	-1.49808	-0.91532
C	3.06939	-2.02410	0.33507
H	2.78372	-3.04721	0.08373
H	3.74648	-2.06222	1.19574
H	4.31047	0.71156	-0.06945
H	1.42097	-1.27093	1.67271
H	1.29563	3.62263	0.29970
H	-0.38499	2.21559	1.47354
H	1.59239	3.02978	2.62963
Si	1.01512	2.62199	1.33452

Frequencies

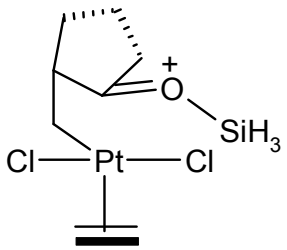
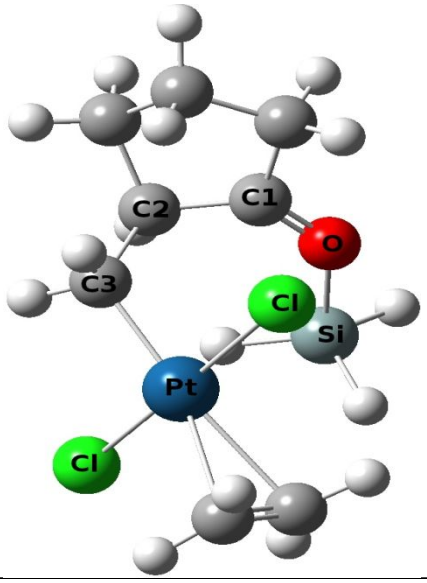
-115.8127	31.5136	43.4562
86.8123	95.3436	102.3878
103.3619	130.7021	134.7698
138.7166	171.1753	176.4259
192.7275	222.2829	248.5832
263.1763	274.6180	281.7790
313.7823	375.6559	409.2408
421.0731	516.2476	560.5384
611.9809	662.3245	689.6675
715.0485	729.2062	802.3766
822.8346	832.8645	850.0718
899.6594	911.1228	935.3406
952.1320	965.5202	980.4074
989.0554	1015.8724	1024.1241
1041.0622	1059.3098	1065.6815
1087.0025	1158.2684	1198.8691
1220.6817	1239.3046	1241.4500
1262.4552	1274.4697	1314.7465
1324.4842	1355.5637	1355.7757
1368.2711	1431.2134	1465.3254
1466.1953	1505.9056	1522.5053
1645.7952	1714.2007	2286.8030
2333.3742	2389.8674	3083.2302
3084.1204	3084.7435	3119.8903
3136.0330	3140.2008	3157.0072
3161.5478	3173.2484	3173.6865
3188.5481	3269.9280	3292.4651

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm

Zero-point correction= 0.225714 Electronic Energy = -1718.36215322

Internal Energy (E)= -1718.11945222	Enthalpy (H)= -1718.11850822
Gibbs Free Energy (G)=-1718.18290922	Gibbs Free Energy of Solvation=-1718.22015212

St.Pt.	General Structure	Ball & Stick model
$2MI_4$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-2.79747	-1.21331	-1.10402
C	-2.56534	-1.68821	0.14758
Pt	-1.02018	0.10203	-0.20997
Cl	-2.52660	1.63739	0.64267
Cl	0.78534	-1.48926	-1.01026
H	-1.93685	-2.55869	0.31348
H	-3.10741	-1.29492	1.00165
H	-3.53045	-0.43182	-1.27555
H	-2.36284	-1.68950	-1.97804
C	1.74200	1.04390	-0.59431
O	2.22079	-0.65276	1.09266
C	2.14005	-0.38150	-0.23485
C	0.43699	1.50797	0.02871
H	0.55097	1.71229	1.09799
H	0.09175	2.43351	-0.43930
C	3.49367	-0.58818	-0.89087
H	4.01190	-1.44603	-0.46112
C	4.18336	0.77495	-0.60351
H	4.89898	0.67885	0.21482
H	4.73649	1.11103	-1.48275
C	3.04598	1.77145	-0.22540
H	3.05366	1.97222	0.85007
H	3.13268	2.72856	-0.74288
H	3.36291	-0.74680	-1.96325
H	1.64240	1.05291	-1.68737
H	2.02968	-1.49706	3.40469
H	0.51812	0.30408	2.86210
H	0.13270	-1.92198	1.95842
Si	1.15065	-0.93027	2.36236

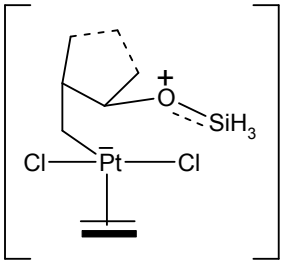
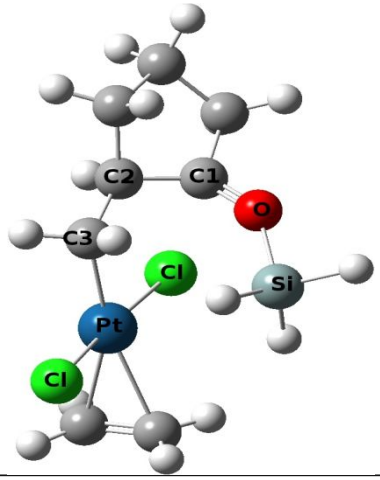
Frequencies

39.0444	62.9117	67.4153
82.0062	83.2225	104.2807
109.5490	136.5449	164.3161
173.5958	181.5470	189.0081
207.4705	218.0029	241.2098
288.9677	341.5677	356.7094
360.2199	366.6158	395.7558
540.9595	571.8085	601.7523
655.7415	666.8416	717.2191
728.9466	764.9842	776.0421
797.4699	825.7222	859.6164
913.5961	954.1208	958.4033
981.9580	997.5931	1011.7618
1012.1547	1020.2608	1023.5893
1062.0990	1064.7955	1110.8409
1115.0153	1189.6504	1199.3830
1208.8680	1217.0072	1232.0408
1260.0976	1292.1185	1324.4458
1332.2167	1351.7061	1354.9747
1376.2928	1409.5012	1469.9969
1487.1957	1491.8414	1502.3655
1525.2789	1646.8333	2272.8577
2286.9068	2289.9642	3074.2115
3095.9059	3102.0677	3110.4034
3118.6121	3148.7037	3155.6940
3163.7737	3167.2753	3180.1460
3182.5100	3261.6498	3283.7733

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm

Zero-point correction= 0.227064	Electronic Energy = -1718.37401511
Internal Energy (E)= -1718.12983911	Enthalpy (H)= -1718.12889511
Gibbs Free Energy (G)=-1718.19339611	Gibbs Free Energy of Solvation=-1718.22009057

St.Pt.	General Structure	Ball & Stick model
$2MTS_4$		

Cartesian co-ordinate

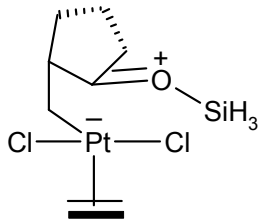
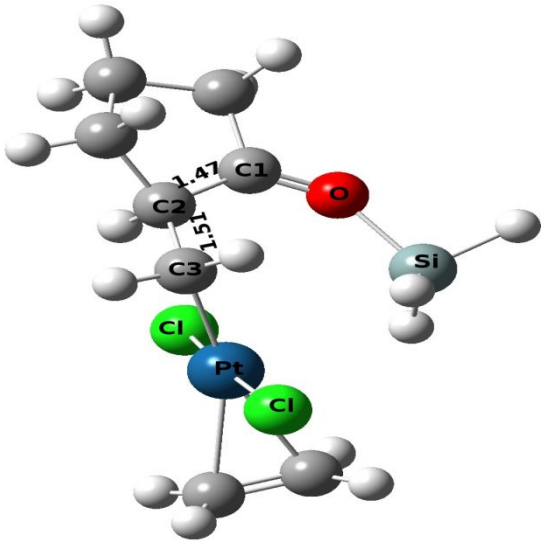
Atoms	X	Y	Z
C	-2.83643	-1.19736	-0.91749
C	-2.61682	-1.47941	0.39640
Pt	-0.96216	0.05597	-0.28769
Cl	-2.32536	1.85007	0.36303
Cl	0.49566	-1.85025	-0.78959
H	-2.04786	-2.35810	0.68444
H	-3.12373	-0.92065	1.17675
H	-3.52088	-0.40738	-1.20985
H	-2.44534	-1.84356	-1.69717
C	1.89682	0.76053	-0.69247
O	2.01984	-0.46363	1.45223
C	2.36814	-0.30291	0.24271
C	0.57392	1.40811	-0.37455
H	0.61865	1.99544	0.54839
H	0.31075	2.10854	-1.17346
C	3.73762	-0.76978	-0.16180
H	4.30541	-1.05561	0.72469
C	4.29516	0.47736	-0.90624
H	5.27165	0.77252	-0.51983
H	4.41014	0.25960	-1.97018
C	3.21847	1.57369	-0.70962
H	3.35604	2.10073	0.24184
H	3.20724	2.31728	-1.50811
H	3.63858	-1.64611	-0.80771
H	1.84449	0.27049	-1.67196
H	1.37395	-0.50262	3.80525
H	0.05739	1.03851	2.48585
H	-0.24445	-1.42490	2.25542
Si	0.65439	-0.29853	2.53195

Frequencies

-117.3324	46.3118	71.5226
83.7325	102.0531	116.3595
119.9352	137.3554	146.0408
165.9570	173.2281	192.7741
208.3189	220.3159	243.7991
251.1492	263.1045	285.1077
323.0193	369.3106	385.3421
544.5046	570.3171	582.2082
586.9737	644.7363	673.5575
686.1201	718.3152	771.5828
788.9028	828.4841	837.1173
913.5007	918.2187	921.2650
968.0304	990.8513	999.6507
1009.0506	1023.4022	1025.5393
1034.7591	1064.8536	1087.8912
1114.2268	1176.3560	1199.2008
1214.2614	1222.2472	1239.9097
1246.0191	1304.4879	1310.4302
1314.6302	1345.0257	1349.7749
1434.2493	1466.1864	1468.1396
1486.1391	1502.3221	1518.1138
1636.7751	1638.8247	2286.7154
2344.8857	2373.2703	3076.3880
3089.3116	3097.5295	3109.0186
3118.3567	3140.1624	3155.2015
3164.5352	3173.0962	3183.0893
3189.3966	3268.1656	3292.0434

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.226320 Electronic Energy = -1718.36290578
Internal Energy (E)= -1718.11992778 Enthalpy (H)= -1718.11898378
Gibbs Free Energy (G)=-1718.18174178 Gibbs Free Energy of Solvation=-1718.21486308

St.Pt.	General Structure	Ball & Stick model
$2MI_5$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	2.99291	0.34150	-1.21704
C	2.75174	1.31051	-0.28970
Pt	0.97243	-0.22013	-0.21125
Cl	2.11131	-1.45419	1.45176
Cl	-0.18054	1.17256	-1.81363
H	2.27734	2.24286	-0.58002
H	3.16352	1.23275	0.71169
H	3.59721	-0.52507	-0.96851
H	2.70967	0.48550	-2.25476
C	-2.01487	-0.82962	-0.24429
O	-2.03996	1.30732	0.99728
C	-2.58923	0.39894	0.32486
C	-0.68134	-1.32360	0.27358
H	-0.71946	-1.48761	1.35618
H	-0.48889	-2.30373	-0.17768
C	-4.06644	0.47441	0.08310
H	-4.53432	0.50176	1.07640
C	-4.39377	-0.82340	-0.67114
H	-5.38215	-1.21031	-0.42052
H	-4.36452	-0.64427	-1.74970
C	-3.24560	-1.76530	-0.27104
H	-3.41111	-2.19560	0.72347
H	-3.09577	-2.58647	-0.97290
H	-4.33031	1.41097	-0.41668
H	-1.88054	-0.48346	-1.29378
H	-1.15366	2.65532	2.82428
H	0.04997	0.58237	2.46913
H	0.27019	2.52322	0.87451
Si	-0.54149	1.75720	1.82285

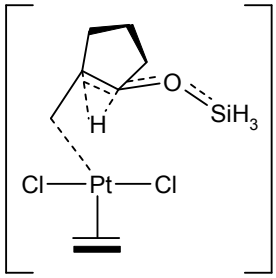
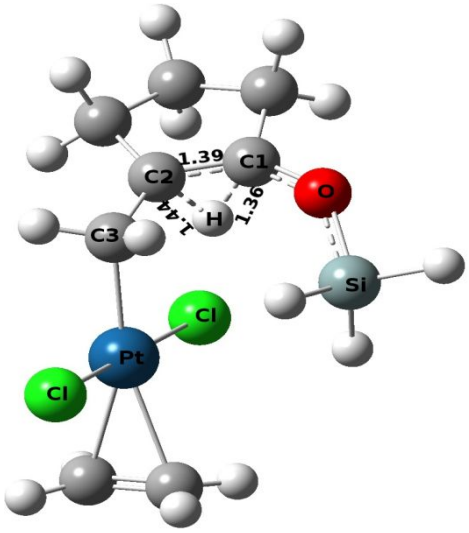
Frequencies

33.7550	46.9522	73.2920
90.7891	104.7089	115.9777
125.8055	138.7219	150.0007
165.6524	172.7473	184.2361
215.7564	224.8842	236.7876
271.8630	280.1703	295.7681
313.4062	375.1652	397.2950
483.1493	567.7131	588.9441
606.6657	626.4217	657.4244
688.3309	698.6332	752.0182
805.8786	836.1840	859.8038
903.1026	915.7653	942.4867
947.3691	968.6532	1007.4455
1016.9303	1020.5057	1025.5297
1048.4429	1058.7815	1093.8972
1120.6563	1159.3318	1199.3925
1212.6556	1227.7974	1238.2940
1241.3532	1270.5459	1317.6559
1327.1260	1347.0003	1349.4854
1407.4392	1434.9408	1462.4001
1474.9927	1507.2834	1521.3469
1632.9198	1696.0040	2278.0422
2359.5186	2393.8271	2936.0714
3070.8929	3076.9859	3090.2859
3100.6800	3127.0087	3135.8806
3161.1771	3167.6967	3173.3383
3184.4067	3270.5356	3290.7319

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm

Zero-point correction= 0.225765	Electronic Energy = -1718.36427637
Internal Energy (E)= -1718.12103937	Enthalpy (H)= -1718.12009537
Gibbs Free Energy (G)=-1718.18529837	Gibbs Free Energy of Solvation=-1718.22310871

St.Pt.	General Structure	Ball & Stick model
$2MTS_5$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	2.75398	-0.94527	-1.22310
C	2.53821	0.37929	-1.51501
Pt	1.00259	-0.24846	0.02429
Cl	2.44664	0.41072	1.74473
Cl	-0.53329	-0.86199	-1.76290
H	1.95754	0.66640	-2.38616
H	3.09666	1.15541	-1.00206
H	3.48626	-1.23356	-0.47585
H	2.34932	-1.72609	-1.85937
C	-1.86080	-0.40919	0.94343
O	-2.39597	1.74929	-0.08720
C	-2.64284	0.47039	0.19846
C	-0.51549	-0.17486	1.46966
H	-0.42139	0.80422	1.94311
H	-0.24817	-0.95053	2.19063
C	-4.01544	-0.09204	-0.09022
H	-4.71692	0.33970	0.63249
C	-3.80634	-1.60147	0.12099
H	-4.70079	-2.10706	0.48545
H	-3.52161	-2.06154	-0.82958
C	-2.62199	-1.70441	1.10473
H	-2.95578	-1.74782	2.14866
H	-1.97682	-2.56884	0.92541
H	-4.35531	0.17534	-1.09251
H	-1.82143	-0.35755	-0.50293
H	-1.66246	4.03717	-0.63417
H	-0.13030	2.77692	0.75603
H	-0.34785	2.25053	-1.61626
Si	-1.04055	2.71924	-0.40174

Frequencies

-360.4065	33.0200	52.5418
62.3870	89.3121	97.4226
120.2014	137.0455	141.0776
158.1323	165.4982	180.7488
188.8726	191.6852	201.7266
259.3945	275.0249	281.0923
326.9641	375.5574	404.9954
428.9622	541.1123	588.2769
631.6997	652.9610	687.5862
710.1710	733.4747	736.7072
771.5320	836.1204	845.1358
883.3436	940.7037	942.9676
964.1307	976.5118	987.7076
1020.8723	1031.4096	1038.2435
1046.8746	1057.8867	1068.6800
1105.5694	1151.6459	1183.0104
1227.3113	1229.9999	1235.8615
1239.8649	1273.9507	1318.4336
1332.7584	1344.4023	1354.0848
1388.1410	1435.0821	1468.1694
1482.5803	1493.9254	1498.6425
1517.2541	1616.0960	1703.1233
2277.5442	2291.3066	2306.8228
3081.4581	3095.7622	3105.0913
3115.4495	3141.9143	3155.0050
3169.9861	3173.8623	3184.8543
3194.3091	3269.7059	3295.9570

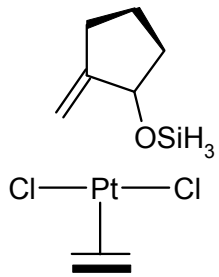
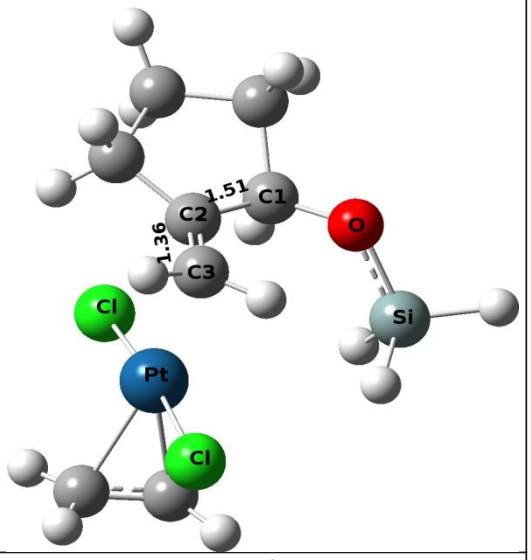
Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm

Zero-point correction= 0.221722 Electronic Energy = -1718.35438845

Internal Energy (E)= -1718.11562045 Enthalpy (H)= -1718.11467645

Gibbs Free Energy (G)=-1718.17921845 Gibbs Free Energy of Solvation=-1718.21035325

St.Pt.	General Structure	Ball & Stick model
$2MI_6$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	2.77175	-1.00831	-0.66483
C	2.34410	0.03719	-1.48505
Pt	0.90491	-0.24514	0.09212
Cl	2.18150	1.27143	1.38433
Cl	-0.15014	-1.84963	-1.31580
H	1.81931	-0.17589	-2.41086
H	2.74344	1.03654	-1.34485
H	3.50632	-0.82283	0.11182
H	2.58375	-2.03722	-0.95326
C	-1.59191	-0.23061	0.91909
O	-2.33407	1.80714	-0.22264
C	-2.40249	0.40764	-0.19367
C	-0.69262	0.44649	1.68235
H	-0.55248	1.51400	1.54680
H	-0.28582	0.00940	2.59037
C	-3.79691	-0.15712	0.08945
H	-4.21329	0.34587	0.96967
C	-3.48225	-1.63158	0.38149
H	-4.29495	-2.14892	0.89352
H	-3.28609	-2.15670	-0.55816
C	-2.18664	-1.58876	1.22544
H	-2.40378	-1.62934	2.29795
H	-1.50384	-2.40560	0.98537
H	-4.47688	-0.00745	-0.75108
H	-2.05715	-0.02617	-1.14488
H	-1.87383	3.85709	-1.64630
H	-0.01235	2.97982	-0.37557
H	-0.82451	1.75110	-2.29313
Si	-1.22069	2.62572	-1.15800

Frequencies

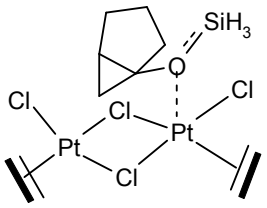
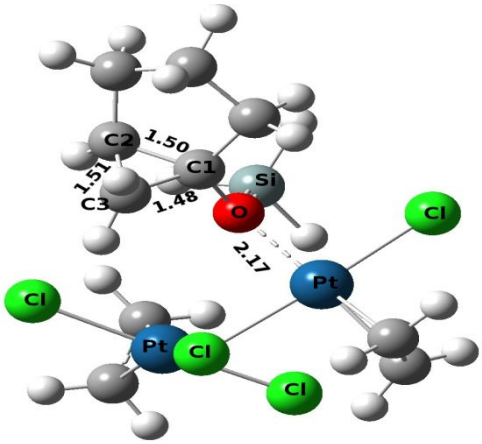
28.5562	43.8150	64.7438
69.8211	104.9949	111.1154
131.4826	156.0435	172.8344
182.9529	201.8576	206.0246
223.1218	251.8899	268.4368
299.6021	305.8270	321.2729
364.3678	376.6065	405.0036
487.3214	510.4327	583.9555
604.6588	732.2646	738.3796
757.9879	773.2908	830.7898
846.3405	858.7198	879.2825
902.9121	924.9713	946.9939
975.1998	987.4640	1005.7142
1021.5537	1035.0250	1037.1181
1039.5306	1077.5304	1081.9634
1092.0650	1166.7266	1204.9637
1229.9566	1236.2475	1240.6122
1260.1761	1298.0810	1318.3436
1324.4673	1337.2437	1351.1849
1430.4274	1445.3999	1464.0628
1469.8309	1504.5103	1520.4429
1581.1175	1672.4320	2249.7537
2258.1812	2274.7545	3060.4314
3083.1750	3088.1208	3100.2743
3152.7829	3153.4567	3172.6234
3179.3974	3184.8953	3192.4573
3278.8157	3283.8220	3299.7128

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm

Zero-point correction= 0.228023 Electronic Energy = -1718.38996547

Internal Energy (E)= -1718.14498647	Enthalpy (H)= -1718.14404247
Gibbs Free Energy (G)=-1718.20844847	Gibbs Free Energy of Solvation=-1718.23996996

St.Pt.	General Structure	Ball & Stick model
$2DI_1$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.75284	-2.94122	-1.33491
C	-0.73092	-3.28460	-0.44388
Pt	-1.19404	-1.21609	-0.22418
Cl	-2.78776	-1.68551	1.39995
Cl	0.48294	-0.60632	-1.83999
H	0.30486	-3.32774	-0.76628
H	-0.96673	-3.74679	0.50978
H	-2.78802	-3.15227	-1.08619
H	-1.52388	-2.73842	-2.37688
Pt	2.09597	0.21262	-0.09363
Cl	2.04110	2.38360	-0.99565
Cl	2.11857	-1.93430	0.89710
H	4.47275	1.34222	0.12452
C	3.99098	0.60597	0.76015
C	2.99045	1.00505	1.65886
H	4.48347	-0.35298	0.88588
H	2.71659	0.35459	2.48401
H	2.71097	2.05178	1.72236
C	-1.59081	3.20895	-0.21512
O	-1.09909	0.82062	0.53930
C	-1.96225	1.75652	-0.10699
C	-1.54168	2.29988	-1.42578
H	-2.28796	2.39003	-2.20977
H	-0.53976	2.04569	-1.75327
C	-3.44544	1.63769	0.18345
H	-3.91601	0.80872	-0.35507
C	-4.00340	3.01659	-0.21921
H	-4.27267	3.01404	-1.27918
H	-4.90636	3.27294	0.33820
C	-2.85325	4.01631	0.02876
H	-2.92756	4.89838	-0.61362
H	-2.86402	4.36149	1.06902
H	-3.58793	1.45316	1.25403
H	-0.62623	3.55574	0.14319
H	0.01659	-0.13030	2.59648
H	0.21099	2.27726	2.21343
H	-1.90260	1.36531	2.95520

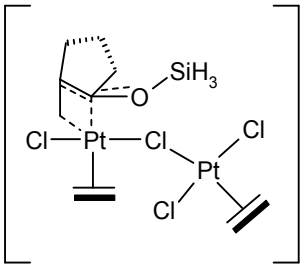
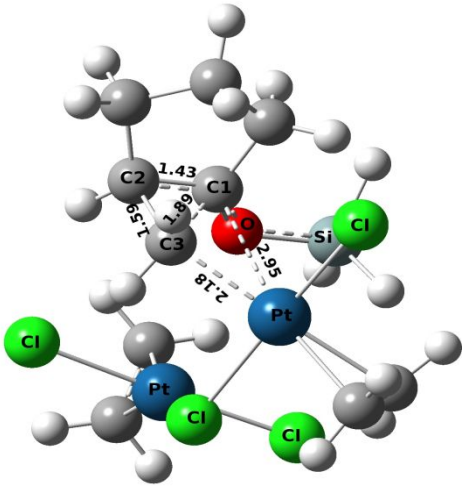
Frequencies

14.5043	35.4889	51.0108
62.9612	69.8840	75.1540
81.2779	94.4883	95.4710
102.8919	112.1942	125.8987
138.5968	149.8350	159.8290
162.1078	167.1817	178.8576
189.7919	195.8421	206.1925
208.9733	230.7490	255.5238
278.8199	283.9976	314.8938
325.7377	344.1361	382.7201
402.5997	413.3160	443.9414
455.3551	509.3372	518.1794
540.9533	618.6513	660.0618
709.0908	766.9229	770.9190
788.1966	809.3916	827.5739
844.4495	846.8357	871.4128
897.2012	922.8478	949.6671
960.5665	978.1467	981.8886
990.9489	1016.2596	1023.0133
1023.7436	1038.4909	1065.7158
1077.1153	1083.0376	1085.1933
1091.2172	1095.7435	1098.8084
1131.9218	1190.7182	1213.6222
1226.0263	1235.5373	1251.4321
1269.7757	1284.3086	1297.2156
1299.2594	1346.8560	1354.2716
1369.7463	1416.9372	1466.0482
1479.3108	1496.8986	1503.4565
1511.4092	1533.9255	1569.1239
1582.5251	2277.3051	2292.3309
2318.3905	3077.3989	3084.1846
3107.0629	3131.2943	3133.6250
3161.6551	3172.0217	3179.4881
3183.5885	3188.1903	3190.4944
3217.3385	3272.7622	3278.4726
3282.6506	3293.4738	3297.2037

Si	-0.67870	1.09709	2.17592	

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.288054 Electronic Energy = -2836.39105627
Internal Energy (E)= -2836.07782927 Enthalpy (H)= -2836.07688527
Gibbs Free Energy (G)=-2836.16115827 Gibbs Free Energy of Solvation=-2836.21974765

St.Pt.	General Structure	Ball & Stick model
$2DTS_1$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-2.07859	-2.98521	-0.52129
C	-1.53617	-2.72317	0.72310
Pt	-1.65906	-0.81632	-0.39505
Cl	-3.84294	-0.49545	0.37725
Cl	0.48583	-1.30942	-1.41822
H	-0.47270	-2.85488	0.91294
H	-2.19059	-2.59248	1.57948
H	-3.15380	-3.05987	-0.64722
H	-1.45203	-3.34606	-1.33084
Pt	2.22436	-0.07035	-0.16269
Cl	2.20553	1.63552	-1.79638
Cl	2.17780	-1.73874	1.50871
H	4.66681	0.84927	-0.57242
C	4.22632	0.42424	0.32379
C	3.35718	1.18951	1.11347
H	4.68289	-0.47175	0.73234
H	3.15907	0.88669	2.13637
H	3.12490	2.21254	0.83594
C	-1.02161	2.66641	-0.63782
O	-0.12125	1.42224	1.23639
C	-1.15928	1.92740	0.57943
C	-1.47989	1.22938	-1.15493
H	-2.46444	1.33155	-1.60620
H	-0.67626	0.97505	-1.84566
C	-2.44573	2.30918	1.27792
H	-2.98973	1.47633	1.72362
C	-3.23464	3.08675	0.21831
H	-3.87597	2.39265	-0.33091
H	-3.87592	3.84943	0.66221
C	-2.14702	3.68649	-0.69622
H	-2.49317	3.86292	-1.71745
H	-1.78101	4.63705	-0.29263
H	-2.11129	2.98156	2.08135
H	-0.02156	2.90710	-0.98877
H	-0.73300	-0.77643	2.51443

Frequencies

-262.4137	22.3483	33.9021
50.1672	58.9295	70.2863
81.2918	93.6386	97.9023
112.5264	118.3354	129.1823
135.6270	146.4031	155.4025
162.9187	166.7438	169.6382
182.4348	192.1043	197.9115
232.4033	243.7327	249.3971
277.6260	294.6621	305.0571
314.0062	316.1565	319.2542
328.9370	382.1979	410.0186
413.7763	454.9206	487.3639
518.9761	535.8107	627.0102
685.1184	690.5573	702.0970
751.7604	773.6255	775.1425
803.2116	837.4744	841.0144
841.3597	891.7597	913.3184
930.3942	941.1096	973.6254
983.6648	993.7382	1016.3302
1040.1590	1042.7674	1049.4574
1056.1448	1066.0909	1066.7113
1073.4370	1119.9995	1133.3892
1169.9084	1193.0272	1231.8838
1232.3080	1233.6862	1258.0496
1286.4391	1294.7498	1311.1151
1321.3909	1341.7480	1351.1823
1388.6334	1402.7134	1466.4007
1469.1222	1469.6475	1502.6796
1520.6847	1559.0619	1572.4059
1600.2169	2270.8503	2309.8020
2354.1001	3056.6264	3092.3756
3111.3369	3118.1124	3146.9248
3160.5294	3165.4992	3174.3030
3178.3721	3181.2643	3188.8375
3206.1306	3235.5705	3262.5564
3277.4750	3285.3143	3295.9267

H	1.16747	0.61660	3.24313	
H	-1.10396	1.35367	3.60905	
Si	-0.20416	0.58024	2.72472	

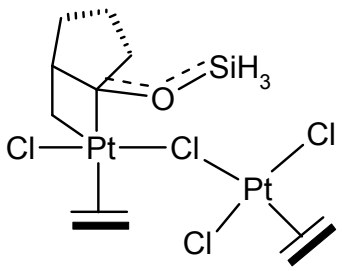
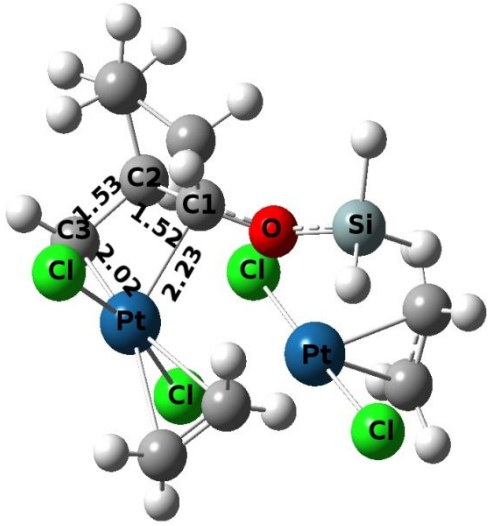
Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm

Zero-point correction= 0.285526 Electronic Energy = -2836.36186683

Internal Energy (E)= -2836.05138083 Enthalpy (H)= -2836.05043683

Gibbs Free Energy (G)=-2836.13340783 Gibbs Free Energy of Solvation=-2836.1900671

St.Pt.	General Structure	Ball & Stick model
$2DI_2$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.89405	-3.05299	-0.18111
C	-1.46525	-2.57152	1.00110
Pt	-1.86900	-0.50985	-0.52681
Cl	-4.13661	-0.51210	0.02882
Cl	0.31480	-0.75052	-1.54449
H	-0.40066	-2.47264	1.20393
H	-2.17207	-2.33924	1.79397
H	-2.95006	-3.21995	-0.37451
H	-1.18157	-3.34529	-0.94835
Pt	2.32195	-0.02976	-0.21468
Cl	2.39774	1.99666	-1.40267
Cl	2.20383	-2.02765	1.05673
H	4.79532	0.50812	-0.95691
C	4.42649	-0.03971	-0.09539
C	3.90087	0.65319	1.00933
H	4.73689	-1.07461	0.01042
H	3.82917	0.14960	1.96818
H	3.87751	1.73819	1.00598
C	-1.24123	2.13609	-0.36692
O	-0.07705	0.78292	1.32577
C	-1.24896	1.16371	0.81087
C	-1.97651	1.29968	-1.42417
H	-3.02445	1.57215	-1.55417
H	-1.44796	1.22981	-2.37451
C	-2.36907	1.56388	1.76840
H	-2.97488	0.72913	2.12295
C	-3.14639	2.65573	1.02202
H	-3.93250	2.20295	0.41311
H	-3.61772	3.35616	1.71417
C	-2.07343	3.31956	0.14160
H	-2.49289	3.89975	-0.68446
H	-1.44650	3.98759	0.74262
H	-1.86077	2.01638	2.62899
H	-0.21680	2.36704	-0.67117

Frequencies

6.6773	38.9675	47.6529
57.6057	63.2830	73.1755
87.2002	95.7839	108.8221
114.8466	117.3698	123.2746
140.4689	145.1917	150.2073
158.5255	163.8407	167.1875
174.5176	184.5170	200.8595
217.0482	222.6944	244.8078
253.2673	277.1500	288.2700
301.9285	310.5144	326.6820
333.5971	352.8242	418.2629
419.6259	425.5033	504.8943
524.0491	542.8139	595.6152
661.1890	717.0219	726.3324
774.7683	784.8148	816.3741
830.8145	845.5419	849.8975
862.0428	877.7295	923.3161
937.6954	957.8635	985.6406
998.5994	1011.8610	1014.2991
1032.0856	1041.1779	1044.8197
1065.5278	1067.5279	1082.1278
1086.5664	1103.9845	1160.1848
1182.7160	1197.0842	1217.5351
1228.5049	1248.2176	1259.7449
1274.6219	1283.5344	1314.8823
1330.9650	1339.4289	1360.9672
1378.4111	1413.4196	1458.5810
1463.1654	1467.4421	1475.6029
1497.5961	1520.7652	1562.3062
1673.2951	2260.9013	2303.8493
2362.0430	3080.2345	3087.3172
3114.3755	3122.3505	3144.3075
3146.8689	3152.0633	3168.4293
3168.8534	3172.4851	3175.0811
3177.5852	3205.9825	3252.8742
3271.2478	3272.6252	3286.0058

H	-0.27151	1.23155	3.85865	
H	-0.34285	-1.07292	3.15294	
H	1.74173	0.23563	2.99011	
Si	0.27918	0.23945	2.90865	

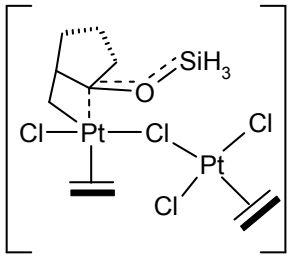
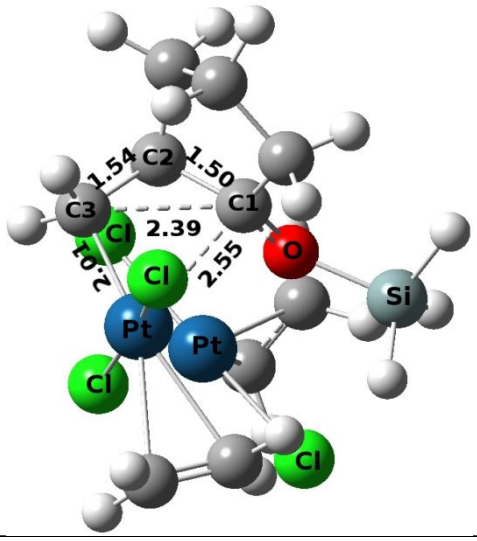
Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm

Zero-point correction= 0.285485 Electronic Energy = -2836.36942292

Internal Energy (E)= -2836.05801092 Enthalpy (H)= -2836.05706692

Gibbs Free Energy (G)=-2836.14345092 Gibbs Free Energy of Solvation=-2836.20108534

St.Pt.	General Structure	Ball & Stick model
$2DTS_2$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-2.14424	-3.02796	-0.24545
C	-1.61501	-2.61837	0.92678
Pt	-1.84050	-0.57054	-0.52996
Cl	-4.08078	-0.30432	0.08670
Cl	0.36071	-1.01643	-1.45597
H	-0.53890	-2.62406	1.09028
H	-2.26270	-2.35068	1.75730
H	-3.21906	-3.09251	-0.38546
H	-1.50491	-3.37819	-1.05127
Pt	2.29669	-0.08070	-0.21636
Cl	2.43934	1.69991	-1.74505
Cl	2.10921	-1.82693	1.37783
H	4.81907	0.47619	-0.76761
C	4.37819	0.06821	0.13624
C	3.69773	0.90966	1.02843
H	4.71529	-0.91088	0.46186
H	3.52802	0.58011	2.04849
H	3.62295	1.97224	0.82119
C	-1.02848	2.17119	-0.43223
O	-0.06590	0.92828	1.43705
C	-1.12061	1.43204	0.87556
C	-1.76296	1.23935	-1.42134
H	-2.78014	1.57932	-1.62104
H	-1.19478	1.12354	-2.34551
C	-2.30626	1.91851	1.67800
H	-2.95677	1.11595	2.03105
C	-2.98296	2.94459	0.75839
H	-3.75398	2.44546	0.16774
H	-3.45559	3.74594	1.32868
C	-1.83538	3.44616	-0.13841
H	-2.18586	3.91185	-1.06248
H	-1.21776	4.17456	0.39920
H	-1.86667	2.42078	2.55067

Frequencies

-113.1162	20.0044	46.3181
53.6723	60.5327	68.6741
82.5869	87.6415	100.8556
112.9892	122.4948	123.1078
138.7987	147.5783	152.7436
155.2783	168.2425	171.5311
178.7295	197.0212	198.3566
218.0318	226.5654	250.5659
274.2120	284.0943	303.3333
310.1702	313.5438	325.2929
326.0334	336.6574	408.9895
416.7063	468.8412	483.0933
518.2288	542.8788	595.2635
667.6605	705.8103	727.2464
762.0986	780.0867	799.4047
836.2721	839.8417	849.9066
859.1786	871.5029	922.0159
934.8236	960.6186	973.6467
996.3303	1014.1781	1019.5787
1034.5039	1040.2850	1050.8505
1059.0875	1063.5415	1079.8824
1088.4198	1099.5923	1168.3262
1176.6989	1208.9592	1230.9637
1239.4538	1246.7705	1269.0656
1283.4537	1301.1239	1309.6969
1321.8541	1346.9238	1360.5740
1373.5245	1445.0219	1464.6492
1468.4688	1471.3651	1499.0045
1524.1970	1543.2769	1569.5161
1666.8788	2271.0128	2359.0601
2383.0934	3062.9618	3079.8166
3111.1406	3124.2149	3139.1250
3151.7148	3153.6784	3157.0447
3173.5862	3174.2152	3177.3893
3181.2864	3191.6652	3255.2613
3272.6183	3277.3828	3289.0405

H	0.01510	2.31918	-0.72397
H	-0.72364	1.09626	3.91301
H	-0.47075	-1.12647	2.99546
H	1.50159	0.34979	3.34593
Si	0.07926	0.23238	3.02050

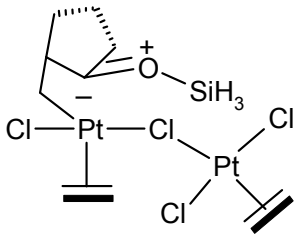
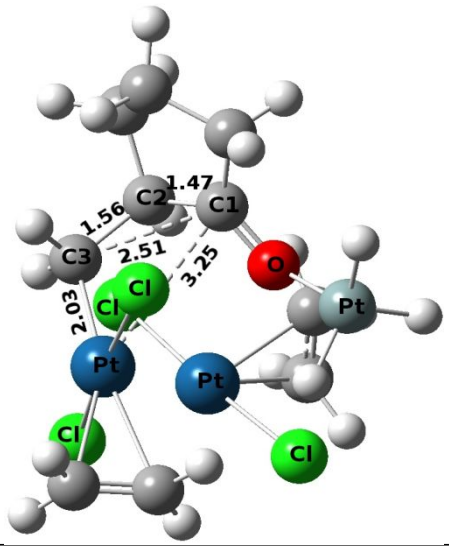
Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm

Zero-point correction= 0.285913 Electronic Energy = -2836.36815795

Internal Energy (E)= -2836.05723695 Enthalpy (H)= -2836.05629295

Gibbs Free Energy (G)=-2836.13925495 Gibbs Free Energy of Solvation=-2836.19615919

St.Pt.	General Structure	Ball & Stick model
$2DI_3$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-2.02978	-3.22254	-0.03639
C	-1.42281	-2.79599	1.09899
Pt	-1.32485	-0.99625	-0.52014
Cl	-3.33528	-0.05477	0.34294
Cl	0.82712	-1.81184	-1.25670
H	-0.37018	-2.97652	1.29148
H	-2.00818	-2.35121	1.89786
H	-3.10388	-3.13066	-0.16702
H	-1.48109	-3.78048	-0.78928
Pt	2.01602	-0.05328	0.03291
Cl	2.59584	1.00582	-1.98557
Cl	1.39371	-0.99642	2.12484
H	4.43374	1.00453	0.20381
C	3.68493	0.84541	0.97290
C	2.58302	1.70751	1.06936
H	3.95117	0.21061	1.81177
H	2.00763	1.74491	1.98866
H	2.49509	2.54309	0.38183
C	-0.74062	2.04218	-0.97551
O	-0.70270	1.52007	1.35169
C	-1.27467	2.12377	0.40105
C	-1.12026	0.67919	-1.65058
H	-2.09069	0.81122	-2.14025
H	-0.35172	0.50779	-2.40993
C	-2.41697	3.08023	0.51572
H	-3.22516	2.70278	1.14236
C	-2.76881	3.36426	-0.95091
H	-3.46017	2.59094	-1.29853
H	-3.24148	4.33798	-1.08461
C	-1.41396	3.24116	-1.67130
H	-1.51192	3.07579	-2.74553
H	-0.82328	4.15212	-1.52135
H	-1.99185	3.97639	0.99773
H	0.35369	2.08374	-0.94120

Frequencies

43.4535	49.7138	55.6665
69.4058	73.7769	86.2845
92.9828	93.3983	98.3406
108.6983	114.5424	124.4540
134.5568	149.4855	156.0858
160.6371	177.7184	181.2431
183.8584	199.2490	207.3067
212.3194	233.3037	242.0831
261.4999	264.3750	281.0096
291.4358	304.8926	324.5070
333.4558	357.6585	396.7551
411.1038	502.7945	524.3260
533.2251	538.2497	595.8672
662.7529	684.9745	735.1896
749.2067	792.8566	807.8076
814.5289	836.0680	856.8954
864.6966	891.3021	919.1263
952.5890	957.3736	959.1000
976.6017	990.8712	1022.4239
1022.6459	1029.1692	1040.0993
1061.5883	1064.9200	1074.2687
1087.2644	1113.3041	1168.2125
1200.9512	1219.8640	1234.5134
1238.1151	1241.6164	1269.5203
1274.9345	1285.5669	1316.7976
1323.9853	1361.2373	1365.1221
1366.5832	1423.9126	1470.5432
1473.7805	1476.3275	1504.3750
1517.7464	1573.8363	1652.7840
1673.5701	2287.7948	2327.8154
2399.4680	3029.8094	3080.5039
3087.7897	3111.1935	3114.8686
3159.9403	3162.8636	3174.4360
3175.4204	3176.6074	3181.1004
3189.2970	3191.9172	3269.3536
3275.5095	3296.3000	3297.1150

H	-2.45516	1.83721	3.21447
H	-1.49185	-0.40453	2.91123
H	-0.13027	1.45485	3.80102
Si	-1.24702	1.03525	2.94090

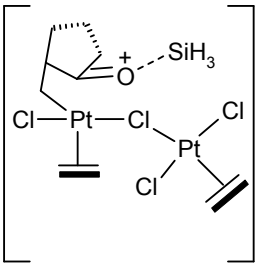
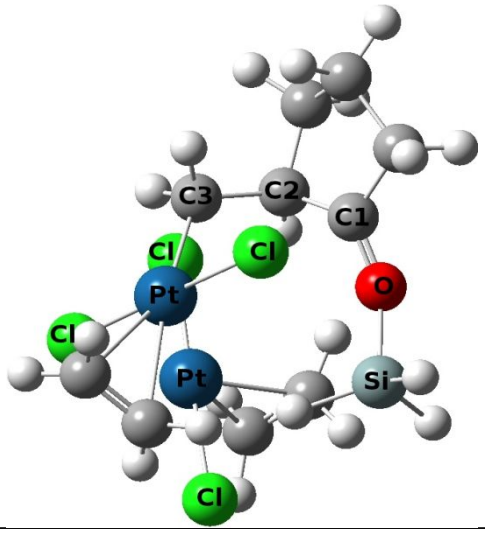
Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm

Zero-point correction= 0.286503 Electronic Energy = -2836.38047637

Internal Energy (E)= -2836.06831937 Enthalpy (H)= -2836.06737437

Gibbs Free Energy (G)=-2836.15087637 Gibbs Free Energy of Solvation=-2836.21089468

St.Pt.	General Structure	Ball & Stick model
$2DTS_3$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.52296	-3.41715	-0.48161
C	-0.97219	-3.10219	0.71505
Pt	-1.23637	-1.02547	-0.57271
Cl	-3.31824	-0.57681	0.48832
Cl	0.91984	-1.36930	-1.60446
H	0.10292	-3.11183	0.87483
H	-1.61015	-2.92415	1.57593
H	-2.59937	-3.50046	-0.59882
H	-0.90371	-3.71304	-1.32302
Pt	2.08721	0.15918	-0.04242
Cl	2.07341	1.86209	-1.67960
Cl	2.14947	-1.49568	1.64603
H	4.26805	1.65028	0.09861
C	3.74602	1.10466	0.87794
C	2.56165	1.61981	1.42314
H	4.29385	0.33060	1.40550
H	2.20925	1.25365	2.38210
H	2.18166	2.57455	1.07357
C	-1.19274	2.06621	-0.47657
O	-1.45311	1.53394	1.87612
C	-1.92778	2.00061	0.80634
C	-1.36485	0.81233	-1.38737
H	-2.35368	0.85967	-1.85566
H	-0.59357	0.92172	-2.15522
C	-3.18427	2.80684	0.79126
H	-4.01580	2.24399	1.22134
C	-3.31098	3.23471	-0.67586
H	-3.85875	2.46788	-1.23054
H	-3.83901	4.18180	-0.79212
C	-1.84536	3.29850	-1.14560
H	-1.73417	3.25912	-2.23063
H	-1.37471	4.22184	-0.78976
H	-2.98759	3.66962	1.44584
H	-0.12268	2.17155	-0.26819

Frequencies

-111.9992	16.5363	41.8634
42.4612	58.1323	63.9456
78.5480	83.8386	90.0723
99.3340	109.6340	115.3903
123.0488	130.2370	142.8339
154.2304	156.5208	169.3889
174.7296	190.8869	199.2413
209.1259	227.8804	243.0751
244.5660	260.6192	287.9111
297.3076	312.0653	313.3893
317.0989	337.1874	409.1444
416.8553	430.4969	514.0496
520.8019	527.8883	601.0436
655.6164	685.2621	716.2230
740.4809	793.8510	813.2650
822.6171	836.4814	854.1968
864.2249	899.9435	916.8218
947.6096	962.4844	962.9103
980.9304	989.1544	1025.6740
1026.9202	1032.3735	1033.6501
1061.3090	1070.8681	1075.6503
1085.8844	1116.6979	1180.7172
1193.4442	1218.8585	1236.1662
1238.5048	1239.8964	1270.4307
1284.8564	1290.6255	1311.4311
1330.3389	1355.8428	1360.0480
1363.7087	1428.9862	1471.1563
1471.7374	1472.9727	1504.7207
1516.1450	1574.7971	1658.2025
1690.7997	2295.9119	2340.0775
2403.3183	3054.6874	3085.0783
3086.7931	3108.4780	3111.2420
3156.8601	3161.6970	3162.8488
3166.1286	3170.5999	3185.4015
3189.6293	3195.2982	3263.1838
3285.3271	3287.0778	3303.2755

H	-2.37644	-0.05140	3.66235	
H	-0.57059	-0.89794	2.19258	
H	-0.13127	0.86145	3.83996	
Si	-1.11857	0.22418	2.95054	

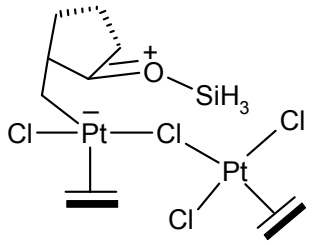
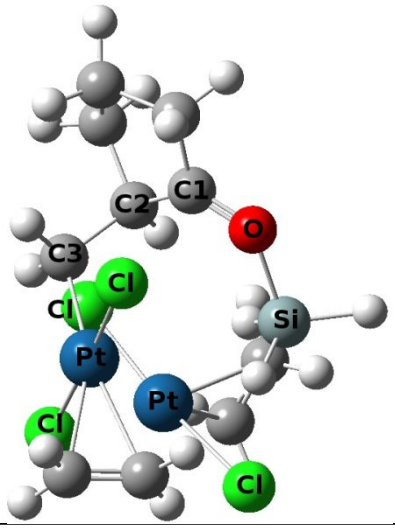
Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm

Zero-point correction= 0.285591 Electronic Energy = -2836.37107538

Internal Energy (E)= -2836.06001838 Enthalpy (H)= -2836.05907338

Gibbs Free Energy (G)=-2836.14388438 Gibbs Free Energy of Solvation=-2836.20279866

St.Pt.	General Structure	Ball & Stick model
$2DI_4$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.54831	-3.40778	-0.47402
C	-1.03283	-3.08106	0.74161
Pt	-1.37180	-1.00084	-0.50197
Cl	-3.54261	-0.67466	0.44848
Cl	0.82478	-1.30607	-1.57307
H	0.03979	-3.03720	0.91858
H	-1.69320	-2.96240	1.59646
H	-2.61691	-3.55053	-0.60792
H	-0.89890	-3.65541	-1.30896
Pt	2.20483	0.13167	-0.09732
Cl	2.07972	1.89243	-1.69870
Cl	2.13023	-1.49507	1.69517
H	4.58101	1.33092	-0.27159
C	4.11124	0.85966	0.58631
C	3.09601	1.53365	1.29093
H	4.61822	0.01510	1.04352
H	2.84126	1.21089	2.29563
H	2.79426	2.52923	0.98098
C	-1.32430	2.08832	-0.22344
O	-1.89814	1.39777	2.09541
C	-2.19503	1.96079	0.98857
C	-1.50946	0.89253	-1.22597
H	-2.49916	0.97237	-1.68943
H	-0.72796	1.03544	-1.98247
C	-3.48012	2.72604	0.84164
H	-4.32323	2.05773	1.03858
C	-3.41145	3.30500	-0.59237
H	-3.88730	2.61048	-1.28916
H	-3.90285	4.27567	-0.66825
C	-1.88435	3.38605	-0.87770
H	-1.64567	3.41092	-1.94243
H	-1.45581	4.27075	-0.39388
H	-3.47807	3.52081	1.60174
H	-0.26106	2.15264	0.03198

Frequencies

45.6999	57.6969	61.0622
69.0866	82.7116	89.3426
94.4296	103.9443	108.8858
118.5214	122.4062	129.0263
136.1196	152.4074	152.7727
158.0919	172.1792	179.5968
183.2535	190.9492	206.4568
228.1112	229.7455	242.5948
250.2956	257.5753	277.7153
282.0231	298.1143	308.6021
323.8873	346.8550	362.0849
373.4345	489.2393	518.4790
533.6288	538.8635	605.1895
675.0640	687.4034	698.5505
761.0788	774.9620	790.0592
812.0110	835.4342	844.9008
847.4254	895.3074	899.4647
918.4991	933.9653	951.7181
970.6714	987.0119	1011.3821
1025.7459	1028.4759	1034.4418
1057.8843	1058.5560	1068.0738
1074.9735	1104.6753	1174.7223
1181.2690	1219.9171	1232.4198
1237.5393	1239.0098	1266.9276
1268.5234	1278.9219	1298.8041
1313.0075	1343.0940	1347.0662
1355.0841	1428.5056	1463.0286
1470.0708	1471.3393	1500.6653
1516.9488	1561.6700	1605.6496
1643.8437	2288.9832	2339.1456
2398.3491	3064.2355	3075.3352
3082.6619	3116.5290	3123.5091
3150.5490	3150.9641	3157.3554
3168.8014	3173.3093	3177.0722
3178.9717	3179.6977	3255.5653
3274.0389	3277.4433	3289.9292

H	-0.95900	-1.01487	2.39948
H	0.53322	0.88335	1.62359
H	-0.26525	0.77203	3.93824
Si	-0.49136	0.36594	2.53654

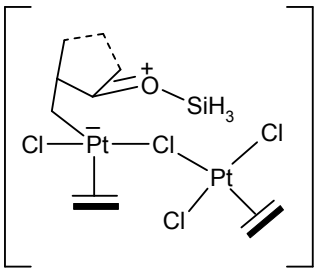
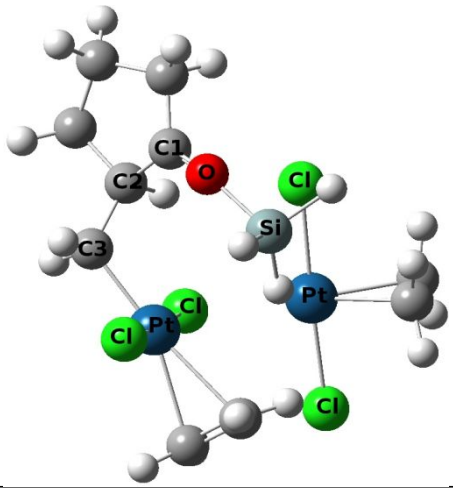
Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm

Zero-point correction= 0.285157 Electronic Energy = -2836.37628080

Internal Energy (E)= -2836.0653758 Enthalpy (H)= -2836.0644318

Gibbs Free Energy (G)=-2836.1476888 Gibbs Free Energy of Solvation=-2836.20388407

St.Pt.	General Structure	Ball & Stick model
$2DTS_4$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	0.43698	-3.27302	-0.13234
C	0.60253	-2.63730	1.05195
Pt	-1.08347	-1.40165	-0.27073
Cl	-2.65733	-2.28982	1.22594
Cl	0.48489	-0.30962	-1.82676
H	1.43483	-1.95254	1.19027
H	-0.00782	-2.88901	1.91334
H	-0.29800	-4.06443	-0.24571
H	1.12357	-3.08896	-0.95447
Pt	2.04474	0.59951	-0.14652
Cl	3.48574	-1.18626	-0.58401
Cl	0.62198	2.46731	0.37574
H	3.47346	-0.02443	2.00670
C	3.05300	0.92779	1.69895
C	3.67713	1.67460	0.69255
H	2.34771	1.40805	2.37036
H	3.45165	2.73006	0.57886
H	4.57671	1.29752	0.21689
C	-2.32885	1.27057	-0.98420
O	-2.23991	1.45719	1.47013
C	-2.49578	1.91965	0.33434
C	-2.54111	-0.24361	-1.04902
H	-3.50839	-0.50623	-0.61025
H	-2.56944	-0.50899	-2.11272
C	-3.03456	3.30206	0.20745
H	-3.61183	3.59486	1.08638
C	-3.77140	3.32129	-1.13774
H	-4.84507	3.21443	-0.96858
H	-3.61877	4.26413	-1.66346
C	-3.22590	2.10544	-1.93573
H	-4.04772	1.48175	-2.29588
H	-2.65115	2.41812	-2.80881
H	-2.12549	3.92553	0.19082
H	-1.26732	1.48620	-1.20596
H	-0.66537	1.77323	3.36751
H	-2.19149	-0.11852	3.41106

Frequencies

-90.2053	20.9641	31.7653
45.7450	58.2475	66.0335
74.2763	77.3823	84.0309
93.7786	105.5237	115.4722
123.2930	131.4841	132.9868
149.9784	154.6997	166.1906
168.1916	170.8402	188.0509
201.1541	206.9436	233.3904
237.1866	246.8223	249.9751
272.3788	286.4704	318.8422
329.7021	336.7222	386.8473
403.6292	464.3533	515.8186
519.1360	528.8058	617.3688
635.6743	670.6853	708.7608
712.7278	775.1768	784.0538
800.5156	816.1386	825.0992
844.7647	915.5844	929.9133
938.6136	955.0199	971.5171
985.7441	1010.9941	1022.2906
1024.4373	1032.8750	1057.5526
1070.7217	1073.0858	1077.2703
1098.4097	1112.9602	1204.1523
1214.3790	1215.1819	1226.2304
1245.3317	1250.5613	1261.9483
1280.9726	1287.4241	1309.4151
1329.1091	1352.6905	1362.0185
1382.2234	1441.0112	1460.4298
1463.8423	1477.1243	1506.4403
1530.6227	1569.2415	1653.0451
1718.4140	2289.2233	2364.6169
2388.6304	3011.7599	3046.4318
3075.7788	3107.1000	3114.7999
3139.6594	3156.2702	3167.2754
3172.4696	3174.0316	3176.7383
3179.2251	3180.3163	3269.0173
3271.8626	3286.6281	3288.0770

H	-0.16114	-0.17045	1.99346	
Si	-1.21652	0.63195	2.61447	

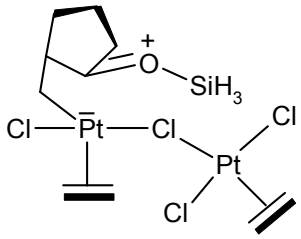
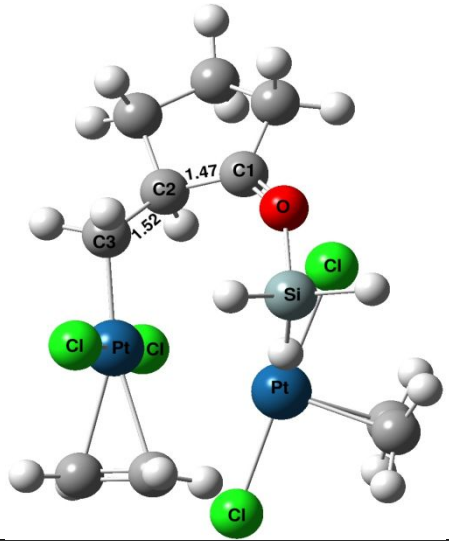
Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm

Zero-point correction= 0.284695 Electronic Energy = -2836.36849583

Internal Energy (E)= -2836.05796083 Enthalpy (H)= -2836.05701683

Gibbs Free Energy (G)=-2836.14290583 Gibbs Free Energy of Solvation=-2836.20159351

St.Pt.	General Structure	Ball & Stick model
$2DI_5$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.69396	-3.30800	-0.41793
C	-0.35003	-2.85558	0.81666
Pt	-1.57383	-1.10492	-0.26478
Cl	-3.45267	-1.86391	0.90642
Cl	0.31229	-0.36259	-1.68707
H	0.64167	-2.44681	0.98985
H	-0.99414	-3.03356	1.67226
H	-1.61634	-3.85932	-0.57394
H	0.01356	-3.24653	-1.24002
Pt	2.16195	0.08194	-0.11740
Cl	2.91612	-2.10970	-0.42480
Cl	1.46517	2.35188	0.22725
H	3.40165	-0.80333	2.05976
C	3.30804	0.20580	1.67143
C	4.09662	0.61488	0.58944
H	2.83418	0.94854	2.30568
H	4.22772	1.67180	0.38077
H	4.79611	-0.07938	0.13528
C	-1.83673	1.90345	-0.78441
O	-1.44064	2.23646	1.63398
C	-1.56154	2.65891	0.45322
C	-2.61454	0.59550	-0.68767
H	-3.45734	0.69686	0.00397
H	-3.04319	0.40119	-1.67892
C	-1.51028	4.12998	0.20723
H	-2.41382	4.54016	0.68321
C	-1.58370	4.25078	-1.31956
H	-2.03770	5.18766	-1.64428
H	-0.57374	4.19072	-1.73634
C	-2.38838	3.00596	-1.71904
H	-3.45918	3.14961	-1.53024
H	-2.26330	2.72372	-2.76534
H	-0.64362	4.57492	0.70209
H	-0.80592	1.70915	-1.14078

Frequencies

20.9540	35.2405	40.2650
56.9345	58.5630	70.6547
75.5534	82.7571	99.0688
102.2545	113.2162	121.5959
129.5520	143.3997	158.4854
166.2681	174.7544	179.0247
182.6519	190.0001	205.2327
209.1658	214.0709	222.8606
234.0514	237.6664	256.4627
289.6844	297.1861	322.3363
335.0602	365.5459	380.6654
400.9596	479.6275	512.7383
552.1464	566.9928	597.2834
622.8078	674.8161	679.7211
697.2308	749.8285	775.9644
814.2525	830.9561	838.8379
865.7380	903.4965	913.0769
942.6931	952.7369	955.3480
986.4176	1015.2498	1021.4996
1030.6389	1032.3327	1047.1226
1070.5446	1071.7746	1080.4709
1093.1982	1120.3064	1165.2302
1203.8501	1210.0812	1227.8103
1234.0588	1239.7362	1241.8615
1285.7918	1289.0499	1316.7568
1329.0641	1353.3034	1354.3634
1391.0655	1423.6828	1458.8499
1466.1506	1470.7192	1504.8800
1518.6784	1573.7467	1640.0540
1686.3396	2290.0207	2309.4421
2365.9755	2995.9414	3051.8966
3070.3128	3079.2227	3103.3501
3126.2855	3150.1722	3157.7561
3169.3713	3169.7057	3175.2750
3176.4028	3185.3543	3264.4023
3273.8182	3281.9638	3292.6800

H	-0.74634	1.35488	3.82635
H	-2.42330	0.04703	2.62067
H	-0.02316	0.04716	1.91257
Si	-1.14646	0.76071	2.53777

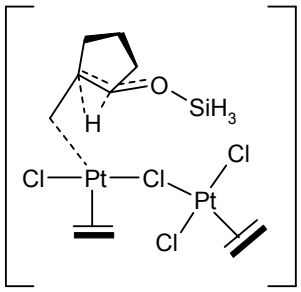
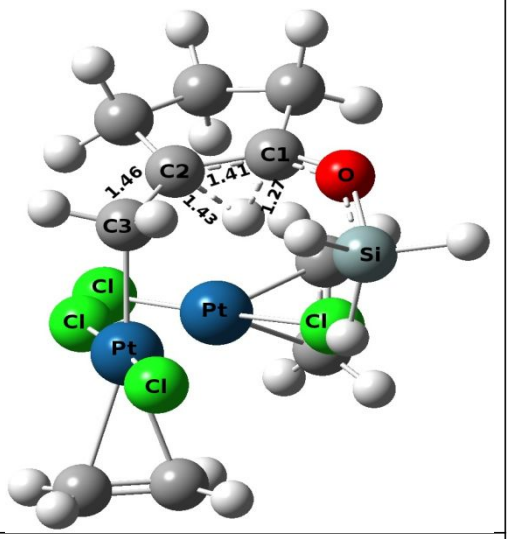
Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm

Zero-point correction= 0.284640 Electronic Energy = -2836.37492095

Internal Energy (E)= -2836.06403795 Enthalpy (H)= -2836.06309295

Gibbs Free Energy (G)=-2836.14974395 Gibbs Free Energy of Solvation=-2836.20916997

St.Pt.	General Structure	Ball & Stick model
$2DTS_5$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	1.86354	-3.04031	-0.40017
C	1.44756	-2.25742	-1.44728
Pt	1.86790	-0.87825	0.30797
Cl	4.10268	-0.70059	-0.34649
Cl	-0.42637	-1.21924	1.13344
H	0.39214	-2.10491	-1.65320
H	2.15200	-1.91609	-2.19914
H	2.90479	-3.33094	-0.30686
H	1.14278	-3.53523	0.24353
Pt	-2.20827	-0.28666	-0.28755
Cl	-3.78034	-1.20260	1.17569
Cl	-0.62101	0.71726	-1.75975
H	-4.41201	-0.95096	-1.59799
C	-3.69235	-0.16447	-1.80125
C	-3.71143	1.01466	-1.04465
H	-3.17519	-0.18989	-2.75533
H	-3.21281	1.90393	-1.41798
H	-4.44816	1.14134	-0.25797
C	0.99613	1.75664	1.39659
O	1.46785	3.12965	-0.60459
C	0.71402	2.72638	0.40879
C	2.13517	0.84371	1.46627
H	3.06640	1.31442	1.14843
H	2.23461	0.46268	2.48653
C	-0.49708	3.55791	0.77461
H	-0.13270	4.50804	1.18123
C	-1.19944	2.69639	1.83342
H	-1.74683	3.28407	2.57037
H	-1.91344	2.02042	1.34776
C	-0.06879	1.86370	2.46274
H	0.41344	2.40628	3.28721
H	-0.38411	0.88861	2.83660
H	-1.09971	3.77358	-0.11006
H	0.20283	1.56998	0.21577

Frequencies

-600.2785	16.5455	32.7465
39.3372	57.5725	68.3260
79.2782	86.0460	91.8355
96.7180	102.0642	119.1720
131.0642	132.6460	138.1102
152.7300	159.0346	164.7263
173.2132	181.8604	197.6529
200.3886	215.4808	235.8009
237.2059	257.9830	278.3824
279.3627	304.0506	328.3810
341.5769	372.3938	391.4663
403.6829	419.8770	512.6629
544.2424	565.6330	626.9986
629.7100	695.0924	709.5695
731.0197	737.0672	778.6871
790.6118	828.2860	840.2154
843.4216	877.1135	927.8648
943.8447	951.4251	973.2717
1000.6565	1007.5247	1019.1177
1030.1836	1036.3989	1039.6721
1049.8712	1064.7244	1073.5863
1078.6026	1088.1543	1145.3112
1185.7759	1210.6592	1227.9922
1233.0925	1234.4656	1247.1339
1270.5548	1286.9153	1316.2828
1335.2601	1340.5010	1351.7457
1422.3932	1468.3556	1468.5122
1479.2629	1488.9531	1504.9718
1512.2719	1574.1105	1598.3011
1618.0963	2007.0369	2285.3624
2300.3611	2333.2117	3072.0292
3084.6413	3098.6702	3104.7309
3159.2977	3165.5107	3174.0958
3176.7647	3177.3463	3180.1830
3182.2048	3183.2651	3267.9108
3274.6089	3285.5248	3289.4357

H	2.86405	3.46891	-2.61743
H	3.95151	2.39589	-0.74017
H	2.30283	1.15722	-2.08122
Si	2.72176	2.46163	-1.54855

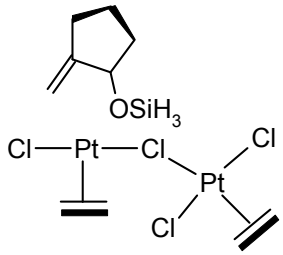
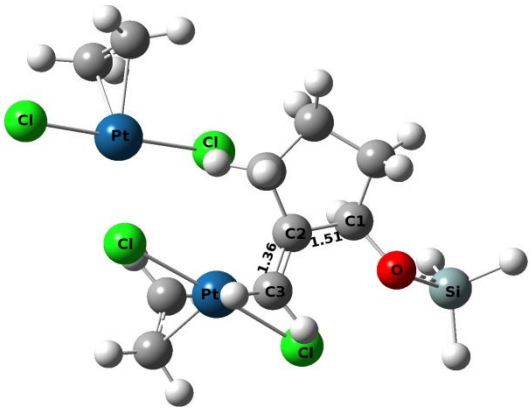
Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm

Zero-point correction= 0.282049 Electronic Energy = -2836.35555207

Internal Energy (E)= -2836.04792407 Enthalpy (H)= -2836.04698007

Gibbs Free Energy (G)=-2836.13235007 Gibbs Free Energy of Solvation=-2836.19170293

St.Pt.	General Structure	Ball & Stick model
$2DI_6$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.84288	-3.23558	0.49534
C	-0.39634	-2.35643	1.47427
Pt	-1.20196	-1.21323	-0.21828
Cl	-3.30695	-1.32004	0.77914
Cl	0.99309	-1.19273	-1.22395
H	0.65251	-2.08663	1.54341
H	-1.03039	-2.09056	2.31385
H	-1.82777	-3.68497	0.57091
H	-0.14012	-3.67760	-0.20447
Pt	2.44567	0.25701	0.19474
Cl	4.22666	-0.25086	-1.23074
Cl	0.64787	0.80465	1.66376
H	4.75192	0.33290	1.48975
C	3.82954	0.87284	1.67751
C	3.48796	1.97179	0.87570
H	3.35077	0.73434	2.64165
H	2.74363	2.68268	1.22037
H	4.14614	2.28058	0.07006
C	-1.69532	1.14393	-1.22314
O	-3.93670	1.59675	-0.46148
C	-2.58658	1.86661	-0.22792
C	-2.09830	0.04858	-1.93490
H	-3.12881	-0.28364	-1.84282
H	-1.50905	-0.29622	-2.78095
C	-2.17986	3.33431	-0.41970
H	-2.67516	3.70861	-1.32307
C	-0.66255	3.24949	-0.61496
H	-0.24105	4.14480	-1.07534
H	-0.16982	3.09313	0.34861
C	-0.47764	1.99905	-1.49471
H	-0.50285	2.26052	-2.55949
H	0.46415	1.47416	-1.32295
H	-2.48446	3.95668	0.42521
H	-2.27852	1.54547	0.78326
H	-5.80382	2.91959	0.71642
H	-6.04735	0.53300	0.50553
H	-4.41674	1.48332	2.06599

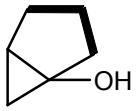
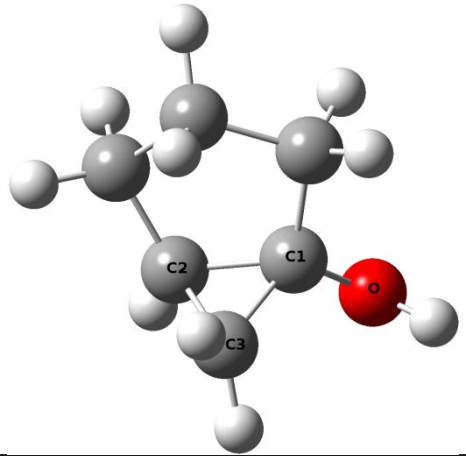
Frequencies

20.6200	30.0643	44.8951
55.4207	67.7040	69.6869
83.5087	94.3543	96.2216
100.0624	114.1416	122.9679
133.6198	141.3335	163.4788
167.1407	168.3817	180.1865
183.7931	198.0541	204.9951
207.3359	237.0878	246.4251
259.2003	287.2489	288.6019
303.5735	336.8093	339.2932
356.7635	383.0329	410.4240
432.7493	454.5912	481.1802
515.1979	577.4463	595.1605
721.4598	724.7497	725.9391
767.0737	777.7337	842.3693
844.0680	852.9900	868.2395
877.1973	903.0284	927.6864
949.1462	953.8890	996.9046
1004.8928	1008.9021	1019.0244
1030.1966	1038.8336	1042.0841
1070.1539	1073.8824	1075.4800
1079.1520	1088.8413	1166.3181
1203.6135	1230.8091	1231.9097
1237.6383	1240.4676	1262.8926
1284.1467	1309.3102	1316.9282
1323.6771	1337.9601	1356.9332
1408.7943	1437.4577	1455.3969
1471.7426	1473.1187	1501.5635
1518.6104	1575.2258	1589.8115
1641.4531	2245.4663	2251.8265
2296.0832	3019.9957	3082.6446
3085.7816	3106.6795	3150.7915
3155.9379	3160.7185	3163.2741
3180.1940	3184.2652	3189.8653
3195.2962	3265.3244	3277.9674
3286.3624	3292.9807	3302.3050

Si	-5.08347	1.62259	0.74979	

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.286790 Electronic Energy = -2836.39236936
Internal Energy (E)= -2836.07990236 Enthalpy (H)= -2836.07895836
Gibbs Free Energy (G)=-2836.16437536 Gibbs Free Energy of Solvation=-2836.22075825

St.Pt.	General Structure	Ball & Stick model
1		

Cartesian co-ordinate

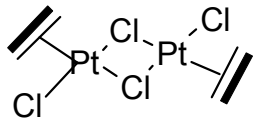
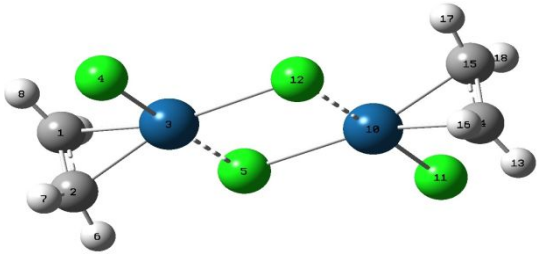
Atoms	X	Y	Z
C	-0.02874	-1.04625	-0.41140
O	1.99353	0.39244	-0.53034
C	0.74411	0.15361	0.03190
C	0.57671	-1.00247	0.97215
H	-0.06760	-0.91641	1.84608
H	1.46249	-1.61597	1.11507
H	2.55044	0.78959	0.14776
C	-0.21998	1.31359	0.15396
H	-0.00451	1.98067	0.99962
C	-1.60178	0.65758	0.25215
H	-1.83704	0.43149	1.30014
H	-2.40501	1.30620	-0.11250
C	-1.47999	-0.64601	-0.55430
H	-2.18458	-1.41405	-0.21083
H	-1.69662	-0.45897	-1.61513
H	-0.12958	1.90688	-0.76685
H	0.42174	-1.72921	-1.12738

Frequencies

217.1381	260.4429	279.5237
365.2713	394.5579	464.1024
546.8045	615.7427	700.8082
818.1708	837.6690	881.5795
907.0705	921.6870	946.9379
974.4526	999.2673	1017.8852
1047.2865	1085.0363	1109.8609
1156.5982	1196.0371	1234.5889
1258.3597	1270.3203	1309.9180
1330.3640	1341.7480	1352.6812
1413.2496	1468.2907	1476.5127
1493.8876	1515.8050	3031.2374
3036.0396	3054.6162	3083.1835
3087.0744	3114.6564	3124.6172
3180.2878	3222.6634	3881.3009

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.150417 Electronic Energy = -309.644879854
Internal Energy (E)= -309.488126854 Enthalpy (H)= -309.487182854
Gibbs Free Energy (G)=-309.524068854 Gibbs Free Energy of Solvation=-309.527141755

St.Pt.	General Structure	Ball & Stick model
b		

Cartesian co-ordinate

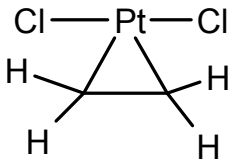
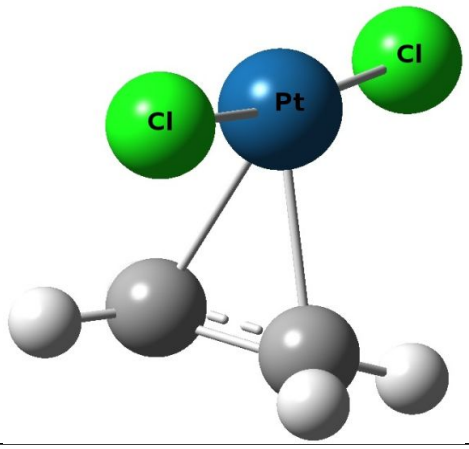
Atoms	X	Y	Z
C	-3.16324	-1.56406	-0.70042
C	-3.16341	-1.56395	0.70031
Pt	-1.77909	-0.07918	0.00000
Cl	-3.48186	1.49911	-0.00047
Cl	0.06173	-1.66790	0.00052
H	-2.58984	-2.30421	1.25636
H	-3.94427	-1.03846	1.24695
H	-3.94399	-1.03868	-1.24732
H	-2.58953	-2.30441	-1.25620
Pt	1.77909	0.07918	0.00000
Cl	3.48186	-1.49911	-0.00041
Cl	-0.06174	1.66790	0.00047
H	3.94427	1.03850	1.24693
C	3.16341	1.56397	0.70027
C	3.16325	1.56404	-0.70046
H	2.58984	2.30425	1.25629
H	2.58954	2.30437	-1.25626
H	3.94399	1.03864	-1.24734

Frequencies

16.7812	57.3971	83.4611
89.4958	95.9356	112.3590
128.3620	128.9969	174.9616
175.1650	191.4876	194.7292
248.3676	263.1560	283.0715
284.6913	357.7089	359.1469
393.5372	394.8806	467.2203
467.2624	726.5266	726.7192
826.0055	826.0502	975.8408
976.2062	1029.4951	1029.5557
1032.8103	1033.0539	1200.9967
1201.0421	1262.3914	1263.2146
1432.6769	1432.7982	1531.3010
1532.4162	3142.2375	3142.2692
3144.5248	3144.5613	3241.1654
3241.1782	3257.0540	3257.0609

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.115224 Electronic Energy = -2236.15949615
Internal Energy (E)= -2236.02872015 Enthalpy (H)= -2236.02777615
Gibbs Free Energy (G)=-2236.09111615 Gibbs Free Energy of Solvation=-2236.14255742

St.Pt.	General Structure	Ball & Stick model
c		

Cartesian co-ordinate

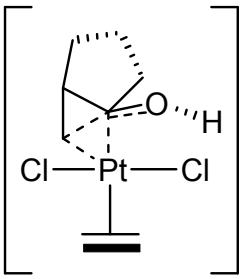
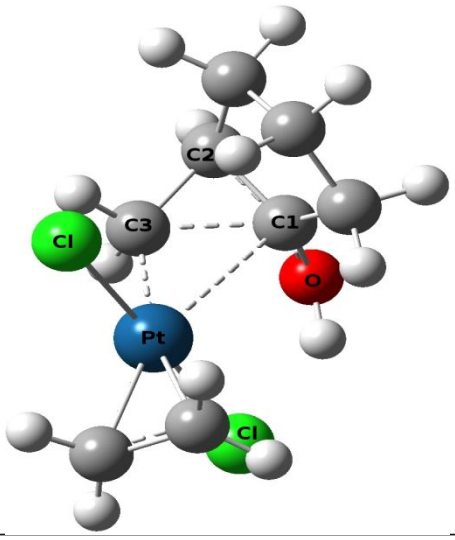
Atoms	X	Y	Z
Pt	0.00002	0.21970	0.00002
Cl	-2.32706	0.33871	0.00012
Cl	2.32709	0.33862	-0.00020
H	-0.92957	-1.91865	1.25376
C	-0.00006	-1.74806	0.71228
C	-0.00017	-1.74805	-0.71227
H	0.92951	-1.91877	1.25361
H	0.92932	-1.91876	-1.25375
H	-0.92977	-1.91863	-1.25360
Pt	1.77909	0.07918	0.00000
Cl	3.48186	-1.49911	-0.00041
Cl	-0.06174	1.66790	0.00047
H	3.94427	1.03850	1.24693
C	3.16341	1.56397	0.70027
C	3.16325	1.56404	-0.70046
H	2.58984	2.30425	1.25629
H	2.58954	2.30437	-1.25626
H	3.94399	1.03864	-1.24734

Frequencies

115.8772	129.5588	136.2589
150.4350	340.4505	363.0286
459.6862	499.2095	780.0821
823.8908	939.0218	1055.2448
1057.7554	1197.3888	1219.3178
1423.1821	1502.4458	3141.3942
3141.5787	3242.6592	3257.8357

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.056900 Electronic Energy = -1118.03818476
Internal Energy (E)= -1117.97425176 Enthalpy (H)= -1117.97330776
Gibbs Free Energy (G)=-1118.01492176 Gibbs Free Energy of Solvation=-1118.0562792

St.Pt.	General Structure	Ball & Stick model
$1MTS_1$		

Cartesian co-ordinate

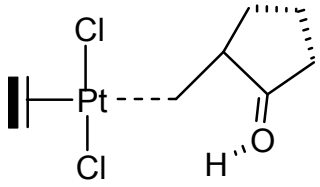
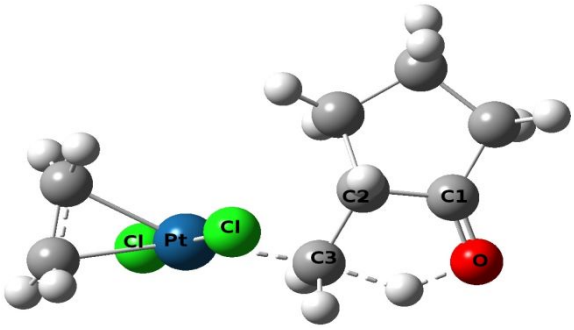
Atoms	X	Y	Z
C	2.87271	-0.21450	0.11753
C	2.27783	-0.23895	1.36927
Pt	0.68555	-0.05048	-0.15529
Cl	0.58373	-2.41704	-0.25770
Cl	0.93851	2.32607	0.00353
H	2.22602	0.66560	1.97241
H	2.08594	-1.18627	1.86917
H	3.15431	-1.14124	-0.37782
H	3.29022	0.70943	-0.27756
C	-2.73653	0.06713	-0.83852
O	-1.97909	2.21165	-0.13559
C	-2.09024	0.92731	0.10742
C	-1.22501	-0.03047	-1.28238
H	-1.08575	-1.07035	-1.59273
H	-1.05049	0.71377	-2.06140
H	-1.13222	2.56008	0.23225
C	-2.05255	0.30984	1.47547
H	-1.11921	0.47272	2.02434
C	-2.42763	-1.15417	1.23528
H	-1.52313	-1.75912	1.11262
H	-2.99512	-1.57486	2.07012
C	-3.23860	-1.14459	-0.07526
H	-3.12348	-2.07509	-0.64245
H	-4.30953	-1.00878	0.12587
H	-2.85166	0.84070	2.01925
H	-3.36431	0.51435	-1.60852

Frequencies

-194.0986	58.7326	69.9782
105.6146	123.3557	135.4526
161.7855	181.9439	187.5237
208.2740	218.8850	281.1056
298.7612	318.7451	338.0322
358.1342	391.0736	411.0886
440.6192	441.4616	577.7554
645.0397	681.0713	692.8294
705.7588	768.3825	821.8720
830.3688	873.8518	888.6549
924.7326	948.3089	1007.1457
1014.3815	1018.9822	1020.6941
1023.0877	1067.1335	1105.2470
1121.6180	1178.6001	1206.2644
1206.7564	1217.6842	1242.2176
1286.8900	1294.6983	1324.6594
1328.1662	1345.2221	1378.9488
1419.4454	1431.3526	1437.3139
1461.6303	1474.8307	1550.8544
1590.3943	3018.4374	3053.6107
3077.7030	3084.5727	3115.8519
3116.5286	3142.9341	3143.3711
3149.6208	3163.5399	3197.4401
3243.3157	3260.5978	3473.7171

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.207506 Electronic Energy = -1427.71314639
Internal Energy (E)= -1427.49156639 Enthalpy (H)= -1427.49062139
Gibbs Free Energy (G)=-1427.54723239 Gibbs Free Energy of Solvation=-1427.57235612

St.Pt.	General Structure	Ball & Stick model
$1MTS_{7a}$		

Cartesian co-ordinate

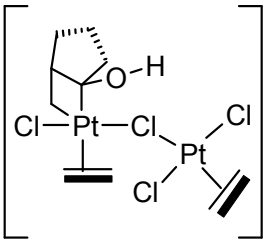
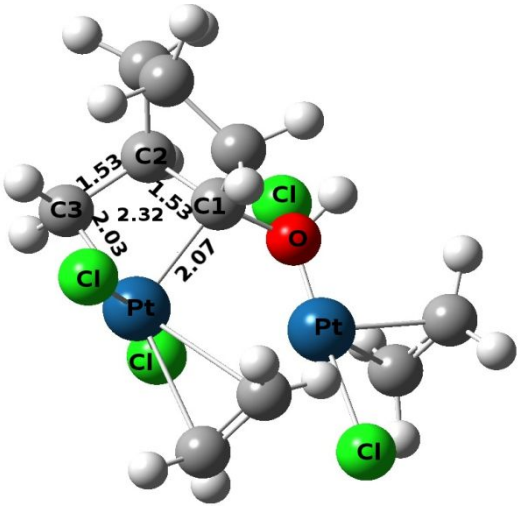
Atoms	X	Y	Z
C	2.50704	0.21145	1.40939
C	3.11849	0.25022	0.16333
Pt	0.95798	0.00650	-0.12692
Cl	0.65373	2.36693	-0.16452
Cl	1.18842	-2.34994	-0.04494
H	3.57321	-0.64572	-0.25462
H	3.37349	1.20263	-0.29792
H	2.28177	1.13558	1.93852
H	2.48573	-0.71275	1.98364
C	-1.96689	0.26627	-0.03893
O	-3.41047	-0.24094	-1.79189
C	-3.33296	0.03582	-0.58451
C	-0.99941	-0.21589	-1.09876
H	-1.84010	1.35845	0.09372
H	-0.90325	-1.29297	-1.27056
H	-0.64888	0.49012	-1.86315
C	-2.10470	-0.36495	1.35233
C	-3.53249	0.04054	1.76776
C	-4.36994	-0.03827	0.47360
H	-2.16582	-0.27642	-1.94041
H	-1.33526	-0.00815	2.04340
H	-4.89101	-0.99819	0.35668
H	-5.13279	0.74051	0.36023
H	-3.94170	-0.58788	2.56275
H	-3.52552	1.07232	2.13992
H	-2.00034	-1.45683	1.27861

Frequencies

-1018.1884	34.7359	53.7573
66.5566	100.6218	121.1979
129.5212	147.6084	156.1685
170.5996	188.3819	211.0255
250.9504	310.1865	312.1508
328.7007	354.1327	442.0772
457.7739	565.9743	592.6920
639.8452	701.4139	707.5949
754.2156	800.3921	812.6786
831.5513	845.3725	908.0392
935.6609	942.6363	960.4495
1001.7514	1008.0602	1010.9872
1015.2169	1045.9575	1133.7854
1161.2536	1175.1097	1194.0067
1204.8585	1217.6624	1254.1847
1265.8386	1281.2518	1282.4193
1296.8588	1328.4586	1344.4710
1406.8450	1409.6523	1425.9760
1465.7086	1477.0312	1544.7606
1671.2171	1817.7990	2973.8953
3048.7399	3058.2534	3059.9050
3070.9265	3114.6834	3131.6641
3142.9534	3145.0171	3148.4147
3179.9403	3242.3474	3259.7855

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.202420 Electronic Energy = -1427.68494750
Internal Energy (E)= -1427.4678345 Enthalpy (H)= -1427.4668895
Gibbs Free Energy (G)=-1427.5264365 Gibbs Free Energy of Solvation=-1427.55834167

St.Pt.	General Structure	Ball & Stick model
$1DTS_2$	 $1DTS_2$	

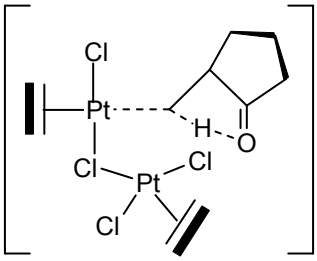
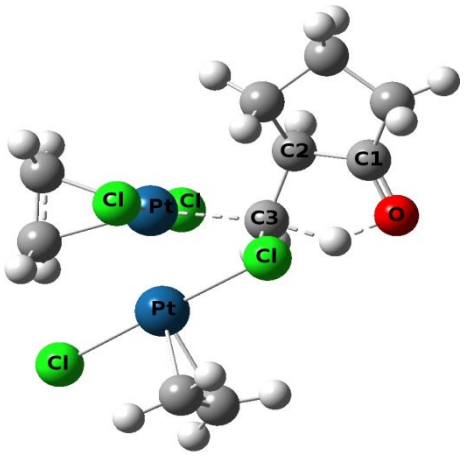
Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.30511	-2.90692	0.22514
C	-1.21347	-2.23894	1.39759
Pt	-1.79279	-0.54991	-0.40675
Cl	-4.03171	-0.80335	0.24958
Cl	0.33026	-0.48305	-1.56031
H	-0.24407	-1.89748	1.75915
H	-2.08578	-2.10156	2.03430
H	-2.24903	-3.34020	-0.10458
H	-0.40767	-3.11719	-0.35527
Pt	2.27718	0.03281	-0.02286
Cl	2.28193	2.30511	-0.69161
Cl	2.25659	-2.20685	0.73777
H	4.74832	0.75234	-0.70073
C	4.39874	0.01940	0.02458
C	3.90362	0.44164	1.27580
H	4.72806	-1.00869	-0.11585
H	3.86391	-0.26270	2.10527
H	3.89667	1.50234	1.52146
C	-1.46030	2.13282	-0.32863
O	-0.03447	0.76757	1.26559
C	-1.28045	1.12898	0.81414
C	-2.18843	1.24707	-1.34357
H	-3.27136	1.39231	-1.38101
H	-1.73578	1.21461	-2.33702
H	0.31863	1.44191	1.86443
C	-2.28420	1.46189	1.90406
H	-2.76607	0.58619	2.34756
C	-3.23036	2.48328	1.27913
H	-4.05289	1.96636	0.77030
H	-3.67508	3.14729	2.02658
C	-2.34102	3.22761	0.27590
H	-2.90741	3.76716	-0.49157
H	-1.71204	3.96190	0.79873
H	-1.69280	1.94039	2.70418
H	-0.48648	2.46563	-0.70838

Frequencies

-482.8469	36.5920	46.4976
63.5151	74.5724	79.1444
90.9422	105.4337	113.4535
121.1576	127.4182	152.1481
155.5634	174.6890	181.2878
184.4219	195.3222	206.5858
211.5930	214.1802	222.6078
254.5608	285.0462	293.6769
295.9910	303.0098	317.6329
332.4126	340.8956	360.7285
422.2007	438.0454	495.6795
513.6168	527.5180	567.8802
619.4355	630.9825	763.4901
793.3440	821.3487	823.8627
839.2731	842.2579	848.1268
908.3397	942.6476	965.5908
993.3154	997.1925	1020.2834
1030.2610	1037.4544	1039.2726
1046.1690	1065.7633	1080.7354
1105.7149	1136.8081	1159.2392
1176.6818	1204.9634	1211.2960
1221.6051	1228.2077	1242.9080
1254.5336	1275.0551	1311.9340
1318.7095	1340.7966	1344.8988
1357.4398	1409.3287	1425.7621
1427.2190	1437.2938	1463.4430
1480.8472	1516.9430	1626.6938
3002.0887	3044.7528	3071.1681
3089.8456	3097.1357	3112.7951
3131.0421	3132.7360	3137.5800
3139.2095	3141.2900	3152.1662
3189.3354	3237.7422	3238.2219
3253.4002	3264.2271	3815.0753

Statistical Thermodynamic Analysis	
Temperature=298.15 K	Pressure=1 atm
Zero-point correction= 0.265505	Electronic Energy = -2545.79436837
Internal Energy (E)= -2545.50601937	Enthalpy (H)= -2545.50507537
Gibbs Free Energy (G)=-2545.58237237	Gibbs Free Energy of Solvation=-2545.63245017

St.Pt.	General Structure	Ball & Stick model
$1DTS_{6a}$		

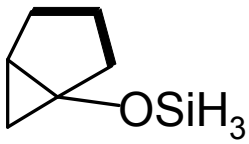
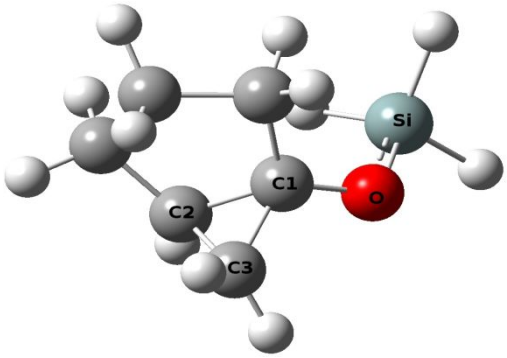
Cartesian co-ordinate

Atoms	X	Y	Z
C	0.81027	-3.22439	-0.37709
C	1.78298	-2.85900	-1.29630
Pt	1.38140	-1.12570	0.00961
Cl	3.08118	-1.83437	1.45819
Cl	-0.26466	-0.39110	-1.61068
H	1.50473	-2.55695	-2.30458
H	2.82628	-3.11963	-1.12882
H	1.08634	-3.76066	0.52879
H	-0.25209	-3.18233	-0.62141
Pt	-2.08597	0.19369	-0.08321
Cl	-2.66956	-2.08051	0.11846
Cl	-1.48737	2.49466	-0.24884
H	-4.71416	-0.06618	0.32275
C	-4.04712	0.74930	0.59643
C	-3.20108	0.62586	1.70386
H	-4.25717	1.72975	0.17265
H	-2.75525	1.51248	2.15126
H	-3.20770	-0.28484	2.29992
C	2.33144	1.72950	0.18437
O	1.57733	3.20879	1.83349
C	2.14176	3.11174	0.74081
C	1.42369	0.84158	1.01713
C	2.49389	4.16506	-0.24587
H	1.57352	4.74260	-0.41584
C	2.90009	3.34928	-1.48541
H	2.64117	3.85575	-2.41862
H	3.98697	3.19366	-1.48859
C	2.17867	1.99972	-1.31879
H	1.11301	2.08770	-1.57133
H	2.60369	1.20235	-1.93613
H	3.24159	4.87057	0.13196
H	3.38337	1.44726	0.37644
H	1.28513	1.89665	1.85422
H	0.33779	0.97579	0.91334
H	1.83996	0.34346	1.90038

Frequencies

-1164.0198	22.8575	36.6038
48.1396	60.0995	62.8687
78.8136	82.9935	88.6286
103.5412	124.1073	128.8835
143.4864	160.6985	169.1095
173.1290	176.9322	187.5115
198.2839	201.5467	226.7950
254.9427	263.5314	278.1523
313.5142	331.0663	336.6243
339.5050	343.9592	393.5992
432.2261	455.1564	471.4578
555.9548	582.7873	641.0543
683.8623	697.2275	737.1080
753.4696	816.0906	816.7513
823.5190	829.5548	841.3355
915.5051	939.7163	947.1140
981.7300	989.1650	1006.1565
1014.7049	1015.2002	1029.9885
1034.8676	1036.4072	1038.7079
1130.1944	1160.3203	1176.6651
1190.8241	1201.5796	1204.0251
1214.0714	1258.5388	1264.5537
1275.6048	1284.3382	1286.4041
1297.0257	1325.0632	1344.3038
1395.4006	1413.7039	1426.8211
1435.6652	1451.1674	1474.9125
1529.5774	1550.1844	1648.0521
1811.7650	2996.2547	3044.2768
3055.1466	3061.0936	3078.0234
3120.1151	3127.0128	3138.0982
3141.8978	3143.5226	3143.9255
3144.0055	3169.3281	3234.9029
3241.4151	3253.0283	3256.9621

Statistical Thermodynamic Analysis	
Temperature=298.15 K	Pressure=1 atm
Zero-point correction= 0.260888	Electronic Energy = -2545.78015172
Internal Energy (E)= -2545.49609972	Enthalpy (H)= -2545.49515572
Gibbs Free Energy (G)=-2545.57503772	Gibbs Free Energy of Solvation=-2545.63381852

St.Pt.	General Structure	Ball & Stick model
2		

Cartesian co-ordinate

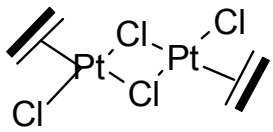
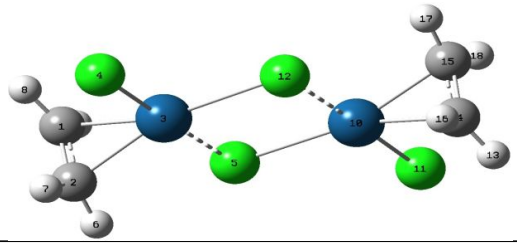
Atoms	X	Y	Z
C	-0.84929	0.80002	0.78844
O	1.29111	0.57417	-0.55253
C	-0.08162	0.36522	-0.43220
C	-0.95219	1.56870	-0.50964
H	-1.87370	1.54832	-1.08943
H	-0.41704	2.51389	-0.53732
C	-0.65028	-0.95878	-0.89323
H	-0.67545	-1.06366	-1.98467
C	-2.03558	-1.02864	-0.24360
H	-2.77835	-0.54705	-0.89148
H	-2.37837	-2.05706	-0.09115
C	-1.89856	-0.24946	1.07511
H	-2.85708	0.16243	1.41554
H	-1.52949	-0.91275	1.87099
H	-0.00832	-1.76602	-0.50496
H	-0.32727	1.28527	1.61075
H	3.65213	0.38793	0.28850
H	1.89325	-0.54276	1.69846
H	2.57270	-1.68846	-0.30965
Si	2.37166	-0.34970	0.30253

Frequencies

-64.9829	106.9780	132.1657
243.0256	259.7381	357.2639
406.3416	456.0562	514.1953
610.0253	662.8021	733.6958
768.4077	810.2767	814.9997
862.6499	877.1533	910.9454
953.1021	963.7857	972.3776
979.8378	988.8437	1005.9316
1012.0153	1032.5957	1057.3774
1105.5127	1113.5360	1169.3389
1198.0354	1248.2562	1266.0883
1284.3519	1326.9218	1337.4172
1353.1683	1396.5261	1464.7891
1470.9606	1486.1143	1509.3963
2267.7083	2278.5152	2315.5390
3015.6562	3026.6055	3060.4644
3082.8605	3090.3868	3117.4025
3125.8485	3169.7338	3225.4169

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.166304 Electronic Energy = -600.345219215
Internal Energy (E)= -600.171275215 Enthalpy (H)= -600.170331215
Gibbs Free Energy (G)=-600.211065215 Gibbs Free Energy of Solvation=-600.21317576

St.Pt.	General Structure	Ball & Stick model
b		

Cartesian co-ordinate

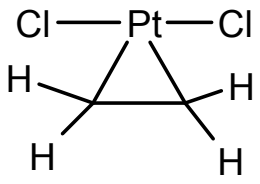
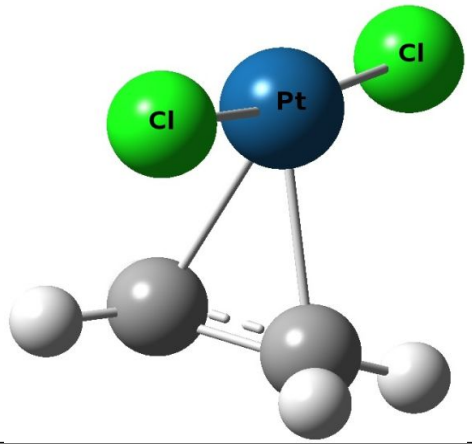
Atoms	X	Y	Z
C	-3.16324	-1.56406	-0.70042
C	-3.16341	-1.56395	0.70031
Pt	-1.77909	-0.07918	0.00000
Cl	-3.48186	1.49911	-0.00047
Cl	0.06173	-1.66790	0.00052
H	-2.58984	-2.30421	1.25636
H	-3.94427	-1.03846	1.24695
H	-3.94399	-1.03868	-1.24732
H	-2.58953	-2.30441	-1.25620
Pt	1.77909	0.07918	0.00000
Cl	3.48186	-1.49911	-0.00041
Cl	-0.06174	1.66790	0.00047
H	3.94427	1.03850	1.24693
C	3.16341	1.56397	0.70027
C	3.16325	1.56404	-0.70046
H	2.58984	2.30425	1.25629
H	2.58954	2.30437	-1.25626
H	3.94399	1.03864	-1.24734
H	2.57270	-1.68846	-0.30965
Si	2.37166	-0.34970	0.30253

Frequencies

16.7812	57.3971	83.4611
89.4958	95.9356	112.3590
128.3620	128.9969	174.9616
175.1650	191.4876	194.7292
248.3676	263.1560	283.0715
284.6913	357.7089	359.1469
393.5372	394.8806	467.2203
467.2624	726.5266	726.7192
826.0055	826.0502	975.8408
976.2062	1029.4951	1029.5557
1032.8103	1033.0539	1200.9967
1201.0421	1262.3914	1263.2146
1432.6769	1432.7982	1531.3010
1532.4162	3142.2375	3142.2692
3144.5248	3144.5613	3241.1654
3241.1782	3257.0540	3257.0609

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.115224 Electronic Energy = -2236.15949615
Internal Energy (E)= -2236.02872015 Enthalpy (H)= -2236.02777615
Gibbs Free Energy (G)=-2236.09111615 Gibbs Free Energy of Solvation=-2236.14698202

St.Pt.	General Structure	Ball & Stick model
c		

Cartesian co-ordinate

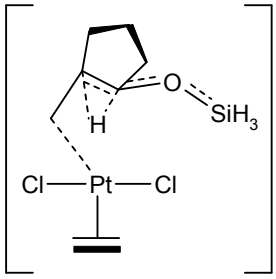
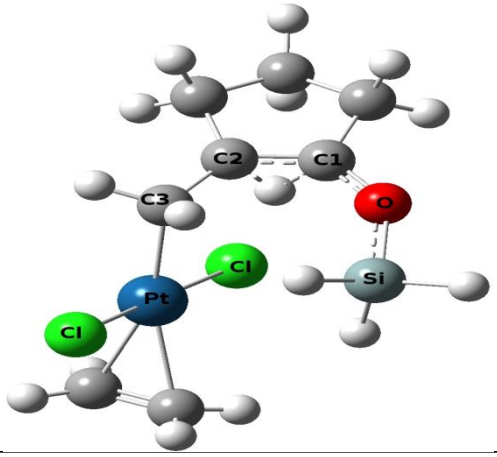
Atoms	X	Y	Z
Pt	0.00002	0.21970	0.00002
Cl	-2.32706	0.33871	0.00012
Cl	2.32709	0.33862	-0.00020
H	-0.92957	-1.91865	1.25376
C	-0.00006	-1.74806	0.71228
C	-0.00017	-1.74805	-0.71227
H	0.92951	-1.91877	1.25361
H	0.92932	-1.91876	-1.25375
H	-0.92977	-1.91863	-1.25360
Pt	1.77909	0.07918	0.00000
Cl	3.48186	-1.49911	-0.00041
Cl	-0.06174	1.66790	0.00047
H	3.94427	1.03850	1.24693
C	3.16341	1.56397	0.70027
C	3.16325	1.56404	-0.70046
H	2.58984	2.30425	1.25629
H	2.58954	2.30437	-1.25626
H	3.94399	1.03864	-1.24734
H	2.57270	-1.68846	-0.30965
Si	2.37166	-0.34970	0.30253

Frequencies

115.8772	129.5588	136.2589
150.4350	340.4505	363.0286
459.6862	499.2095	780.0821
823.8908	939.0218	1055.2448
1057.7554	1197.3888	1219.3178
1423.1821	1502.4458	3141.3942
3141.5787	3242.6592	3257.8357

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.056900 Electronic Energy = -1118.03818476
Internal Energy (E)= -1117.97425176 Enthalpy (H)= -1117.97330776
Gibbs Free Energy (G)=-1118.01492176 Gibbs Free Energy of Solvation=-1118.063618

St.Pt.	General Structure	Ball & Stick model
$2MTS_5$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-2.81207	-1.16653	0.90424
C	-2.54910	0.02862	1.53827
Pt	-1.00528	-0.26046	-0.07868
Cl	-2.36589	0.91201	-1.59887
Cl	0.42386	-1.39519	1.50431
H	-1.98947	0.05205	2.47186
H	-3.07401	0.93658	1.24775
H	-3.54823	-1.21823	0.10461
H	-2.46677	-2.10868	1.32559
C	1.91207	-0.20529	-0.93210
O	2.35058	1.67505	0.58201
C	2.66284	0.54442	-0.01845
C	0.57322	0.08269	-1.44604
H	0.46389	1.12041	-1.77565
H	0.33554	-0.58125	-2.28508
C	4.04481	-0.01799	0.16203
H	4.73113	0.59354	-0.44078
C	3.90935	-1.44552	-0.37808
H	4.83486	-1.82839	-0.81457
H	3.62796	-2.11674	0.44298
C	2.75292	-1.37191	-1.38571
H	3.10004	-1.14843	-2.40456
H	2.15454	-2.28919	-1.43726
H	4.37612	0.04673	1.20286
H	1.84668	-0.49804	0.38713
H	1.54867	3.84732	1.40986
H	0.28271	2.92694	-0.44528
H	0.07127	1.96049	1.80668
Si	0.95447	2.62457	0.83051

Frequencies

-573.7448	40.0397	52.6199
73.3681	89.9623	92.2164
119.3750	138.3662	142.3183
158.6968	171.4262	177.1271
191.1287	199.9790	222.0503
279.3193	296.4955	306.3441
335.3055	359.3427	400.8647
414.4190	531.2263	570.3708
620.8804	647.3749	678.4177
700.4578	715.1659	731.8388
742.9288	817.1158	839.2493
874.2340	929.8724	937.9481
942.4434	973.3954	983.9153
992.3097	994.4997	1007.9053
1011.6907	1029.8470	1060.3293
1065.0585	1147.6883	1177.1762
1206.2546	1212.7150	1224.2277
1259.6471	1264.5634	1295.3645
1307.2501	1328.0104	1335.1414
1416.5619	1424.9500	1453.1645
1456.5087	1466.0374	1479.9110
1554.7677	1566.2885	1771.8099
2330.0402	2338.5654	2364.7118
3046.7036	3050.4250	3069.0396
3083.4812	3107.8788	3126.9486
3141.4078	3143.1967	3147.4563
3154.6169	3239.4995	3257.4606

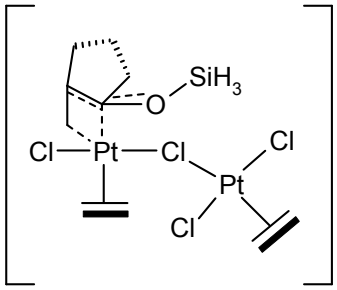
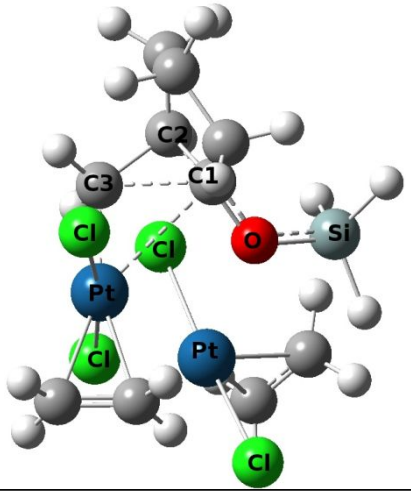
Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm

Zero-point correction= 0.220091 Electronic Energy = -1718.39336781

Internal Energy (E)= -1718.15627681 Enthalpy (H)= -1718.15533281

Gibbs Free Energy (G)=-1718.21942581 Gibbs Free Energy of Solvation=-1718.25040221

St.Pt.	General Structure	Ball & Stick model
$2DTS_1$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-2.09785	-3.06996	0.11930
C	-1.64019	-2.48981	1.28450
Pt	-1.83330	-0.86057	-0.24768
Cl	-4.10116	-0.57417	0.29063
Cl	0.37657	-1.38814	-1.06628
H	-0.57870	-2.49006	1.53548
H	-2.33974	-2.20866	2.06945
H	-3.15913	-3.25770	-0.02872
H	-1.40663	-3.55771	-0.56527
Pt	2.30539	-0.17657	-0.17549
Cl	2.11141	1.43834	-1.90239
Cl	2.40652	-1.67632	1.64338
H	4.71127	0.25274	-1.23169
C	4.44383	-0.02092	-0.21247
C	3.94348	0.94206	0.67124
H	4.82409	-0.96862	0.16536
H	3.96309	0.75004	1.74289
H	3.85058	1.97602	0.34234
C	-1.29401	2.43984	-0.72724
O	-0.40141	1.32716	1.27430
C	-1.39582	1.82185	0.57177
C	-1.71395	1.03069	-1.28815
H	-2.70869	1.11018	-1.73210
H	-0.92044	0.75583	-1.98827
C	-2.68423	2.18398	1.23617
H	-3.19863	1.34572	1.71382
C	-3.48239	2.91581	0.15846
H	-4.13419	2.19654	-0.34997
H	-4.12136	3.70085	0.57160
C	-2.41255	3.46645	-0.79980
H	-2.77986	3.60514	-1.82221
H	-2.03543	4.43633	-0.44691
H	-2.35691	2.87553	2.03404
H	-0.29315	2.71102	-1.07165
H	1.68590	1.30665	2.68756
H	1.58552	2.97241	0.85717

Frequencies

-211.6415	30.0328	39.4400
47.3258	49.2341	74.8379
81.0455	95.1857	97.9873
107.5600	120.9163	129.9598
137.5762	141.2689	149.2016
156.9276	164.1535	166.4409
171.3759	193.9628	194.5539
222.5282	252.7067	276.8323
296.4424	297.3109	306.4960
315.0078	322.8531	335.0808
337.5786	388.2036	410.9665
414.1409	437.0256	467.2268
485.9713	550.2058	621.8863
656.2974	715.8593	730.1358
737.8298	743.0408	749.7987
791.2820	820.7729	826.8367
828.9765	878.5803	897.0517
926.9863	966.5414	970.7420
978.7268	992.0854	1001.1189
1003.8267	1010.9668	1020.1535
1021.8714	1037.1560	1038.3341
1041.7401	1078.7297	1108.1239
1150.5466	1190.3845	1206.6240
1212.2674	1218.9739	1240.5562
1264.9927	1265.2639	1294.9958
1299.3907	1317.5124	1325.3466
1348.5727	1383.6884	1414.4275
1423.8046	1431.4957	1466.3817
1478.0656	1529.5483	1534.5088
1560.9745	2297.2774	2332.0253
2382.9545	2993.5944	3046.8195
3078.8344	3084.2899	3118.3936
3134.8486	3134.9809	3136.1644
3140.3605	3143.1445	3144.6670
3149.7745	3194.9350	3237.3150
3238.8343	3253.6187	3258.7846

H	0.20113	3.24201	2.82065	
Si	0.86532	2.25786	1.92970	

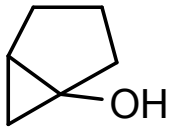
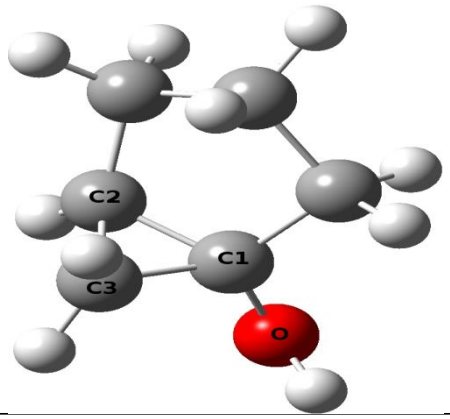
Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm

Zero-point correction= 0.281857 Electronic Energy = -2836.48683554

Internal Energy (E)= -2836.17994354 Enthalpy (H)= -2836.17899854

Gibbs Free Energy (G)=-2836.26193854 Gibbs Free Energy of Solvation=-2836.31602428

St.Pt.	General Structure	Ball & Stick model
1		

Cartesian co-ordinate

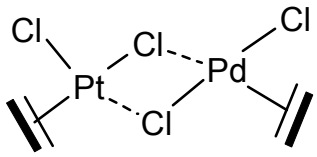
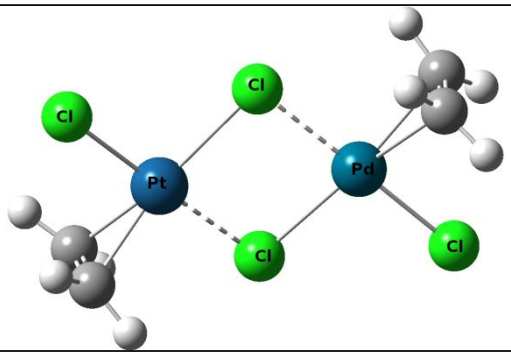
Atoms	X	Y	Z
C	-0.03028	-1.05068	-0.41217
O	2.00227	0.38667	-0.52845
C	0.74672	0.15044	0.02888
C	0.57091	-1.00145	0.97587
H	-0.07826	-0.90477	1.84133
H	1.45155	-1.61605	1.12589
H	2.55325	0.78977	0.15229
C	-0.21550	1.31928	0.14884
H	0.00395	1.98045	0.99447
C	-1.60371	0.66350	0.25353
H	-1.83307	0.43898	1.29968
H	-2.40237	1.31192	-0.11380
C	-1.48666	-0.64650	-0.55506
H	-2.18673	-1.41105	-0.20396
H	-1.70299	-0.45950	-1.61272
H	-0.12787	1.90700	-0.77205
H	0.41549	-1.73776	-1.12287

Frequencies

218.7186	249.7708	346.9290
369.7460	389.5136	457.7402
550.7976	618.5293	712.7037
826.0150	847.4259	898.7741
916.2375	921.1445	967.1094
987.7957	1012.3285	1039.2903
1065.7574	1099.6435	1125.4589
1174.1473	1211.8734	1253.4906
1274.9256	1290.3576	1330.2710
1349.9471	1361.9481	1370.9121
1425.9593	1501.3010	1506.3580
1516.1429	1536.0356	3069.6620
3076.7137	3096.2241	3117.9686
3122.9285	3145.5093	3150.0545
3221.3029	3241.3378	3880.0908

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.152288 Electronic Energy = -309.718741856
Internal Energy (E)= -309.560224856 Enthalpy (H)= -309.559280856
Gibbs Free Energy (G)=-309.595983856 Gibbs Free Energy of Solvation=-309.599133984

St.Pt.	General Structure	Ball & Stick model
b_{Pd}		

Cartesian co-ordinate

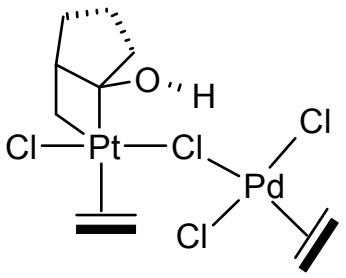
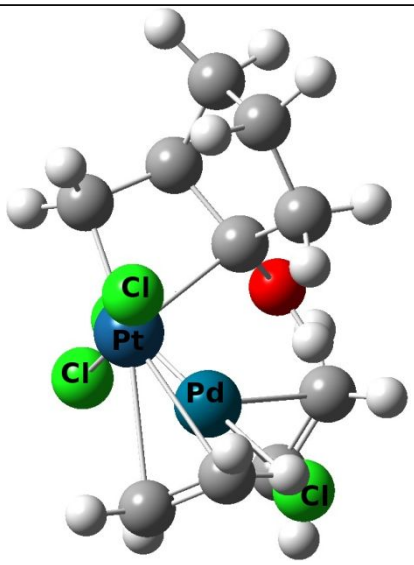
Atoms	X	Y	Z
C	-2.94641	-1.55414	-0.56972
C	-2.81419	-1.53627	0.82573
Pt	-1.52907	-0.07182	-0.01838
Cl	-3.22503	1.49033	0.14284
Cl	0.30351	-1.66640	-0.18215
H	-2.18513	-2.26582	1.32712
H	-3.54090	-1.00610	1.43273
H	-3.77550	-1.03886	-1.04373
H	-2.42196	-2.29872	-1.16119
Cl	3.71962	-1.46273	0.13777
Cl	0.20305	1.69304	-0.18615
H	4.08352	1.03826	1.41772
C	3.40436	1.62225	0.80493
C	3.53376	1.63200	-0.56244
H	2.72855	2.31061	1.30461
H	2.96355	2.32847	-1.17062
H	4.31748	1.05716	-1.04566
	2.02202	0.07766	-0.02452

Frequencies

11.4059	52.7471	80.9671
89.0270	93.8371	110.8168
126.8404	131.6688	143.5943
162.8891	181.6858	192.9596
234.2716	253.8482	271.1481
280.7738	281.8292	350.1532
354.5792	386.0877	407.1973
512.1322	601.5285	771.2757
832.8304	835.2863	1021.0858
1040.9809	1058.0488	1061.0577
1074.0606	1079.0580	1226.0963
1236.8976	1287.3608	1337.1857
1471.6477	1471.9254	1574.7216
1615.1968	3173.1520	3180.5180
3181.6300	3185.6525	3271.8199
3280.7111	3289.6790	3297.2171

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.116567 Electronic Energy = -2243.56719436
Internal Energy (E)= -2243.43473536 Enthalpy (H)= -2243.43379136
Gibbs Free Energy (G)=-2243.49804136 Gibbs Free Energy of Solvation=-2243.51562026

St.Pt.	General Structure	Ball & Stick model
$1PdI_1$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.00639	-2.92739	-0.22786
C	-1.44683	-2.59738	1.00041
Pt	-1.54154	-0.41062	-0.51170
Cl	-3.83058	-0.64899	-0.08027
Cl	0.65221	-0.32190	-1.54432
H	-0.73699	-2.34657	1.78374
H	-2.50190	-2.63387	1.25091
H	-1.69645	-3.26428	-0.99899
H	0.05604	-2.93393	-0.45315
Cl	3.44003	1.55436	-1.48259
Cl	1.83088	-1.68074	1.56630
H	5.28529	-0.14113	-0.16473
C	4.67853	-0.38931	0.70004
C	4.11597	0.60764	1.46233
H	4.65356	-1.42109	1.03688
H	3.64663	0.37240	2.41248
H	4.27729	1.65034	1.20865
C	-1.22429	2.25603	-0.00714
O	0.25703	0.88937	1.32781
C	-1.00916	1.11107	0.97225
C	-1.84590	1.48237	-1.18188
H	-2.91805	1.64250	-1.29969
H	-1.30518	1.59614	-2.12077
H	0.38023	0.07638	1.85864
C	-2.07786	1.16194	2.06172
H	-2.54518	0.20034	2.27790
C	-3.05863	2.24210	1.57754
H	-3.83768	1.78193	0.96554
H	-3.54343	2.75056	2.41316
C	-2.19114	3.19081	0.72997
H	-2.77734	3.80154	0.03868
H	-1.62104	3.86587	1.37770
H	-1.54481	1.50118	2.95928

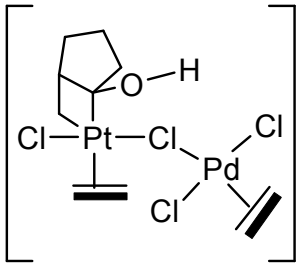
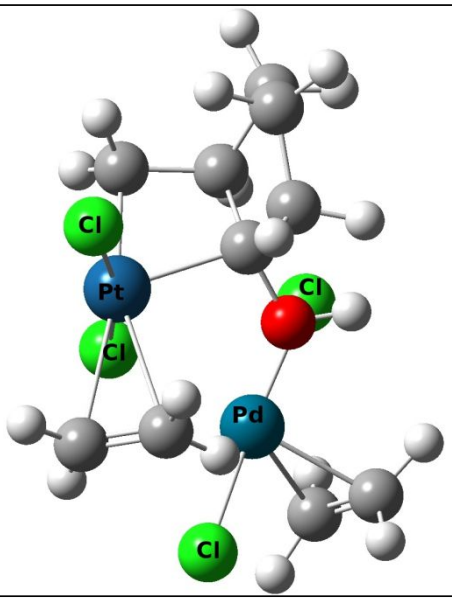
Frequencies

14.6685	44.7163	47.4100
67.9817	76.0388	86.3552
91.8680	99.8159	105.6784
124.5404	134.1971	144.8381
149.1115	159.2624	169.5988
186.0188	192.8834	201.4642
214.2996	228.3859	237.7490
255.6057	268.8199	272.2843
287.9075	297.4135	305.7184
331.2298	336.0700	359.5856
396.0639	436.6850	454.3758
524.0818	573.2989	617.1500
628.0824	656.1536	681.7741
809.6157	831.1665	836.6927
845.8834	862.4710	880.9396
923.0933	956.7357	1008.3958
1034.9491	1037.2913	1045.4343
1046.0844	1050.1643	1064.4445
1072.2125	1086.5344	1107.0260
1135.4444	1165.1091	1190.1482
1203.2604	1237.5631	1241.4216
1245.3114	1281.4793	1300.6496
1320.9807	1327.7416	1331.1166
1359.1300	1369.3900	1371.8507
1435.8885	1459.8824	1462.2681
1469.8703	1484.4886	1502.1874
1529.8508	1607.8417	1671.4064
3074.9155	3083.9500	3122.0446
3126.8966	3136.0820	3146.8285
3164.3158	3167.4432	3176.5045
3178.3322	3181.2488	3194.8258
3211.0400	3268.5538	3282.1436
3287.2791	3304.4523	3624.3096

H	-0.26701	2.70443	-0.28448	
	2.60871	-0.05355	-0.02828	

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.269721 Electronic Energy = -2553.29416455
Internal Energy (E)= -2553.00070855 Enthalpy (H)= -2552.99976355
Gibbs Free Energy (G)=-2553.08008755 Gibbs Free Energy of Solvation=-2553.09687341

St.Pt.	General Structure	Ball & Stick model
$1PdTS_1$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.93837	-2.95093	0.29578
C	-0.86730	-2.25264	1.44587
Pt	-1.53575	-0.54490	-0.40257
Cl	-3.73024	-0.80946	0.35065
Cl	0.54546	-0.46839	-1.60693
H	0.08610	-1.85949	1.78791
H	-1.74437	-2.11914	2.07360
H	-1.87129	-3.41011	-0.02459
H	-0.04024	-3.12933	-0.29021
Cl	2.50884	2.33662	-0.61500
Cl	2.54901	-2.20687	0.62438
H	4.97254	0.86855	-0.60564
C	4.68552	0.09759	0.10274
C	4.15210	0.44080	1.32863
H	4.97987	-0.92705	-0.10082
H	4.03358	-0.31186	2.10131
H	4.03326	1.48624	1.59415
C	-1.18507	2.10057	-0.37875
O	0.26299	0.75235	1.21651
C	-1.00037	1.09578	0.77029
C	-1.97281	1.20106	-1.34462
H	-3.05223	1.35168	-1.32705
H	-1.57155	1.15500	-2.35589
H	0.56000	1.41188	1.86066
C	-1.98144	1.46808	1.88173
H	-2.48071	0.61144	2.33432
C	-2.91781	2.50751	1.25630
H	-3.75206	2.00218	0.76159
H	-3.33544	3.18471	2.00397
C	-2.02368	3.22795	0.23192
H	-2.59042	3.77344	-0.52716
H	-1.36611	3.94372	0.73865
H	-1.37137	1.94716	2.66246

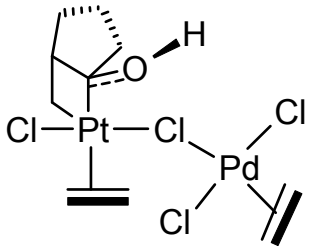
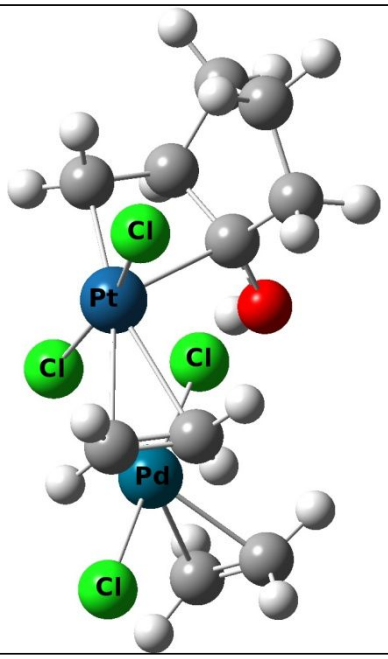
Frequencies

-415.3168	34.1558	43.5094
57.8161	68.0117	79.2132
84.4533	95.0319	114.6458
121.7297	127.9008	143.5888
148.2554	152.5157	167.6906
176.1466	180.9581	185.7458
196.8499	215.5786	240.4237
250.9521	281.9512	287.8531
291.8849	298.3860	306.7845
314.7967	325.6339	339.0302
372.3674	418.6050	431.5147
436.0198	553.6261	579.0443
635.1718	636.4543	660.8598
811.1842	836.7442	840.7638
845.4843	855.7679	881.3622
924.5992	953.9587	1005.2598
1029.0086	1034.3609	1039.9948
1046.2548	1047.0846	1058.5885
1066.4631	1085.7400	1095.8462
1142.8848	1148.6410	1179.7787
1197.8317	1240.4738	1242.3458
1244.8711	1250.3469	1284.3198
1292.8113	1322.6242	1332.6765
1337.8153	1368.1042	1372.3778
1374.2001	1457.3388	1465.8580
1475.9753	1476.4635	1500.0498
1522.4570	1600.3870	1667.2501
3038.7897	3076.4788	3116.8404
3128.8108	3141.4874	3149.9291
3160.9210	3168.7664	3174.1551
3174.8833	3183.3698	3187.0787
3215.3388	3262.2188	3284.1352
3285.1608	3301.0423	3826.2371

H	-0.21967	2.39612	-0.79678	
	2.49713	0.04372	-0.05575	

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.268567 Electronic Energy = -2553.27977345
Internal Energy (E)= -2552.98795045 Enthalpy (H)= -2552.98700645
Gibbs Free Energy (G)=-2553.06530645 Gibbs Free Energy of Solvation=-2553.08421885

St.Pt.	General Structure	Ball & Stick model
$1PdI_2$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.47189	-2.81320	0.58656
C	-0.32507	-1.91266	1.58073
Pt	-1.42733	-0.67378	-0.33009
Cl	-3.52122	-1.35722	0.43555
Cl	0.65785	-0.25341	-1.52844
H	0.61568	-1.38316	1.70961
H	-1.10174	-1.76503	2.32573
H	-1.37618	-3.41003	0.50577
H	0.34848	-3.01138	-0.09857
Cl	2.24253	2.50159	-0.36176
Cl	3.01122	-2.11845	0.18347
H	4.96115	1.49062	-0.07515
C	4.74977	0.56327	0.44879
C	3.99962	0.56701	1.59777
H	5.26183	-0.33906	0.12909
H	3.91397	-0.33215	2.19979
H	3.60949	1.49797	1.99758
C	-1.82132	2.03393	-0.58513
O	-0.15376	1.48332	1.19582
C	-1.36912	1.37802	0.71470
C	-2.23735	0.81496	-1.43387
H	-3.31847	0.68600	-1.49596
H	-1.77881	0.80884	-2.42323
H	0.50151	1.81909	0.53255
C	-2.48145	1.44913	1.74657
H	-2.69748	0.49853	2.23292
C	-3.66655	2.05553	0.98139
H	-4.27376	1.25505	0.55191
H	-4.30708	2.65249	1.63310
C	-3.00710	2.89631	-0.12726
H	-3.68295	3.12039	-0.95643
H	-2.64106	3.84500	0.28077

Frequencies

27.9465	37.8830	50.7394
64.5516	73.9943	76.3504
96.9931	112.4180	117.4425
134.0851	140.0213	144.1941
150.1906	154.7064	160.8227
170.8864	174.1955	179.1997
184.3879	228.3377	232.5281
262.0085	271.3646	277.3534
288.6447	293.5089	296.5670
334.0034	335.7746	359.1489
380.5767	453.8271	467.5324
514.2634	573.2942	593.7498
623.5686	664.7249	781.4769
809.6436	835.5642	839.5277
841.8084	856.9690	875.7912
917.7346	954.7105	1008.9354
1031.4952	1037.3954	1038.0006
1046.8139	1053.7263	1059.1719
1061.5225	1078.7599	1100.7504
1146.2117	1176.9389	1182.5697
1202.1649	1239.6052	1243.2598
1249.1325	1289.3583	1311.3685
1323.0304	1329.4940	1334.5374
1359.9890	1369.3363	1394.6417
1461.9413	1464.1625	1465.7602
1474.0057	1500.0238	1507.9782
1521.5872	1611.5643	1663.4185
3087.0446	3088.2955	3117.1401
3119.9218	3123.5341	3146.2623
3167.1347	3174.0274	3174.6310
3180.0248	3184.5271	3191.2706
3198.3039	3263.8241	3281.0362
3281.3894	3301.3375	3327.5760

H	-2.10306	2.14607	2.50433	
H	-1.00030	2.58648	-1.05278	
	2.62558	0.15643	-0.12548	

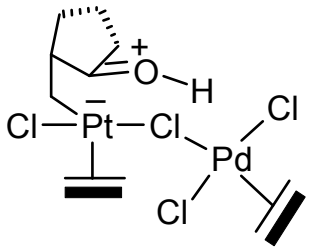
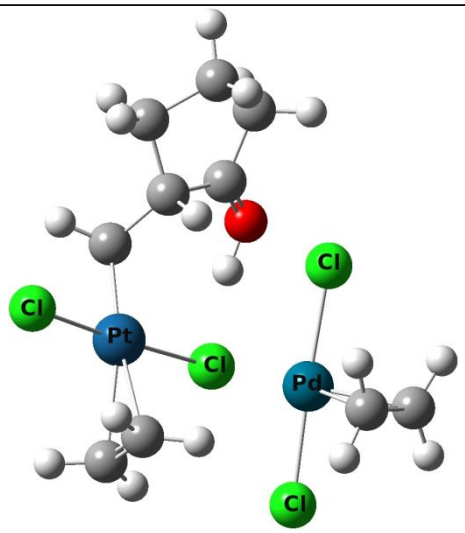
Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm

Zero-point correction= 0.269190 Electronic Energy = -2553.30283733

Internal Energy (E)= -2553.00985033 Enthalpy (H)= -2553.00890633

Gibbs Free Energy (G)=-2553.08898233 Gibbs Free Energy of Solvation=-2553.10441906

St.Pt.	General Structure	Ball & Stick model
$1PdI_3$		

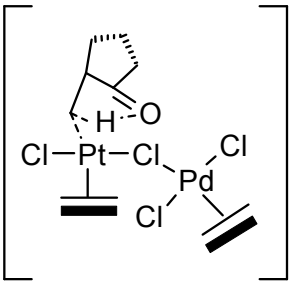
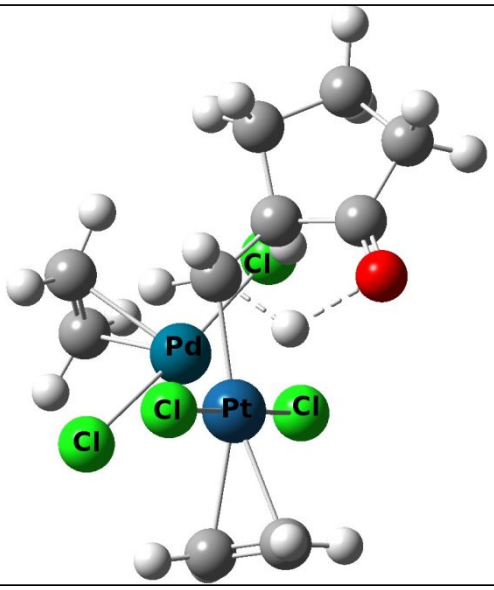
Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.58428	-3.16525	0.13482
C	-0.76544	-2.52966	-1.04976
Pt	0.97037	-1.33953	0.14720
Cl	2.47383	-2.41180	-1.27529
Cl	-0.53305	-0.09294	1.69453
H	-1.58040	-1.82173	-1.16982
H	-0.19781	-2.80556	-1.93197
H	0.12549	-3.98142	0.22845
H	-1.24166	-2.95949	0.97560
Cl	-3.61079	-0.99256	0.67977
Cl	-0.76411	2.45416	-0.83519
H	-3.75627	-0.13657	-2.02545
C	-3.34607	0.86016	-1.89600
C	-3.89000	1.71759	-0.96883
H	-2.61328	1.21802	-2.61250
H	-3.59102	2.76087	-0.94441
H	-4.73040	1.40496	-0.35714
C	2.38543	1.27879	-0.04996
O	1.07692	2.35309	1.73115
C	1.86856	2.41167	0.75292
C	2.47446	-0.07962	0.66058
H	1.66167	1.23757	-0.88575
H	3.41793	-0.54863	0.37376
H	2.48887	0.05128	1.75090
C	3.68343	1.88309	-0.63249
C	3.31872	3.35517	-0.87542
C	2.47557	3.71252	0.35923
H	0.62092	1.45074	1.82446
H	3.98980	1.34794	-1.53204
H	3.10559	4.02832	1.20281
H	1.69950	4.47070	0.22654
H	4.18659	4.00556	-0.98931
H	2.70341	3.44389	-1.77583
H	4.48977	1.79638	0.10551
	-2.16142	0.69049	-0.01935

Frequencies

22.8944	37.5820	50.8590
56.6938	60.5876	70.3776
81.7779	85.2731	105.6637
119.0624	125.6906	130.2316
147.3536	159.5388	170.4207
172.6262	185.1624	197.0658
197.3972	218.1678	223.0402
229.1925	242.4963	273.1009
282.9191	294.5421	321.5958
328.6451	333.0827	348.5229
393.4455	450.8752	529.7685
543.4863	570.0722	609.2687
618.8878	660.1355	728.1580
790.2464	836.1154	853.9326
864.4793	898.8099	915.6935
942.0169	977.3220	1018.1894
1021.8361	1025.3511	1039.6410
1041.4716	1060.7607	1065.2529
1073.5776	1096.5153	1122.2863
1160.0859	1190.3618	1202.7178
1214.7992	1239.1917	1246.4297
1247.8804	1280.5387	1314.8863
1320.6962	1331.2317	1332.4112
1352.4953	1357.8777	1434.9320
1457.8400	1465.2906	1470.1439
1483.1900	1505.5798	1519.8994
1610.0536	1648.5932	1703.7619
2915.0435	3004.5179	3059.1202
3069.1410	3084.5536	3105.5960
3151.7340	3157.8558	3166.5952
3171.3615	3172.3732	3188.5514
3191.8724	3196.6388	3268.5354
3291.8635	3292.9221	3307.9615

Statistical Thermodynamic Analysis	
Temperature=298.15 K	Pressure=1 atm
Zero-point correction= 0.268610	Electronic Energy = -2553.30177525
Internal Energy (E)= -2553.00919425	Enthalpy (H)= -2553.00825025
Gibbs Free Energy (G)=-2553.08966225	Gibbs Free Energy of Solvation=-2553.10892561

St.Pt.	General Structure	Ball & Stick model
$1PdTS_3$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	2.39847	-2.25633	-0.89950
C	3.05823	-1.25573	-1.55908
Pt	1.60554	-0.24566	-0.05948
Cl	3.31435	-0.22536	1.51550
Cl	-0.17798	-0.28596	-1.69975
H	2.70686	-0.89831	-2.52252
H	4.02006	-0.89539	-1.20855
H	2.82346	-2.70941	-0.00866
H	1.50616	-2.71215	-1.31647
Cl	-0.52556	-2.66716	0.77717
Cl	-3.40047	0.65222	-0.91945
H	-3.37564	-3.15082	0.68064
C	-3.71214	-2.11866	0.68912
C	-3.26667	-1.24950	1.65501
H	-4.51514	-1.82994	0.01787
H	-3.71680	-0.26709	1.75719
H	-2.57475	-1.58820	2.41994
C	-0.39596	2.20586	0.52694
O	1.50463	2.91943	-0.73050
C	0.39200	3.18273	-0.31572
C	0.54701	1.20468	1.15656
H	1.22094	1.65863	1.88658
H	0.01735	0.37853	1.64611
C	-0.35273	4.49425	-0.42252
H	0.29861	5.27246	-0.00944
C	-1.61386	4.26640	0.43152
H	-1.94575	5.17316	0.93941
H	-2.43363	3.91276	-0.20110
C	-1.22547	3.14202	1.41560
H	-0.61066	3.53484	2.23476
H	-2.09683	2.64323	1.84506
H	-0.54450	4.75109	-1.46705
H	-1.09807	1.71578	-0.16330
H	1.54915	1.40176	-0.00463

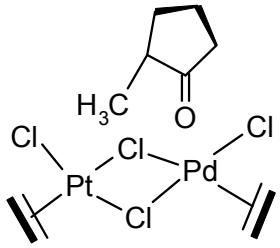
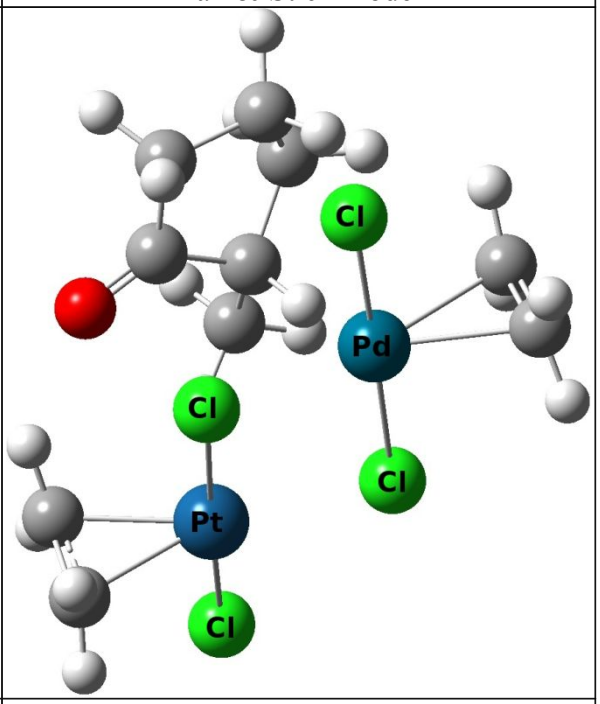
Frequencies

-783.3486	26.0416	31.3910
41.4196	44.6664	58.8061
70.8677	83.4842	89.8655
95.6029	102.0107	124.2734
129.2112	141.1384	155.5134
157.9032	163.8881	165.6311
172.7229	187.1745	213.0425
244.2388	258.5807	266.2829
269.2421	279.8245	291.7030
317.1827	330.4031	348.3508
380.6908	391.7318	448.1101
559.7412	576.3114	592.7592
603.2646	609.4299	613.6364
741.1407	810.7433	845.7274
846.8753	861.3757	904.0585
928.5135	956.9582	968.7500
1021.3391	1036.8036	1040.8563
1052.3197	1054.5058	1061.8540
1064.0057	1065.8941	1091.1120
1145.6945	1179.1971	1191.8308
1202.7767	1211.5989	1238.1533
1238.9605	1243.2536	1309.1884
1315.3600	1324.4285	1334.8603
1343.9289	1353.8158	1394.1270
1455.0470	1461.0737	1466.0222
1477.1072	1498.9973	1513.4157
1526.5149	1611.8538	1627.0631
1876.2284	3067.8739	3086.8306
3089.5213	3090.0774	3098.0358
3146.3913	3153.5597	3163.0890
3167.0489	3180.7690	3182.5094
3191.6290	3195.3969	3280.0725
3284.1423	3300.8720	3302.2616

-1.95759	-1.02897	-0.14258	

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.263150 Electronic Energy = -2553.27564186
Internal Energy (E)= -2552.98846286 Enthalpy (H)= -2552.98751886
Gibbs Free Energy (G)=-2553.06963186 Gibbs Free Energy of Solvation=-2553.08581068

St.Pt.	General Structure	Ball & Stick model
$1PdI_4$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	3.20746	-0.46697	-1.66834
C	2.82247	0.86510	-1.46864
Pt	1.73953	-0.39826	-0.13387
Cl	3.40779	-0.15554	1.44448
Cl	-0.09325	-0.65292	-1.72679
H	2.08794	1.34198	-2.10839
H	3.42427	1.52128	-0.84802
H	4.11559	-0.84912	-1.21310
H	2.78590	-1.04204	-2.48796
Cl	0.12970	-1.25389	1.57243
Cl	-3.49880	-0.80954	-1.44254
H	-2.41588	-2.76943	1.99325
C	-3.10016	-2.12567	1.44775
C	-3.18295	-0.78532	1.73090
H	-3.82053	-2.59276	0.78347
H	-3.97510	-0.18196	1.29830
H	-2.56668	-0.34026	2.50767
C	-0.67936	2.40229	0.97043
O	0.61619	2.70711	-1.06017
C	-0.46345	2.62174	-0.52049
C	0.49740	2.83623	1.82574
H	0.66787	3.91240	1.72361
H	0.32124	2.61043	2.88019
C	-1.81626	2.77452	-1.20521
H	-1.81778	3.73028	-1.73969
C	-2.84368	2.72814	-0.06311
H	-3.68604	3.40401	-0.22253
H	-3.25176	1.71453	0.01360
C	-2.03794	3.07075	1.20575
H	-1.89665	4.15637	1.28550

Frequencies

25.0479	28.0500	33.8876
38.7417	53.4279	68.6776
72.4284	82.3275	90.1415
94.7684	95.5363	116.8115
125.7887	129.3804	132.7686
145.8604	164.4344	173.6736
175.6003	196.3547	200.0018
228.2538	249.2636	252.5266
266.3537	276.9820	280.8453
339.6083	347.7664	354.0082
383.8375	406.9343	458.4644
506.0736	560.1126	579.7407
596.1326	600.1567	723.9408
768.2732	819.6678	826.6137
831.4410	869.5097	910.2046
948.2073	958.8904	994.6287
1029.9023	1038.5801	1039.9582
1053.7851	1056.5217	1071.3981
1075.5068	1095.2699	1164.0306
1186.1987	1191.2846	1211.0160
1219.9671	1233.9300	1244.4628
1291.8833	1302.3663	1306.0902
1324.8629	1335.7615	1346.8180
1380.9379	1423.3160	1458.4287
1465.0874	1475.3144	1500.0123
1503.2242	1504.9006	1516.7071
1574.9565	1612.0848	1885.0299
3034.5081	3067.6455	3069.4569
3084.1107	3093.8213	3127.2348
3133.4780	3148.3352	3149.8643
3159.0431	3174.8197	3174.9158
3181.0394	3199.5893	3273.6009
3274.5916	3292.0457	3304.4308

H	-2.52446	2.73627	2.12640
H	-1.94784	1.98173	-1.94923
H	-0.81960	1.31253	1.07819
H	1.40884	2.31820	1.51210
	-1.74339	-1.04913	0.02941

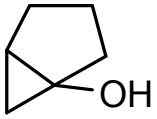
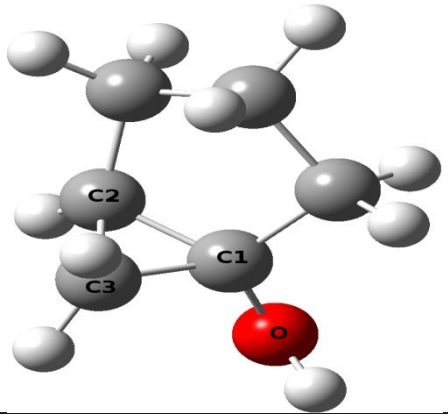
Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm

Zero-point correction= 0.268013 Electronic Energy = -2553.33572097

Internal Energy (E)= -2553.04277497 Enthalpy (H)= -2553.04182997

Gibbs Free Energy (G)=-2553.12679597 Gibbs Free Energy of Solvation=-2553.14341841

St.Pt.	General Structure	Ball & Stick model
1		

Cartesian co-ordinate

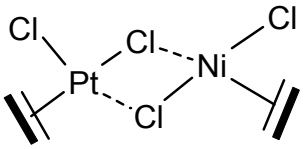
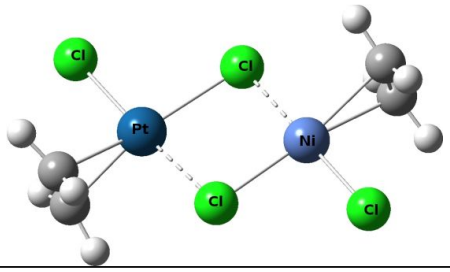
Atoms	X	Y	Z
C	-0.03028	-1.05068	-0.41217
O	2.00227	0.38667	-0.52845
C	0.74672	0.15044	0.02888
C	0.57091	-1.00145	0.97587
H	-0.07826	-0.90477	1.84133
H	1.45155	-1.61605	1.12589
H	2.55325	0.78977	0.15229
C	-0.21550	1.31928	0.14884
H	0.00395	1.98045	0.99447
C	-1.60371	0.66350	0.25353
H	-1.83307	0.43898	1.29968
H	-2.40237	1.31192	-0.11380
C	-1.48666	-0.64650	-0.55506
H	-2.18673	-1.41105	-0.20396
H	-1.70299	-0.45950	-1.61272
H	-0.12787	1.90700	-0.77205
H	0.41549	-1.73776	-1.12287

Frequencies

218.7186	249.7708	346.9290
369.7460	389.5136	457.7402
550.7976	618.5293	712.7037
826.0150	847.4259	898.7741
916.2375	921.1445	967.1094
987.7957	1012.3285	1039.2903
1065.7574	1099.6435	1125.4589
1174.1473	1211.8734	1253.4906
1274.9256	1290.3576	1330.2710
1349.9471	1361.9481	1370.9121
1425.9593	1501.3010	1506.3580
1516.1429	1536.0356	3069.6620
3076.7137	3096.2241	3117.9686
3122.9285	3145.5093	3150.0545
3221.3029	3241.3378	3880.0908

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.152288 Electronic Energy = -309.718741856
Internal Energy (E)= -309.560224856 Enthalpy (H)= -309.559280856
Gibbs Free Energy (G)=-309.595983856 Gibbs Free Energy of Solvation=-309.599133984

St.Pt.	General Structure	Ball & Stick model
b_{Ni}		

Cartesian co-ordinate

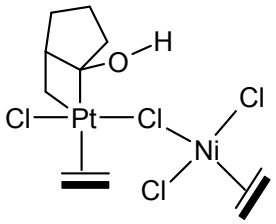
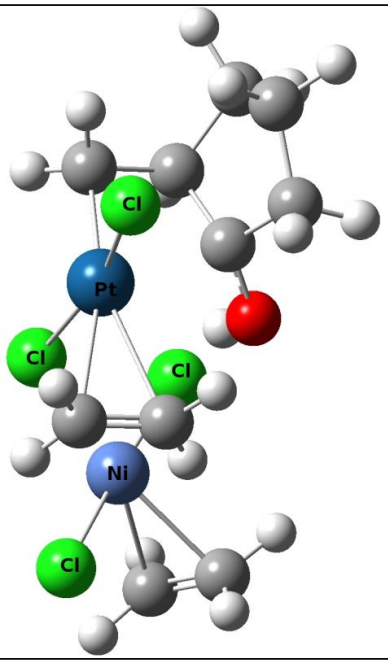
Atoms	X	Y	Z
C	-2.68242	-1.54002	-0.70110
C	-2.68273	-1.54021	0.70052
Pt	-1.32664	-0.06293	0.00020
Cl	-3.03444	1.49492	0.00005
Cl	0.54871	-1.59230	0.00042
H	-2.10368	-2.27562	1.25133
H	-3.46591	-1.01952	1.24182
H	-3.46538	-1.01920	-1.24261
H	-2.10313	-2.27528	-1.25184
Cl	3.73808	-1.42718	-0.00097
Cl	0.46073	1.64104	0.00089
H	4.30637	1.01051	1.22871
C	3.61370	1.63804	0.67626
C	3.61302	1.63806	-0.67802
H	2.96996	2.31060	1.23702
H	2.96869	2.31062	-1.23812
H	4.30511	1.01053	-1.23119
Ni	2.13479	0.06075	-0.00013

Frequencies

14.6871	41.1237	78.0032
92.0705	113.2494	114.6347
145.0093	145.1705	153.8490
174.0219	193.2563	200.5712
244.9249	264.4598	287.6376
301.5910	307.8828	335.7189
356.3977	383.3775	404.2843
464.8156	507.6859	771.7943
830.8142	847.2359	1023.4352
1053.0863	1057.4664	1065.4482
1075.7296	1078.2419	1230.1345
1240.3719	1289.5829	1369.3859
1468.3602	1479.3156	1581.2776
1654.5588	3177.1298	3179.0677
3182.4152	3184.0796	3275.6983
3279.7243	3293.1124	3294.1855

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.116884 Electronic Energy = -2286.25336720
Internal Energy (E)= -2286.1207452 Enthalpy (H)= -2286.1198012
Gibbs Free Energy (G)=-2286.1830642 Gibbs Free Energy of Solvation=-2286.20156192

St.Pt.	General Structure	Ball & Stick model
$1NiI_1$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.15073	-2.97819	0.00884
C	-1.30616	-2.47437	1.24707
Pt	-1.32446	-0.43520	-0.44808
Cl	-3.59744	-0.37913	0.09247
Cl	0.81908	-0.71589	-1.53958
H	-0.43309	-2.29050	1.86746
H	-2.29241	-2.31091	1.67040
H	-2.01253	-3.25287	-0.59578
H	-0.15890	-3.18340	-0.38390
Cl	2.91783	1.73196	-1.29908
Cl	2.16078	-1.89452	1.24353
H	5.15526	0.28829	-0.42387
C	4.72718	-0.15347	0.47078
C	4.09346	0.61864	1.38495
H	4.86113	-1.21761	0.64198
H	3.71886	0.18452	2.30671
H	4.00528	1.69043	1.23822
C	-0.64523	2.18167	-0.14637
O	0.64725	0.71365	1.29158
C	-0.58922	1.08479	0.90822
C	-1.40692	1.42941	-1.25082
H	-2.45329	1.72003	-1.34939
H	-0.88533	1.40374	-2.20686
H	0.65192	-0.06819	1.87506
C	-1.60789	1.38346	2.00727
H	-2.20128	0.52255	2.31751
C	-2.43311	2.55173	1.44651
H	-3.27788	2.16129	0.87417
H	-2.82993	3.18399	2.24320
C	-1.44921	3.29932	0.52864
H	-1.94919	3.94011	-0.20201

Frequencies

43.4593	50.2829	53.8080
67.6308	78.7050	95.9484
101.9862	105.8072	119.7683
135.7188	149.2252	152.2260
169.6882	174.6670	179.4808
186.2285	194.9880	207.6802
218.7550	235.7390	239.5269
255.0670	275.8186	292.5023
295.5804	308.2403	320.5184
323.3671	336.2339	363.1203
371.7564	431.8519	444.0453
465.2120	520.4215	534.0981
578.3688	634.6968	656.8773
809.0618	837.5424	844.3787
847.3932	861.1067	878.9464
922.2967	954.3381	1006.9063
1029.9587	1042.6623	1043.7458
1049.3502	1057.4937	1061.6580
1072.5189	1081.2431	1100.5117
1121.1438	1161.4976	1187.5683
1197.8275	1243.9494	1246.4654
1247.5834	1276.2763	1297.8082
1317.3508	1333.0561	1351.9114
1366.0646	1369.9459	1373.0783
1412.1056	1459.2606	1468.1150
1474.1706	1476.2541	1500.5692
1526.1208	1655.8362	1672.7382
3076.1583	3086.7257	3112.3037
3127.2739	3132.4781	3144.1402
3167.4164	3171.7786	3179.0766
3180.0469	3180.5308	3191.5251
3214.6975	3269.8311	3280.6941
3288.5296	3300.2024	3711.1780

H	-0.77560	3.92655	1.12264
H	-1.00403	1.71902	2.86033
H	0.36217	2.45419	-0.47311
Ni	2.54114	-0.10406	-0.10179

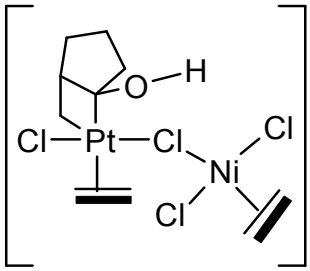
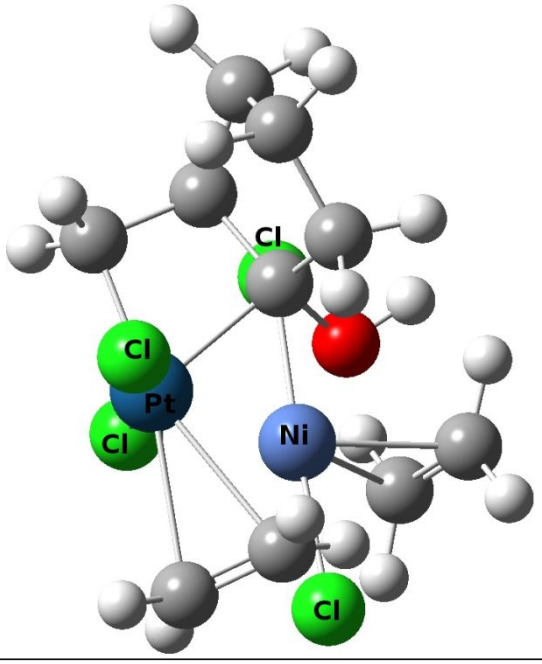
Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm

Zero-point correction= 0.269784 Electronic Energy = -2595.98236528

Internal Energy (E)= -2595.68904228 Enthalpy (H)= -2595.68809828

Gibbs Free Energy (G)=-2595.76608328 Gibbs Free Energy of Solvation=-2595.78325217

St.Pt.	General Structure	Ball & Stick model
$1NiTS_1$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.82038	-2.95340	0.25706
C	-0.79550	-2.29322	1.43199
Pt	-1.30935	-0.52083	-0.40665
Cl	-3.52656	-0.72826	0.29133
Cl	0.79130	-0.49097	-1.59236
H	0.14791	-1.93357	1.83339
H	-1.70277	-2.15943	2.01477
H	-1.74572	-3.37958	-0.12515
H	0.10363	-3.13477	-0.28584
Cl	2.66038	2.12762	-0.82465
Cl	2.53035	-2.08805	0.67472
H	5.08367	0.81532	-0.40305
C	4.76096	0.09893	0.34621
C	4.10097	0.51197	1.45443
H	5.01872	-0.94737	0.21441
H	3.83113	-0.19710	2.23106
H	3.90350	1.56818	1.60956
C	-0.90735	2.12283	-0.33706
O	0.52606	0.72654	1.22991
C	-0.73763	1.08932	0.78797
C	-1.69020	1.25081	-1.33064
H	-2.76706	1.41921	-1.33404
H	-1.26693	1.21075	-2.33323
H	0.83922	1.40284	1.84884
C	-1.71481	1.44675	1.90774
H	-2.22203	0.58511	2.34218
C	-2.64151	2.50820	1.30495
H	-3.48117	2.02235	0.80054
H	-3.05166	3.17345	2.06737
C	-1.74191	3.24151	0.29497

Frequencies

-403.7269	39.4494	43.4190
58.5135	75.4914	82.1553
91.2215	101.2886	117.1379
129.7231	137.8439	150.6632
165.7095	171.0236	177.9096
183.1308	190.9979	198.8810
216.4432	228.9438	238.2625
249.0338	274.7708	286.4805
298.4855	304.0179	311.7018
315.4731	323.4610	338.5417
372.1419	376.3348	437.0285
441.2549	464.7824	551.8564
577.3141	633.9556	657.6382
811.5085	838.4658	842.4375
844.5586	855.0881	880.8583
923.1106	953.4014	1005.2436
1036.2672	1038.0285	1042.0726
1049.7687	1055.4589	1059.8028
1066.8548	1088.4185	1095.6901
1142.0120	1149.6672	1177.7649
1196.8891	1237.3302	1245.0150
1246.1807	1249.8651	1285.2098
1294.3974	1334.3632	1337.5554
1365.1458	1368.1285	1370.2336
1371.9770	1453.9671	1462.2514
1474.5510	1477.1829	1500.1896
1520.9065	1651.6735	1664.5359
3040.2763	3075.3613	3115.4136
3126.9491	3140.0911	3154.2663
3163.7816	3166.5864	3169.4363
3174.7606	3176.1851	3184.6749
3214.8120	3264.8363	3275.4659
3286.3935	3293.3991	3826.6949

H	-2.30448	3.80497	-0.45397
H	-1.08115	3.94439	0.81559
H	-1.09995	1.90136	2.69917
H	0.06204	2.42233	-0.74191
Ni	2.53696	0.00736	-0.10570

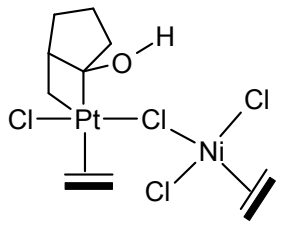
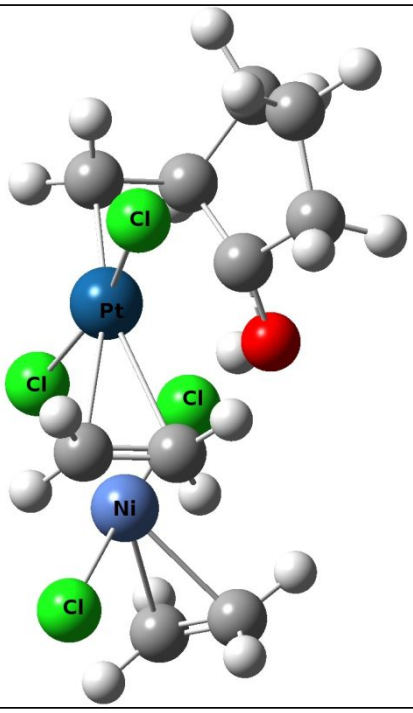
Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm

Zero-point correction= 0.268655 Electronic Energy = -2595.96647739

Internal Energy (E)= -2595.67471239 Enthalpy (H)= -2595.67376839

Gibbs Free Energy (G)=-2595.75089039 Gibbs Free Energy of Solvation=-2595.77057005

St.Pt.	General Structure	Ball & Stick model
$1NiI_2$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-0.31364	-2.82085	0.58414
C	-0.19195	-1.93532	1.59543
Pt	-1.21560	-0.66252	-0.33339
Cl	-3.33254	-1.33527	0.36861
Cl	0.90515	-0.23814	-1.48212
H	0.74852	-1.41576	1.75824
H	-0.98994	-1.79355	2.31874
H	-1.21840	-3.41107	0.46721
H	0.52763	-3.01303	-0.07697
Cl	2.40261	2.39622	-0.39529
Cl	3.07032	-1.98823	0.19505
H	5.07425	1.47335	-0.19596
C	4.89590	0.57026	0.38070
C	4.18938	0.61609	1.53485
H	5.34192	-0.35993	0.04200
H	4.06458	-0.27611	2.14056
H	3.79350	1.55726	1.90426
C	-1.58459	2.04967	-0.56861
O	0.05130	1.46182	1.22811
C	-1.15962	1.37297	0.73045
C	-1.98991	0.84391	-1.44026
H	-3.07023	0.72296	-1.52731
H	-1.50919	0.84448	-2.41901
H	0.71360	1.80004	0.56950
C	-2.28652	1.44441	1.74613
H	-2.51613	0.49227	2.22350
C	-3.45576	2.06570	0.96859
H	-4.06179	1.27372	0.52198
H	-4.10218	2.66072	1.61628
C	-2.77368	2.91292	-0.12136

Frequencies

26.6449	34.4959	55.1358
65.8873	76.5789	78.7543
102.3721	121.1336	134.8549
140.9659	145.4525	154.3422
162.6721	170.5861	172.7304
183.2805	187.0241	196.2096
209.1788	230.7292	234.8852
264.7114	274.9336	291.3615
297.8003	298.7145	312.2643
331.4871	344.8162	360.2846
375.5107	455.4839	459.4984
474.8530	514.7667	574.1486
624.0974	663.9538	793.9093
826.0607	829.0413	841.2073
841.9266	860.0316	880.1268
919.3525	955.2708	1009.7931
1031.8006	1040.9254	1046.9163
1048.0553	1059.1149	1062.7239
1063.6971	1081.2581	1101.0271
1147.7203	1177.6591	1183.4128
1202.9961	1238.9657	1244.3536
1248.6068	1290.1030	1310.5018
1322.5040	1330.8478	1361.5841
1365.4312	1370.0933	1398.0560
1453.9880	1465.3853	1466.4269
1476.1944	1500.8859	1506.5057
1523.9036	1654.2282	1658.9293
3084.4605	3086.9031	3119.0771
3120.2737	3123.1410	3146.2814
3164.5196	3174.0106	3174.3867
3181.0047	3182.5192	3189.5609
3203.2163	3255.1804	3261.7697

H	-3.43480	3.14865	-0.95914	3278.9571	3282.3034	3300.0941
H	-2.40956	3.85597	0.30128			
H	-1.91419	2.13336	2.51426			
H	-0.75227	2.60402	-1.01357			
Ni	2.72747	0.17067	-0.14761			

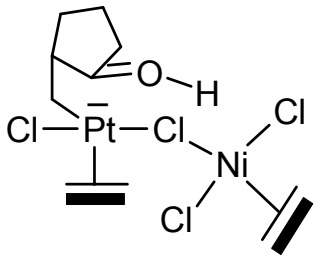
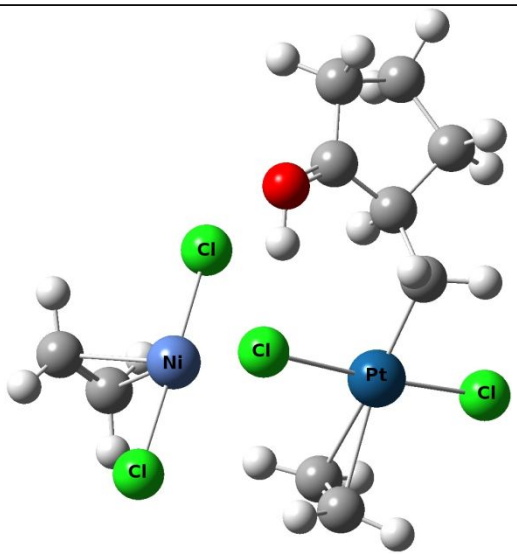
Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm

Zero-point correction= 0.269557 Electronic Energy = -2595.98829040

Internal Energy (E)= -2595.6952274 Enthalpy (H)= -2595.6942834

Gibbs Free Energy (G)=-2595.7730994 Gibbs Free Energy of Solvation=-2595.7885481

St.Pt.	General Structure	Ball & Stick model
$1NiI_3$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.37115	-2.79142	0.09604
C	-1.37786	-2.13159	-1.08964
Pt	0.52504	-1.33298	0.16822
Cl	1.81797	-2.71702	-1.19233
Cl	-0.73262	0.23697	1.64108
H	-2.03441	-1.27811	-1.23694
H	-0.85236	-2.51513	-1.95762
H	-0.84759	-3.73657	0.20343
H	-2.00210	-2.45636	0.91558
Cl	-3.79726	-0.14949	0.82611
Cl	-0.50230	2.26162	-0.98931
H	-3.97554	0.42435	-1.88949
C	-3.37293	1.32740	-1.90422
C	-3.65658	2.35303	-1.06589
H	-2.58458	1.42004	-2.64528
H	-3.09804	3.28247	-1.12069
H	-4.48326	2.28094	-0.36596
C	2.54980	0.85004	-0.03456
O	1.34482	2.32302	1.51710
C	2.23497	2.12324	0.65029
C	2.24926	-0.43661	0.74773
H	1.91482	0.91028	-0.94021
H	3.06591	-1.13763	0.56361
H	2.22146	-0.23535	1.82689
C	4.00352	1.09659	-0.49602
C	4.02764	2.59364	-0.83869
C	3.17016	3.21947	0.27282
H	0.68657	1.55429	1.61439
H	4.26105	0.44686	-1.33320
H	3.76691	3.43944	1.16941
H	2.61678	4.12800	0.02082
H	5.03288	3.01458	-0.87565
H	3.55204	2.76350	-1.80911

Frequencies

30.5138	40.4902	49.2117
58.3919	62.3528	75.0709
79.1747	97.3333	113.8269
120.7758	139.0774	152.9466
158.0680	168.4735	176.2207
188.8974	195.7003	196.8103
211.3972	218.2958	220.9511
238.6298	247.4184	292.4182
300.1103	322.3272	324.8378
332.5202	333.3439	351.3476
380.9674	456.6758	471.4587
530.7060	547.5189	573.2550
617.2714	661.2115	731.9460
797.6596	817.1980	858.5664
867.7341	903.5284	931.9373
947.1486	995.3016	1007.7174
1027.2569	1036.1191	1050.6399
1052.7481	1057.4788	1064.8115
1069.6756	1099.6001	1130.6411
1167.9056	1189.8788	1207.3459
1215.5036	1224.8320	1249.0547
1252.9884	1278.0648	1318.8309
1324.1149	1337.0359	1353.5014
1354.6805	1371.9930	1430.9479
1456.4726	1460.6209	1471.9521
1486.1913	1509.5231	1521.7252
1644.4346	1656.7480	1712.9293
2910.2164	2999.3910	3058.3524
3068.8336	3081.8845	3108.6605
3149.4686	3149.7221	3166.7957
3169.0846	3172.5006	3174.2848
3181.8310	3192.4767	3262.5704
3278.7822	3281.9627	3301.8380

H	4.68967	0.87481	0.32997	
Ni	-2.13363	1.04428	-0.02177	

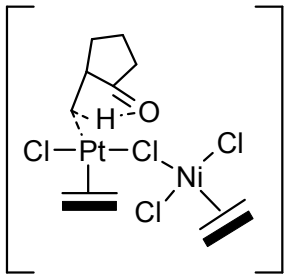
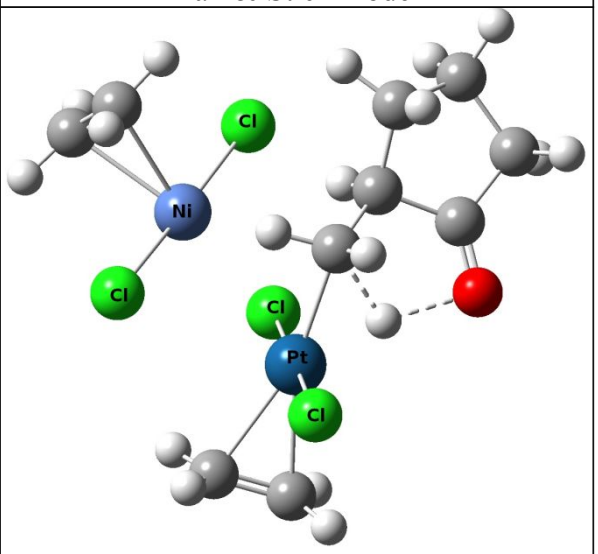
Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm

Zero-point correction= 0.269028 Electronic Energy = -2595.98673467

Internal Energy (E)= -2595.69401167 Enthalpy (H)= -2595.69306767

Gibbs Free Energy (G)=-2595.77295767 Gibbs Free Energy of Solvation=-2595.79277785

St.Pt.	General Structure	Ball & Stick model
$1NiTS_3$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	2.65334	-1.90351	-0.88392
C	3.07351	-0.81752	-1.60070
Pt	1.50196	-0.05873	-0.05767
Cl	3.22144	0.32682	1.45509
Cl	-0.28824	-0.49105	-1.63850
H	2.61904	-0.57115	-2.55605
H	3.95676	-0.26000	-1.30551
H	3.19590	-2.22865	-0.00103
H	1.85181	-2.54082	-1.24409
Cl	-0.19989	-2.59328	0.86100
Cl	-3.44116	-0.17447	-1.03806
H	-2.77901	-3.73875	0.71311
C	-3.35967	-2.82172	0.68100
C	-3.16849	-1.85172	1.60637
H	-4.13290	-2.71951	-0.07423
H	-3.79092	-0.96238	1.60743
H	-2.43468	-1.97955	2.39628
C	-0.91488	1.96996	0.52776
O	0.74462	3.05490	-0.81538
C	-0.37930	3.07663	-0.35586
C	0.22278	1.19622	1.15490
H	0.81600	1.80124	1.84446
H	-0.12105	0.30193	1.68881
C	-1.39782	4.19343	-0.45017
H	-0.92050	5.10288	-0.06868
C	-2.55282	3.71466	0.44778
H	-3.06063	4.53688	0.95402
H	-3.29269	3.17631	-0.15251
C	-1.89821	2.72276	1.43261
H	-1.35780	3.25621	2.22424
H	-2.62616	2.05691	1.90132
H	-1.67230	4.38270	-1.49068
H	-1.51747	1.33242	-0.13547
H	1.16219	1.53292	-0.04116

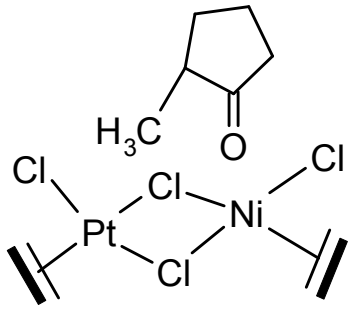
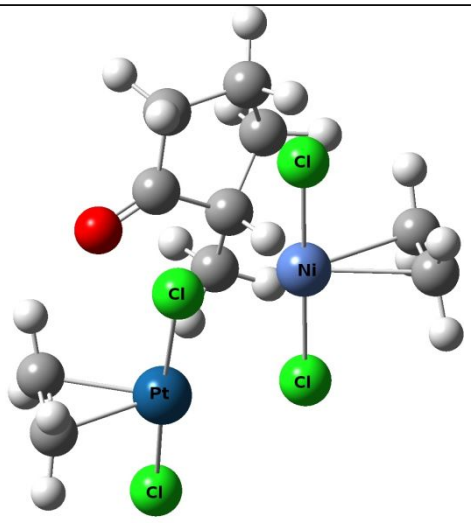
Frequencies

-780.5474	23.8356	32.6669
39.9932	49.1575	56.6206
67.0920	81.5697	99.9037
102.6383	110.9863	121.4291
138.0546	149.3029	154.5038
172.7040	174.7137	180.2167
195.7807	210.6746	214.4877
242.7774	258.3626	270.1510
285.6368	299.8668	309.0387
314.7887	324.9993	352.1206
375.6512	381.3956	442.7018
473.6369	559.4194	576.0608
579.4557	601.6817	612.7359
739.7741	812.9670	831.6428
859.7526	862.8601	883.1619
929.9762	937.8132	970.1425
1020.8926	1034.2886	1051.2191
1053.2698	1059.5017	1060.1742
1064.9462	1067.0392	1101.7482
1146.3660	1184.6611	1199.5054
1200.7173	1220.4578	1232.6913
1238.3788	1253.0763	1309.9628
1321.9880	1332.0007	1345.7053
1355.4849	1372.1772	1408.8785
1454.7689	1469.0808	1471.6343
1472.4921	1502.5048	1517.1495
1610.2989	1628.4327	1656.3004
1884.8815	3070.9092	3083.9121
3089.4130	3090.5559	3099.3696
3151.2236	3151.3693	3170.6336
3174.0629	3181.4904	3186.5532
3190.0217	3197.2097	3278.6610
3289.5916	3295.3718	3307.3045

Ni	-1.80865	-1.40604	-0.15961	

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.263755 Electronic Energy = -2595.96098646
Internal Energy (E)= -2595.67335646 Enthalpy (H)= -2595.67241246
Gibbs Free Energy (G)=-2595.75366946 Gibbs Free Energy of Solvation=-2595.76973814

St.Pt.	General Structure	Ball & Stick model
$1NiI_4$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	3.15380	-0.20008	-1.64738
C	2.60596	1.07809	-1.47705
Pt	1.67676	-0.27827	-0.12095
Cl	3.29822	0.18215	1.45947
Cl	-0.13229	-0.79552	-1.65551
H	1.82114	1.44658	-2.12885
H	3.11731	1.81640	-0.86779
H	4.09941	-0.45602	-1.18000
H	2.81392	-0.83976	-2.45687
Cl	0.10711	-1.25947	1.53660
Cl	-3.28464	-1.25045	-1.41610
H	-2.08017	-3.06997	1.96691
C	-2.85652	-2.52041	1.44151
C	-3.11021	-1.22316	1.73380
H	-3.46379	-3.05404	0.71658
H	-3.93121	-0.69991	1.25301
H	-2.54928	-0.70425	2.50697
C	-1.29280	2.14675	0.96669
O	0.12120	2.52092	-0.97152
C	-0.98742	2.38019	-0.50752
C	-0.20296	2.63622	1.90244
H	-0.08199	3.72003	1.81221
H	-0.44166	2.39944	2.94227
C	-2.29629	2.45974	-1.28154
H	-2.32066	3.42122	-1.80549
C	-3.39313	2.33590	-0.21213
H	-4.27095	2.94693	-0.43025
H	-3.72444	1.29308	-0.15992
C	-2.70104	2.73426	1.10572
H	-2.62879	3.82654	1.18643
H	-3.22833	2.37472	1.99394
H	-2.32804	1.66888	-2.03832
H	-1.38188	1.05025	1.06449
H	0.75519	2.16870	1.65514

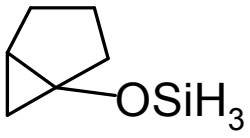
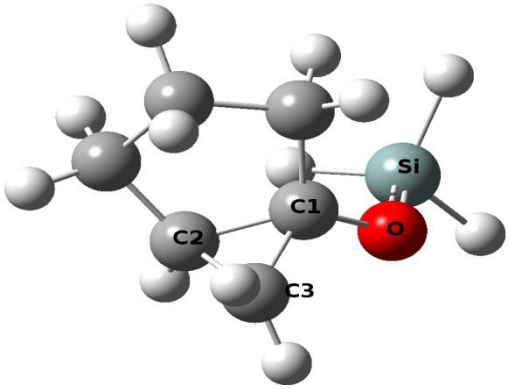
Frequencies

21.3628	37.4913	38.5962
49.1922	64.3373	72.9163
83.1373	89.7493	99.4546
101.1498	112.8133	120.5923
140.0320	150.4421	155.6818
159.8200	170.3662	178.3367
195.7650	198.6395	210.1645
242.8539	253.7107	258.5266
285.0688	294.8852	306.2984
336.5411	340.3036	356.0183
383.6452	406.6350	457.9996
472.5404	506.8574	560.4092
576.0636	602.4747	724.1800
763.5559	821.2738	840.0280
844.6797	869.7726	910.9420
949.5984	956.6416	995.2002
1020.4740	1041.2379	1053.7790
1057.1521	1068.2033	1069.6698
1074.2097	1091.5129	1163.6724
1188.1968	1192.2543	1213.7327
1225.2066	1241.6008	1247.9106
1291.3912	1298.5719	1306.3436
1319.9268	1350.1518	1371.8265
1380.0046	1424.5897	1455.7959
1470.9436	1479.1104	1500.6893
1503.9735	1505.7591	1518.7430
1577.6483	1656.9179	1886.9452
3027.9913	3070.9134	3073.0549
3083.6200	3095.9632	3129.5923
3135.0017	3148.7815	3156.8815
3163.7491	3169.8212	3180.8631
3187.8479	3188.2001	3268.1530
3280.6991	3291.9904	3299.2011

Ni	-1.61614	-1.27287	0.01116	

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.268749 Electronic Energy = -2596.02273361
Internal Energy (E)= -2595.72946261 Enthalpy (H)= -2595.72851861
Gibbs Free Energy (G)=-2595.81122261 Gibbs Free Energy of Solvation=-2595.82791189

St.Pt.	General Structure	Ball & Stick model
2		

Cartesian co-ordinate

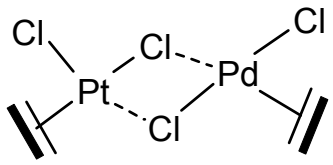
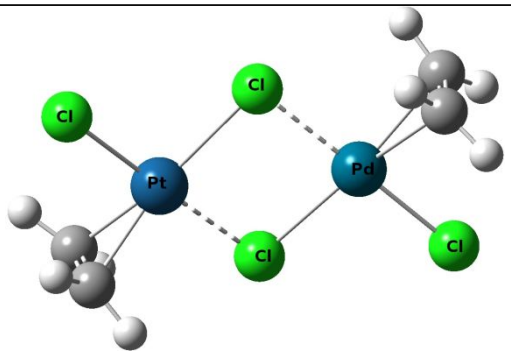
Atoms	X	Y	Z
C	-0.82387	0.80406	0.78579
O	1.29653	0.53614	-0.59065
C	-0.08031	0.34785	-0.44333
C	-0.93806	1.56537	-0.51870
H	-1.86685	1.54693	-1.08105
H	-0.39233	2.50072	-0.56261
C	-0.67963	-0.97251	-0.89477
H	-0.72335	-1.07012	-1.98352
C	-2.06462	-1.00980	-0.22626
H	-2.79922	-0.51298	-0.86677
H	-2.42288	-2.02861	-0.06342
C	-1.89683	-0.22419	1.09259
H	-2.84006	0.21609	1.43070
H	-1.53818	-0.88915	1.88701
H	-0.05079	-1.78840	-0.51358
H	-0.28956	1.28703	1.59732
H	3.66826	0.37054	0.23624
H	1.91830	-0.43706	1.72063
H	2.55476	-1.72213	-0.21136
Si	2.37926	-0.34476	0.31169

Frequencies

50.5800	108.4467	135.7920
235.1995	243.7345	357.1364
398.2266	458.8385	516.8303
613.6786	671.2735	721.3358
761.8710	820.9888	826.5272
870.7087	895.2086	919.7705
956.9564	979.9959	985.1784
991.1530	997.6362	1009.1378
1020.0213	1055.5780	1072.0578
1119.2736	1129.0063	1188.4395
1214.6074	1267.2868	1278.6625
1302.3936	1347.3555	1356.5718
1368.9609	1416.2538	1497.3544
1502.2798	1508.6772	1530.3504
2239.2261	2242.6140	2289.2514
3053.5143	3068.6937	3090.8192
3120.0301	3126.5413	3145.0497
3159.0805	3216.2177	3254.5058

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.167917 Electronic Energy = -600.400552085
Internal Energy (E)= -600.224173085 Enthalpy (H)= -600.223229085
Gibbs Free Energy (G)=-600.266249085 Gibbs Free Energy of Solvation=-600.268488721

St.Pt.	General Structure	Ball & Stick model
b_{Pd}		

Cartesian co-ordinate

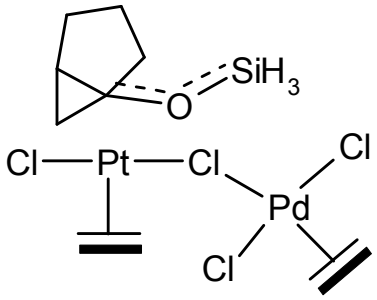
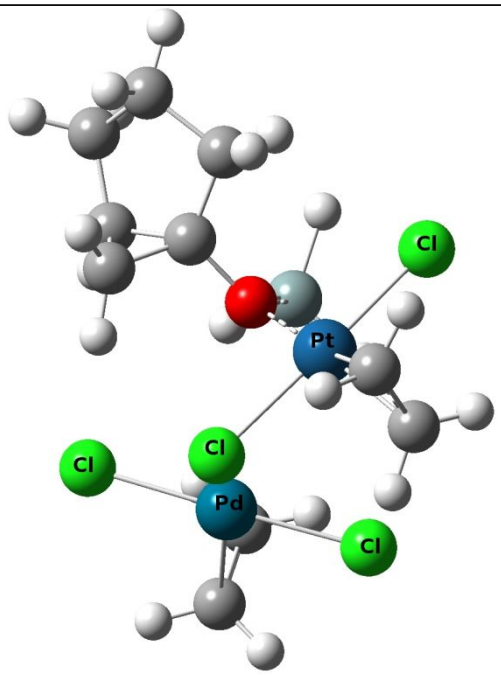
Atoms	X	Y	Z
C	-2.94641	-1.55414	-0.56972
C	-2.81419	-1.53627	0.82573
Pt	-1.52907	-0.07182	-0.01838
Cl	-3.22503	1.49033	0.14284
Cl	0.30351	-1.66640	-0.18215
H	-2.18513	-2.26582	1.32712
H	-3.54090	-1.00610	1.43273
H	-3.77550	-1.03886	-1.04373
H	-2.42196	-2.29872	-1.16119
Cl	3.71962	-1.46273	0.13777
Cl	0.20305	1.69304	-0.18615
H	4.08352	1.03826	1.41772
C	3.40436	1.62225	0.80493
C	3.53376	1.63200	-0.56244
H	2.72855	2.31061	1.30461
H	2.96355	2.32847	-1.17062
H	4.31748	1.05716	-1.04566
	2.02202	0.07766	-0.02452
H	2.55476	-1.72213	-0.21136
Si	2.37926	-0.34476	0.31169

Frequencies

11.4059	52.7471	80.9671
89.0270	93.8371	110.8168
126.8404	131.6688	143.5943
162.8891	181.6858	192.9596
234.2716	253.8482	271.1481
280.7738	281.8292	350.1532
354.5792	386.0877	407.1973
512.1322	601.5285	771.2757
832.8304	835.2863	1021.0858
1040.9809	1058.0488	1061.0577
1074.0606	1079.0580	1226.0963
1236.8976	1287.3608	1337.1857
1471.6477	1471.9254	1574.7216
1615.1968	3173.1520	3180.5180
3181.6300	3185.6525	3271.8199
3280.7111	3289.6790	3297.2171

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.116567 Electronic Energy = -2243.56719436
Internal Energy (E)= -2243.43473536 Enthalpy (H)= -2243.43379136
Gibbs Free Energy (G)=-2243.49804136 Gibbs Free Energy of Solvation=-2243.51562026

St.Pt.	General Structure	Ball & Stick model
$2PdI_1$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.30712	-3.02946	-1.30221
C	-0.23236	-3.28438	-0.44372
Pt	-0.85593	-1.25938	-0.21485
Cl	-2.35495	-1.85376	1.46181
Cl	0.71827	-0.52810	-1.87098
H	0.79211	-3.24572	-0.80050
H	-0.39933	-3.75893	0.51832
H	-2.31372	-3.32046	-1.01913
H	-1.12830	-2.81459	-2.35154
Cl	2.01608	2.58226	-0.98322
Cl	2.52641	-1.72536	0.83186
H	4.57373	1.75685	0.04604
C	4.21964	0.99421	0.73290
C	3.24010	1.28601	1.65162
H	4.75226	0.04926	0.77763
H	2.99580	0.57492	2.43524
H	2.81933	2.28516	1.70272
C	-1.66044	3.11718	-0.23012
O	-0.92099	0.79260	0.52806
C	-1.87945	1.63496	-0.11303
C	-1.52973	2.21123	-1.43765
H	-2.28832	2.22042	-2.21499
H	-0.50960	2.05649	-1.77153
C	-3.33851	1.36497	0.19570
H	-3.72571	0.48929	-0.33518
C	-4.04123	2.67699	-0.20263
H	-4.32323	2.64221	-1.25861
H	-4.95846	2.84172	0.36617
C	-2.99685	3.79119	0.02615
H	-3.17039	4.65719	-0.61901

Frequencies

4.9086	38.1302	54.9856
60.2736	68.3103	75.8875
81.0213	91.5131	97.9196
106.4706	111.9953	128.1689
141.4767	144.2890	149.8246
151.9154	159.2204	164.0136
174.2670	188.2062	192.7287
202.5089	237.9780	256.1071
270.9652	279.1257	285.4656
294.4807	330.8986	342.2605
376.6999	396.2285	404.3707
440.2563	454.5625	510.1588
543.4539	619.1336	620.3447
662.1708	716.5913	770.8834
773.5788	809.0700	825.2062
831.8593	835.0961	870.8704
894.8894	921.6999	947.8646
963.3960	974.1780	982.1651
988.6764	1012.9208	1021.2101
1033.4483	1042.3389	1054.1856
1056.3415	1067.4768	1080.0075
1083.6428	1097.3141	1099.0948
1128.0525	1189.4186	1209.4322
1223.4976	1235.2146	1247.9518
1268.6984	1294.5820	1298.1593
1332.4585	1345.4981	1353.2084
1367.8837	1415.6808	1458.2054
1473.1470	1496.7887	1503.0746
1509.3431	1530.9000	1577.3353
1605.3902	2276.9481	2289.1690
2304.8575	3075.2980	3082.1648
3103.2446	3128.2811	3129.8435
3151.2835	3156.2455	3178.5394

H	-3.03032	4.13934	1.06499	3180.8813	3185.4658	3191.5125
H	-3.44628	1.16885	1.26833	3209.8591	3255.1592	3277.6922
H	-0.73360	3.56535	0.11510	3279.2404	3295.7209	3296.4950
H	0.29292	-0.03522	2.57999			
H	0.28009	2.37020	2.17153			
H	-1.74369	1.29515	2.95103			
Si	-0.51378	1.12229	2.15605			
	2.26837	0.40410	-0.15241			

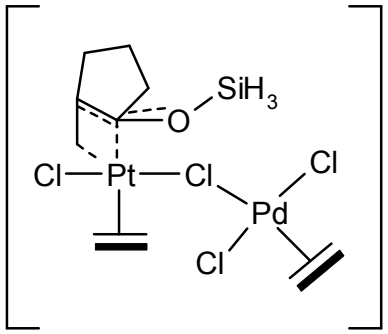
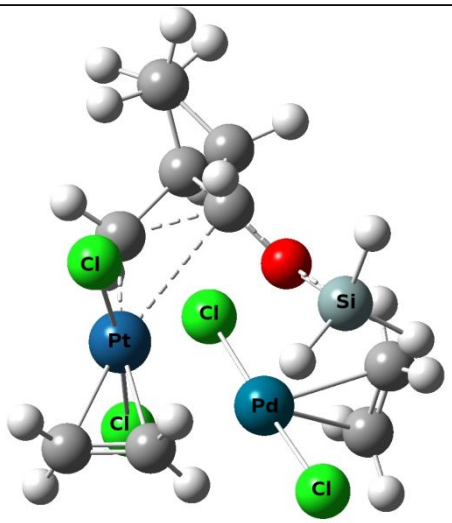
Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm

Zero-point correction= 0.286545 Electronic Energy = -2843.98772451

Internal Energy (E)= -2843.67550451 Enthalpy (H)= -2843.67456051

Gibbs Free Energy (G)=-2843.76050051 Gibbs Free Energy of Solvation=-2843.78123534

St.Pt.	General Structure	Ball & Stick model
$2PdTS_1$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.94169	-2.94566	-0.48138
C	-1.37336	-2.68405	0.75107
Pt	-1.43446	-0.79092	-0.39768
Cl	-3.59497	-0.37022	0.40086
Cl	0.66726	-1.37266	-1.44422
H	-0.31386	-2.85385	0.93205
H	-2.01144	-2.50984	1.61204
H	-3.02052	-2.97722	-0.59306
H	-1.34130	-3.34623	-1.29209
Cl	2.48958	1.50705	-1.89451
Cl	2.30573	-1.74986	1.50884
H	4.91230	0.70983	-0.62044
C	4.50984	0.35282	0.32230
C	3.67934	1.14744	1.07160
H	4.88580	-0.58330	0.72347
H	3.40330	0.84947	2.07778
H	3.41652	2.14535	0.73560
C	-0.64642	2.64650	-0.66146
O	0.20788	1.37092	1.21974
C	-0.80712	1.92705	0.56501
C	-1.18129	1.23528	-1.17493
H	-2.16778	1.38447	-1.60864
H	-0.40327	0.94732	-1.88212
C	-2.06914	2.37533	1.26829
H	-2.64832	1.57340	1.72611
C	-2.82852	3.18185	0.20942
H	-3.50754	2.51642	-0.32939
H	-3.42741	3.97779	0.65421
C	-1.71946	3.72236	-0.71605
H	-2.06336	3.91052	-1.73591
H	-1.30436	4.65567	-0.31972
H	-1.69739	3.03940	2.06210
H	0.35958	2.83723	-1.02579
H	-0.54013	-0.74485	2.58210
H	1.44139	0.56567	3.26517

Frequencies

-260.2554	28.2388	34.4304
53.3439	65.1525	72.2075
84.2654	94.5665	96.5404
112.9784	117.4932	131.8344
137.8403	146.9629	153.9385
161.3269	163.0566	168.3390
184.5582	189.0382	193.7796
238.6493	249.0686	266.6427
269.9843	277.7128	294.8344
296.3252	304.5553	312.8750
324.7629	326.2894	382.5785
396.6572	417.9126	454.7965
490.9651	539.3249	604.5381
627.8643	691.8886	693.3442
699.4466	757.2907	771.0398
800.3616	837.8008	839.3131
844.9632	890.9311	912.2800
927.7121	941.1361	977.0636
991.5068	999.4573	1038.2792
1039.6723	1041.8924	1042.3179
1050.5029	1053.4308	1065.5024
1067.6749	1118.3763	1133.6083
1168.1414	1192.9035	1232.2251
1232.9973	1243.9639	1259.5522
1297.0167	1309.8285	1322.4497
1336.3426	1342.7005	1349.9192
1388.0750	1398.5297	1466.8662
1468.0578	1469.9098	1502.7760
1519.8947	1557.4416	1601.0153
1613.7732	2258.6556	2300.7724
2355.9737	3056.4754	3090.8211
3110.2512	3116.0391	3147.3829
3164.4873	3167.7124	3179.0334
3179.2464	3186.0696	3200.9507
3206.2898	3232.8256	3265.0003
3284.2037	3288.3021	3309.7075

H	-0.77972	1.44264	3.59210
Si	0.07228	0.58316	2.73983
	2.40300	-0.15167	-0.22353

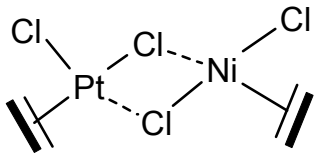
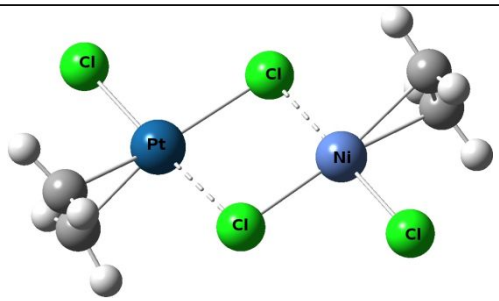
Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm

Zero-point correction= 0.284925 Electronic Energy = -2843.95963999

Internal Energy (E)= -2843.64948599 Enthalpy (H)= -2843.64854199

Gibbs Free Energy (G)=-2843.73130599 Gibbs Free Energy of Solvation=-2843.74986186

St.Pt.	General Structure	Ball & Stick model
b_{Ni}		

Cartesian co-ordinate

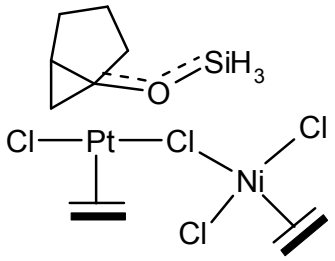
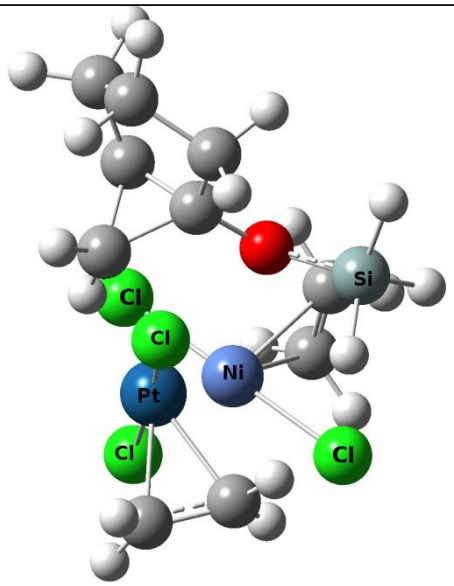
Atoms	X	Y	Z
C	-2.68242	-1.54002	-0.70110
C	-2.68273	-1.54021	0.70052
Pt	-1.32664	-0.06293	0.00020
Cl	-3.03444	1.49492	0.00005
Cl	0.54871	-1.59230	0.00042
H	-2.10368	-2.27562	1.25133
H	-3.46591	-1.01952	1.24182
H	-3.46538	-1.01920	-1.24261
H	-2.10313	-2.27528	-1.25184
Cl	3.73808	-1.42718	-0.00097
Cl	0.46073	1.64104	0.00089
H	4.30637	1.01051	1.22871
C	3.61370	1.63804	0.67626
C	3.61302	1.63806	-0.67802
H	2.96996	2.31060	1.23702
H	2.96869	2.31062	-1.23812
H	4.30511	1.01053	-1.23119
Ni	2.13479	0.06075	-0.00013
H	2.55476	-1.72213	-0.21136
Si	2.37926	-0.34476	0.31169

Frequencies

14.6871	41.1237	78.0032
92.0705	113.2494	114.6347
145.0093	145.1705	153.8490
174.0219	193.2563	200.5712
244.9249	264.4598	287.6376
301.5910	307.8828	335.7189
356.3977	383.3775	404.2843
464.8156	507.6859	771.7943
830.8142	847.2359	1023.4352
1053.0863	1057.4664	1065.4482
1075.7296	1078.2419	1230.1345
1240.3719	1289.5829	1369.3859
1468.3602	1479.3156	1581.2776
1654.5588	3177.1298	3179.0677
3182.4152	3184.0796	3275.6983
3279.7243	3293.1124	3294.1855

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.116884 Electronic Energy = -2286.25336720
Internal Energy (E)= -2286.1207452 Enthalpy (H)= -2286.1198012
Gibbs Free Energy (G)=-2286.1830642 Gibbs Free Energy of Solvation=-2286.20156192

St.Pt.	General Structure	Ball & Stick model
$2NiI_1$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.80533	-2.91126	-0.47500
C	-1.20007	-2.66279	0.76879
Pt	-1.23498	-0.87082	-0.36959
Cl	-3.34211	-0.36343	0.47568
Cl	0.83709	-1.47466	-1.42120
H	-0.14835	-2.88441	0.93769
H	-1.82265	-2.49371	1.64226
H	-2.88724	-2.94170	-0.55439
H	-1.23416	-3.36635	-1.27835
Cl	2.59299	1.19232	-1.92208
Cl	2.23749	-1.67951	1.48899
H	4.93118	0.52021	-0.56258
C	4.50924	0.27005	0.40613
C	3.67168	1.12460	1.03923
H	4.80777	-0.66121	0.87847
H	3.29890	0.89309	2.03170
H	3.40482	2.07826	0.59485
C	-0.28746	2.84681	-0.79161
O	0.41463	1.38185	1.10270
C	-0.59648	1.98166	0.34969
C	-0.88106	1.43732	-1.09334
H	-1.88628	1.44491	-1.50639
H	-0.10397	0.92453	-1.65885
C	-1.78726	2.59862	1.07629
H	-2.46693	1.87065	1.52362
C	-2.45531	3.49604	0.02799
H	-3.16809	2.91365	-0.56328
H	-3.01085	4.31663	0.48525
C	-1.28519	3.98629	-0.84577
H	-1.58626	4.23957	-1.86563
H	-0.82036	4.87475	-0.40316
H	-1.36183	3.21882	1.87400
H	0.73455	2.95587	-1.13762

Frequencies

30.6420	35.4141	60.5301
68.7886	79.1947	83.2552
93.9088	98.4002	104.8874
112.6498	120.9339	138.9200
147.3202	154.7082	156.5706
169.7077	180.7643	186.6909
196.6483	204.1934	209.9419
241.5591	256.0979	259.0343
283.3132	294.7099	299.3715
315.2638	322.5303	342.2406
355.0341	378.1273	399.7907
409.1794	465.5319	467.9203
508.7802	534.5639	627.3461
635.4735	722.8822	745.3724
759.2724	781.7043	814.2947
817.7997	840.2448	859.5514
897.7097	907.2461	929.6611
934.6442	955.6379	961.6924
996.3577	1005.0683	1020.0098
1026.2404	1039.5282	1048.1171
1058.2914	1063.1750	1085.8840
1096.0103	1100.4278	1115.9262
1140.4784	1176.8284	1220.8614
1226.0971	1232.8538	1265.6482
1270.8594	1281.8584	1288.5556
1342.0840	1352.7470	1361.2473
1366.1764	1413.3750	1456.7034
1473.1722	1484.9250	1497.9599
1502.4645	1527.4084	1569.7373
1651.4104	2273.5073	2290.4501
2314.7930	3078.0602	3080.5707
3101.5395	3129.3293	3139.5187
3160.4829	3171.4812	3173.7768
3178.6361	3182.6752	3185.9678
3223.3172	3238.4368	3272.8299

H	-0.54659	-0.54710	2.59246	3277.4660	3288.4619	3295.3160
H	1.49094	0.63674	3.27003			
H	-0.64801	1.69886	3.44465			
Si	0.16221	0.74735	2.65179			
Ni	2.39053	-0.24143	-0.22149			

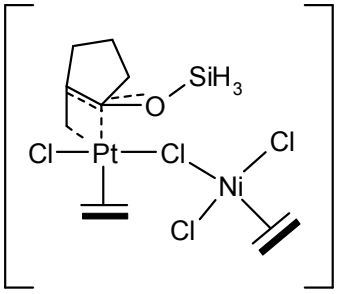
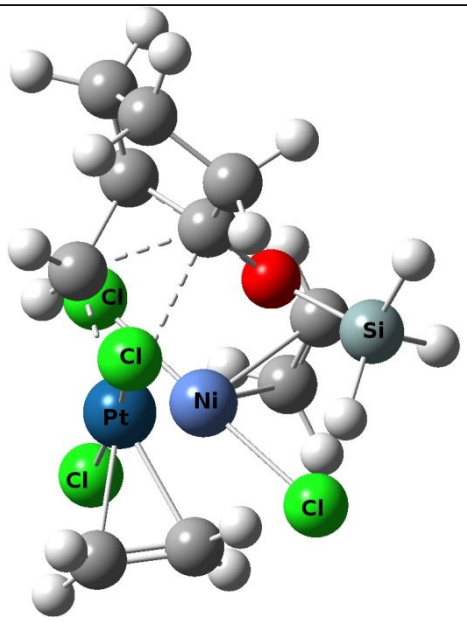
Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm

Zero-point correction= 0.286531 Electronic Energy = -2886.65372477

Internal Energy (E)= -2886.34190277 Enthalpy (H)= -2886.34095877

Gibbs Free Energy (G)=-2886.42334577 Gibbs Free Energy of Solvation=-2886.44173929

St.Pt.	General Structure	Ball & Stick model
$2NiTS_1$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.85530	-2.91361	-0.38884
C	-1.30549	-2.62591	0.84594
Pt	-1.26748	-0.77760	-0.37443
Cl	-3.42244	-0.24048	0.36189
Cl	0.83653	-1.46720	-1.35619
H	-0.25741	-2.82696	1.05700
H	-1.95477	-2.39242	1.68408
H	-2.93165	-2.90761	-0.52580
H	-1.25302	-3.36927	-1.16857
Cl	2.58843	1.18897	-1.98411
Cl	2.31975	-1.62436	1.48928
H	4.97169	0.50725	-0.69349
C	4.57969	0.27502	0.29208
C	3.77026	1.14569	0.93746
H	4.88391	-0.65268	0.76782
H	3.42802	0.93188	1.94490
H	3.50066	2.09532	0.48615
C	-0.33450	2.60333	-0.73752
O	0.46292	1.33660	1.18128
C	-0.52685	1.92268	0.50686
C	-0.93750	1.20861	-1.21459
H	-1.92229	1.39039	-1.63873
H	-0.18146	0.86783	-1.92285
C	-1.76908	2.44732	1.19458
H	-2.38657	1.68549	1.67067
C	-2.48916	3.26236	0.11521
H	-3.19944	2.61793	-0.40828
H	-3.04918	4.09626	0.54085
C	-1.35546	3.72752	-0.82051
H	-1.68820	3.90586	-1.84583
H	-0.89727	4.64985	-0.44647
H	-1.37015	3.11389	1.97247

Frequencies

-255.7367	28.7838	38.2555
64.1081	71.2572	86.3613
88.2885	94.2271	106.7020
117.7413	125.7429	136.5597
146.1214	157.4859	159.8912
176.1667	187.0893	191.2638
194.5001	206.7287	208.4639
238.3733	249.0007	268.3628
291.6910	296.3583	302.3637
307.9471	311.4686	318.1956
324.7650	337.9455	374.8475
380.4506	419.4601	456.4855
458.3709	492.9622	542.7891
630.4032	696.4276	702.2962
725.3534	756.9996	773.0830
799.7544	817.6304	838.3438
840.5522	889.5771	912.2144
933.1444	939.1907	977.5562
994.7027	1004.9527	1040.0517
1044.3435	1048.5731	1051.5497
1056.3502	1058.1606	1062.6235
1067.4453	1122.7167	1131.2440
1167.7354	1191.2222	1231.2797
1233.7731	1235.1049	1259.4714
1290.3170	1303.3819	1325.6434
1339.0310	1344.9300	1366.4521
1383.7494	1393.3622	1455.1768
1463.2623	1473.0226	1502.2272
1522.1700	1551.3769	1603.4351
1653.1635	2275.0332	2334.4920
2363.6460	3060.3886	3085.4588
3110.8426	3116.8067	3146.0831
3166.8677	3174.0620	3179.0022
3179.1355	3179.5601	3185.5557

H	0.67739	2.73488	-1.11016	3206.6360	3231.8646	3270.4063
H	-0.40367	-0.66865	2.64544	3277.5727	3285.9601	3294.7307
H	1.61882	0.59926	3.31633			
H	-0.56105	1.57585	3.52372			
Si	0.27014	0.63336	2.74306			
Ni	2.43626	-0.24099	-0.27020			

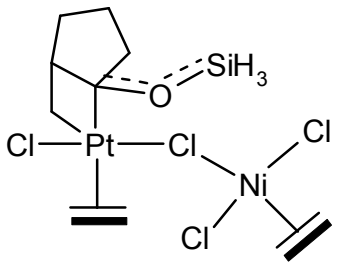
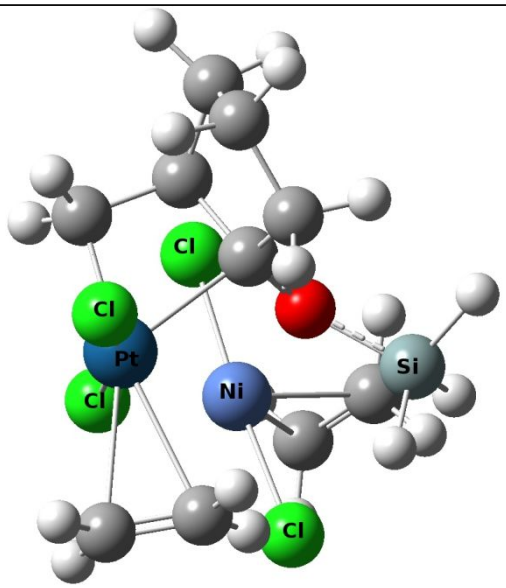
Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm

Zero-point correction= 0.285423 Electronic Energy = -2886.64732484

Internal Energy (E)= -2886.33702184 Enthalpy (H)= -2886.33607684

Gibbs Free Energy (G)=-2886.41707484 Gibbs Free Energy of Solvation=-2886.43573934

St.Pt.	General Structure	Ball & Stick model
$2NiI_2$		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.42440	-3.05919	-0.06044
C	-1.08307	-2.54036	1.13433
Pt	-1.40272	-0.52525	-0.49589
Cl	-3.65640	-0.50085	0.11628
Cl	0.74290	-0.81384	-1.57603
H	-0.03533	-2.44170	1.40651
H	-1.84420	-2.27176	1.86294
H	-2.46428	-3.22811	-0.32761
H	-0.65709	-3.38081	-0.75998
Cl	2.67892	1.80303	-1.53775
Cl	2.46179	-1.89174	0.96918
H	5.05777	0.40589	-1.15659
C	4.82946	-0.08311	-0.21448
C	4.36895	0.62818	0.84089
H	5.01813	-1.14878	-0.12099
H	4.20498	0.14007	1.79597
H	4.23079	1.70250	0.76834
C	-0.78122	2.13174	-0.47951
O	0.45606	0.85882	1.23159
C	-0.73857	1.20743	0.73523
C	-1.53282	1.23989	-1.47761
H	-2.58491	1.49998	-1.60035
H	-1.02207	1.12380	-2.43310
C	-1.82877	1.64324	1.71341
H	-2.40342	0.82233	2.14501
C	-2.65358	2.68026	0.94201
H	-3.44687	2.18331	0.37895
H	-3.11877	3.40241	1.61583
C	-1.62034	3.32202	0.00043
H	-2.07477	3.85547	-0.83856
H	-0.98901	4.02885	0.55058
H	-1.29417	2.15556	2.52279
H	0.22857	2.36488	-0.82421

Frequencies

22.1471	41.1865	53.9921
65.7895	73.6227	80.9747
93.1152	104.6790	106.7081
117.0771	131.6877	141.1578
151.6215	157.9176	162.8508
167.0023	168.9846	181.3951
190.6675	194.7787	207.9561
223.8587	235.0827	257.7737
261.5426	273.6724	281.5196
297.2082	307.3270	311.0070
325.5623	336.3071	354.7714
378.5370	419.2703	421.7480
463.5170	506.1900	542.5134
598.1826	661.2053	707.7977
731.5667	778.7552	816.4061
844.3239	846.0107	847.0710
864.4592	878.3872	925.9442
931.1219	958.0147	985.3494
1000.6043	1016.6222	1029.9746
1042.9700	1045.4536	1048.6198
1057.7256	1063.4635	1072.0772
1086.7668	1107.0907	1161.4795
1183.4392	1199.1290	1218.9225
1246.4760	1248.6889	1260.4984
1279.8136	1316.6057	1331.6988
1339.2932	1363.9496	1371.0256
1377.0615	1407.7258	1456.8020
1463.9925	1465.5823	1476.4074
1499.2886	1522.2142	1656.4082
1672.9839	2270.8461	2322.1365
2369.3371	3081.0449	3088.9160
3120.0753	3124.2243	3146.0422
3153.9497	3154.2942	3165.3651
3168.2760	3177.4667	3179.0734
3191.6037	3205.8801	3255.2679
3273.7456	3279.5012	3300.5087

H	2.27693	0.35974	2.91188
H	0.28682	1.40449	3.74640
H	0.17561	-0.92328	3.13786
Si	0.81421	0.36641	2.83325
Ni	2.56226	-0.08029	-0.35515

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm

Zero-point correction= 0.285467 Electronic Energy = -2886.65387850

Internal Energy (E)= -2886.3424815 Enthalpy (H)= -2886.3415375

Gibbs Free Energy (G)=-2886.4253685 Gibbs Free Energy of Solvation=-2886.44575288