Electronic Supplementary Information

Allylic Amination Reactivity of Ni, Pd, and Pt Heterobimetallic and Monometallic Complexes

Ryan Carlsen and Daniel Ess*

Department of Chemistry and Biochemistry, Brigham Young University, Provo, UT, 84602, United States

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1. XYZ coordinates and absolute energies

M06/6-31G(d,p)[LANL2DZ] optimized geometries in SMD dichloromethane solvent. Energies are reported in hartrees. E large = M06/def2-TZVP single point energies in dichloromethane.

1 – Ground

Lowest Frequency Vibration = 26.3971 cm**-1
Electronic Energy = -3295.27382719
Electronic and Zero-Point Energy = -3294.547995
Enthalpy = -3294.499565
Free Energy = -3294.625778
E large = -4088.46923103

Cl	-0.4260160	-3.9762230	0.7254500
Cl	0.1746820	-2.3857230	-2.0823150
N	-1.5247210	-0.9556310	1.1416520
N	1.6794130	-1.4046780	0.8614110
C	-2.3390980	-1.3735310	2.3420040
C	-3.3106810	-2.4882450	1.9581570
H	-4.0610300	-2.1313750	1.2417000
H	-2.7960010	-3.3483360	1.5200380
H	-3.8411280	-2.8323810	2.8552150
C	-3.1459320	-0.2126940	2.9157430
H	-3.7124130	-0.5861570	3.7775060
H	-2.5089920	0.6058990	3.2654680
H	-3.8775330	0.1868070	2.2038300
C	-1.3606450	-1.8404020	3.4122680
H	-0.7951980	-2.7216820	3.0958090
H	-0.6524610	-1.0382260	3.6622920
H	-1.9106930	-2.1073080	4.3229170
C	2.7443690	-2.2336510	1.5668460
C	2.1522760	-2.7840330	2.8589430
H	1.2882670	-3.4282450	2.6742740
H	2.9124800	-3.3895190	3.3672970
H	1.8532410	-1.9777710	3.5401050
C	3.1592420	-3.3728600	0.6413460
H	3.5867480	-2.9848950	-0.2912820
H	3.9224140	-3.9860280	1.1369290
H	2.3123250	-4.0215120	0.3932530
C	3.9807660	-1.4137040	1.9241740
H	3.7383510	-0.5185890	2.5066030
H	4.6300790	-2.0415350	2.5455690
H	4.5615590	-1.1236700	1.0445400
P	-1.9459260	0.1567170	-0.0332320
P	1.8828410	0.0848270	0.0741920
C	-2.1354960	1.8580780	0.5958280

C	-1.3885210	2.2856660	1.6965090
C	-2.9096430	2.7828300	-0.1144720
C	-1.4489780	3.6122750	2.1079870
H	-0.7597070	1.5770980	2.2338760
C	-2.9634080	4.1099120	0.3002360
H	-3.4713030	2.4763930	-0.9949710
C	-2.2369970	4.5261230	1.4120390
H	-0.8780240	3.9298960	2.9777500
H	-3.5762840	4.8194720	-0.2507690
H	-2.2828450	5.5630390	1.7359370
C	-3.5047300	-0.3490150	-0.8260330
C	-3.4270690	-1.3615150	-1.7885730
C	-4.7561590	0.1271630	-0.4205760
C	-4.5886820	-1.8999430	-2.3307090
H	-2.4532970	-1.7350150	-2.1067690
C	-5.9147250	-0.4122940	-0.9702470
H	-4.8363110	0.9122320	0.3290960
C	-5.8325330	-1.4272810	-1.9198040
H	-4.5204740	-2.6876900	-3.0770480
H	-6.8848840	-0.0412260	-0.6488090
H	-6.7409810	-1.8490420	-2.3433620
C	2.0281090	1.4207610	1.3013440
C	2.2817270	2.7239780	0.8569250
C	1.8020180	1.1841900	2.6588340
C	2.3534250	3.7696760	1.7699800
H	2.4361450	2.9235030	-0.2037040
C	1.8637870	2.2371620	3.5683250
H	1.5719450	0.1774180	3.0051120
C	2.1477970	3.5263570	3.1267080
H	2.5667830	4.7771910	1.4212460
H	1.6930420	2.0459010	4.6251400
H	2.2035500	4.3448560	3.8405570
C	3.4243810	0.0469880	-0.9089860
C	3.4905090	-0.8424310	-1.9879950
C	4.5167520	0.8715710	-0.6264320
C	4.6376450	-0.9055230	-2.7702650
H	2.6443840	-1.4892230	-2.2152080
C	5.6594030	0.8084700	-1.4191430
H	4.4942500	1.5495430	0.2238170
C	5.7223020	-0.0778630	-2.4897170
H	4.6821930	-1.6031340	-3.6031640
H	6.5060450	1.4508970	-1.1892360
H	6.6173390	-0.1244170	-3.1054280
C	-1.1798920	1.3392510	-3.0603470
H	-2.1849790	1.7196860	-2.8816100
H	-1.0971980	0.4416890	-3.6756190

C	1.1929650	1.5744000	-2.9237680
H	1.3532780	0.6867320	-3.5375830
H	2.0816080	2.1411350	-2.6480630
C	-0.2314490	3.6064180	-2.4242370
H	0.1702440	4.2977730	-3.1743600
H	-1.2838550	3.8538330	-2.2605970
H	0.3166620	3.7799070	-1.4892460
C	-0.0712390	2.1968960	-2.9023180
Pd	-0.0045390	0.5501590	-1.3543670
Ti	-0.0519080	-1.8376460	0.1863300

1 – TS1

Lowest Frequency Vibration = -265.0627 cm**-1
Electronic Energy = -3508.91405277
Electronic and Zero-Point Energy = -3508.036561
Enthalpy = -3507.981040
Free Energy = -3508.122012
E large = -4302.17686354

Cl	2.3145090	2.1659690	-3.0162230
Cl	-0.0599750	-0.0941030	-3.0264740
N	2.5626900	0.6962310	-0.1414670
N	-0.0728070	2.5093150	-0.7326790
C	3.9284230	1.2763050	0.1084480
C	4.8929820	0.8494470	-0.9972730
H	5.0794630	-0.2309420	-0.9729580
H	4.5107240	1.1117470	-1.9886420
H	5.8552930	1.3589920	-0.8584190
C	4.4903770	0.8254070	1.4524260
H	5.5025340	1.2341160	1.5615030
H	3.8899460	1.1942520	2.2907200
H	4.5713680	-0.2647230	1.5333960
C	3.7911390	2.7934560	0.1417470
H	3.4954990	3.2013210	-0.8301940
H	3.0482250	3.0944560	0.8928000
H	4.7538350	3.2428220	0.4153760
C	-0.3460720	3.9515890	-1.1019420
C	0.9404510	4.7528050	-0.9468130
H	1.7367100	4.3644390	-1.5887600
H	0.7513500	5.7930140	-1.2393100
H	1.2916280	4.7546510	0.0926310
C	-0.8164640	3.9933880	-2.5526810
H	-1.7490920	3.4301210	-2.6764190
H	-1.0048140	5.0334480	-2.8482870
H	-0.0635980	3.5768490	-3.2307680
C	-1.4199880	4.5814620	-0.2188360
H	-1.1814530	4.5132890	0.8485030

H	-1.4868500	5.6459590	-0.4729670
H	-2.4082400	4.1442220	-0.3902130
P	2.0255660	-0.8533440	0.1897730
P	-1.0253310	1.4583710	0.1874950
C	1.9982040	-1.2677790	1.9684510
C	1.7748490	-0.2748960	2.9259800
C	2.0469740	-2.6095270	2.3667170
C	1.6451600	-0.6151100	4.2681890
H	1.6992340	0.7681590	2.6210330
C	1.9140280	-2.9440310	3.7108610
H	2.1885350	-3.3976630	1.6290360
C	1.7182650	-1.9482720	4.6641550
H	1.4820950	0.1689600	5.0047760
H	1.9660880	-3.9878900	4.0116010
H	1.6201010	-2.2116250	5.7146990
C	3.0880450	-2.0716250	-0.6542960
C	2.8445370	-2.2737870	-2.0172260
C	4.1889160	-2.6903920	-0.0510260
C	3.6981620	-3.0717020	-2.7713280
H	1.9874600	-1.7939470	-2.4914870
C	5.0341850	-3.4953890	-0.8077510
H	4.3990620	-2.5380080	1.0061010
C	4.7938980	-3.6822200	-2.1667540
H	3.5037640	-3.2194620	-3.8310040
H	5.8889500	-3.9720590	-0.3335680
H	5.4606780	-4.3076900	-2.7557400
C	-0.8623120	1.8575060	1.9567810
C	-1.5611630	1.0862070	2.8932000
C	0.0432970	2.8238390	2.3996400
C	-1.3889710	1.3129470	4.2535010
H	-2.2443010	0.3051970	2.5559020
C	0.2218970	3.0403890	3.7640560
H	0.6171780	3.4024230	1.6774750
C	-0.4989100	2.2930160	4.6905640
H	-1.9437040	0.7174240	4.9747700
H	0.9250850	3.7980860	4.1016830
H	-0.3617390	2.4668880	5.7554150
C	-2.7856600	1.6377490	-0.2747060
C	-3.1568080	1.3274910	-1.5886920
C	-3.7637120	2.0237030	0.6458640
C	-4.4895460	1.4114210	-1.9752440
H	-2.4015820	1.0094300	-2.3067080
C	-5.0985180	2.0973150	0.2538140
H	-3.4891590	2.2875250	1.6650600
C	-5.4632730	1.7946970	-1.0543250
H	-4.7674080	1.1763930	-3.0001940

H	-5.8523780	2.4041420	0.9751340
H	-6.5059880	1.8563960	-1.3571020
C	-0.6124580	-3.0277310	-0.1872250
H	0.0878340	-3.6068420	0.4147000
H	-0.5750940	-3.1945820	-1.2657850
C	-2.6584410	-1.7476160	-0.3865140
H	-2.5070670	-1.6610890	-1.4588050
H	-3.3447480	-1.0422660	0.0705280
C	-2.0326690	-2.6672100	1.8845190
H	-2.4612350	-3.6570840	2.0906830
H	-1.1052560	-2.5847850	2.4654580
H	-2.7413840	-1.9160270	2.2532100
C	-1.7753350	-2.5062120	0.4137140
Pd	-0.3326460	-0.8525970	-0.1399000
N	-4.4400130	-3.0304970	-0.7924580
H	-4.9105940	-2.5726920	-1.5749210
C	-3.9443630	-4.3395430	-1.2027000
H	-3.2071500	-4.6710100	-0.4530470
H	-4.7635660	-5.0787140	-1.1815750
C	-5.3324290	-3.0739300	0.3655220
H	-4.7464140	-3.4275850	1.2263660
H	-6.1243930	-3.8251230	0.1995630
C	-5.9560100	-1.7250460	0.6537360
H	-6.4641140	-1.3309690	-0.2360130
H	-6.7035360	-1.8135330	1.4487750
H	-5.2178870	-0.9801190	0.9783930
C	-3.3189330	-4.2957090	-2.5793860
H	-2.9874680	-5.2941500	-2.8819700
H	-4.0412210	-3.9442340	-3.3269890
H	-2.4467540	-3.6304560	-2.6134320
Ti	1.1130480	1.1537760	-1.3920240

1 – Int 1

Lowest Frequency Vibration = 22.2574 cm**-1
Electronic Energy = -3508.94133608
Electronic and Zero-Point Energy = -3508.060504
Enthalpy = -3508.005066
Free Energy = -3508.145776
E large = -4302.20090363

Cl	-2.2371650	-1.9285680	-3.1824020
Cl	0.0621560	0.4120300	-2.9961830
N	-2.5996590	-0.7058820	-0.2292170
N	0.1062350	-2.4309900	-0.9031430
C	-3.9665660	-1.2947890	-0.0562390
C	-4.8959590	-0.7890690	-1.1595640
H	-5.0733830	0.2897000	-1.0687580

H	-4.4805080	-0.9897390	-2.1520630
H	-5.8667690	-1.2962380	-1.0844410
C	-4.5684560	-0.9284860	1.2964710
H	-5.5866280	-1.3335200	1.3513480
H	-3.9945120	-1.3514690	2.1280360
H	-4.6419980	0.1559670	1.4394400
C	-3.8399620	-2.8113210	-0.1253370
H	-3.4920840	-3.1424970	-1.1086980
H	-3.1403220	-3.1773190	0.6386280
H	-4.8180780	-3.2734270	0.0591560
C	0.3729040	-3.8339590	-1.3920640
C	-0.9132990	-4.6476780	-1.3034480
H	-1.7114910	-4.2062460	-1.9080350
H	-0.7263270	-5.6609230	-1.6811760
H	-1.2624130	-4.7342700	-0.2668640
C	0.8422870	-3.7586590	-2.8433820
H	1.7800110	-3.1956270	-2.9198120
H	1.0201530	-4.7710360	-3.2287630
H	0.0943000	-3.2764420	-3.4818780
C	1.4492660	-4.5382330	-0.5690990
H	1.2019140	-4.5811460	0.4973100
H	1.5355410	-5.5704320	-0.9295770
H	2.4323590	-4.0707340	-0.6856670
P	-2.0474380	0.8044890	0.2266720
P	1.0383770	-1.4634120	0.1200610
C	-2.0220630	1.0575020	2.0380180
C	-1.8371210	-0.0214210	2.9067190
C	-2.0223790	2.3588210	2.5566960
C	-1.6904560	0.1945160	4.2729690
H	-1.8019720	-1.0353190	2.5114200
C	-1.8674770	2.5705560	3.9231640
H	-2.1439720	3.2150820	1.8953670
C	-1.7049710	1.4894290	4.7854260
H	-1.5623060	-0.6561580	4.9389260
H	-1.8795620	3.5854870	4.3139790
H	-1.5901480	1.6551010	5.8540890
C	-3.1046960	2.1128120	-0.4829550
C	-2.8530070	2.4726230	-1.8114840
C	-4.1938990	2.6797280	0.1888730
C	-3.6893660	3.3732500	-2.4644990
H	-2.0035100	2.0333300	-2.3366060
C	-5.0223250	3.5854370	-0.4652790
H	-4.4069880	2.4105930	1.2223880
C	-4.7740300	3.9293650	-1.7921170
H	-3.4893780	3.6426610	-3.4989790
H	-5.8684940	4.0200700	0.0618990

H	-5.4267080	4.6346470	-2.3014750
C	0.8778390	-2.0796330	1.8316170
C	1.6254970	-1.4939080	2.8596450
C	-0.0761670	-3.0496430	2.1499080
C	1.4636050	-1.9163850	4.1746370
H	2.3411700	-0.7046590	2.6340570
C	-0.2481750	-3.4600360	3.4693870
H	-0.6916130	-3.4778690	1.3606370
C	0.5301950	-2.9041640	4.4813010
H	2.0622890	-1.4662720	4.9631090
H	-0.9890210	-4.2210680	3.7036430
H	0.4031370	-3.2333410	5.5100740
C	2.7999450	-1.5772000	-0.3719150
C	3.1328560	-1.1589940	-1.6672630
C	3.8119900	-2.0272190	0.4814100
C	4.4526710	-1.2061230	-2.1035920
H	2.3535890	-0.7919470	-2.3353860
C	5.1347330	-2.0559440	0.0442110
H	3.5741730	-2.3826480	1.4817760
C	5.4582440	-1.6506930	-1.2470650
H	4.6951640	-0.8933640	-3.1169080
H	5.9119060	-2.4132430	0.7161870
H	6.4908780	-1.6837360	-1.5866940
C	0.7975790	2.9986930	0.2457530
H	0.1594200	3.3746830	1.0462310
H	0.6191620	3.4149940	-0.7468490
C	3.0184340	2.1230000	-0.5081420
H	2.5602570	2.1166480	-1.5016960
H	3.5453740	1.1725330	-0.3784430
C	2.3674000	2.1370710	2.0030130
H	2.8341860	3.0362480	2.4322090
H	1.4844330	1.9155080	2.6153010
H	3.0806390	1.3113680	2.1236480
C	1.9826700	2.3416360	0.5581300
Pd	0.3393650	0.8525320	-0.0097530
N	4.1315470	3.1768610	-0.5946160
H	4.6613910	2.9151200	-1.4361320
C	3.6171520	4.5700920	-0.8275730
H	2.9246430	4.7907000	-0.0080900
H	4.4824440	5.2324760	-0.7283260
C	5.1308520	3.1450160	0.5332400
H	4.6086430	3.4742950	1.4357790
H	5.8734560	3.9088430	0.2814850
C	5.7912120	1.7978580	0.6930970
H	6.2317650	1.4585240	-0.2528850
H	6.6029590	1.8917430	1.4208860

H	5.1094200	1.0219830	1.0580980
C	2.9795340	4.7247120	-2.1868260
H	2.6992530	5.7726300	-2.3289670
H	3.6816190	4.4580900	-2.9858630
H	2.0740120	4.1208910	-2.3054620
Ti	-1.0694100	-1.0010000	-1.4387840

1 – Int 2

Lowest Frequency Vibration = 30.3049 cm**-1
Electronic Energy = -3755.60916224
Electronic and Zero-Point Energy = -3754.882827
Enthalpy = -3754.832141
Free Energy = -3754.964471
E large = -4548.83414822

Ti	-0.4579100	-1.4597910	-1.0938810
Cl	-1.2804750	-3.1974300	-2.3431600
Cl	0.2108220	-0.3475810	-3.1069560
N	-1.9547890	-1.3136800	0.1897630
N	1.1432940	-2.1618870	-0.2953460
C	-2.9861440	-2.2461090	0.7444990
C	-4.0919610	-2.4824270	-0.2830130
H	-4.6512350	-1.5619170	-0.4890220
H	-3.6817900	-2.8567280	-1.2265620
H	-4.8009190	-3.2273110	0.1023640
C	-3.6051820	-1.6895820	2.0219640
H	-4.3732480	-2.3869580	2.3795030
H	-2.8581090	-1.5763300	2.8162570
H	-4.0922740	-0.7200360	1.8623800
C	-2.3006670	-3.5627400	1.0858350
H	-1.9091030	-4.0561360	0.1906930
H	-1.4754510	-3.3949440	1.7909590
H	-3.0204330	-4.2437930	1.5572340
C	1.9184640	-3.4503600	-0.4141270
C	1.0271890	-4.6106440	0.0146500
H	0.1248720	-4.6657560	-0.6014850
H	1.5759320	-5.5532570	-0.1065600
H	0.7319710	-4.5274900	1.0678640
C	2.3319090	-3.6334790	-1.8729660
H	2.9853250	-2.8153260	-2.2005350
H	2.8841310	-4.5756760	-1.9856130
H	1.4568830	-3.6680940	-2.5322110
C	3.1738880	-3.4540710	0.4552170
H	2.9566660	-3.2384530	1.5076510
H	3.6201870	-4.4547910	0.4078760
H	3.9278130	-2.7459390	0.0977230
P	-2.0084960	0.3521950	0.0610170

P	1.6398660	-0.6680120	0.3217050
C	-2.1145560	1.2390670	1.6608960
C	-1.4989320	0.7338030	2.8109880
C	-2.6701630	2.5248880	1.6961900
C	-1.4770220	1.4853780	3.9809090
H	-1.0287150	-0.2489340	2.7972620
C	-2.6383730	3.2755750	2.8673920
H	-3.1267500	2.9508940	0.8045610
C	-2.0470760	2.7558510	4.0150300
H	-1.0103940	1.0723850	4.8726990
H	-3.0814670	4.2688010	2.8798490
H	-2.0269170	3.3395550	4.9324420
C	-3.4640320	0.8597960	-0.9194480
C	-3.3120420	0.8496330	-2.3097980
C	-4.7201890	1.1395230	-0.3677640
C	-4.4029210	1.0972750	-3.1380430
H	-2.3330670	0.6394160	-2.7433580
C	-5.8062140	1.3931840	-1.1985700
H	-4.8563070	1.1522440	0.7126460
C	-5.6501610	1.3674840	-2.5830620
H	-4.2748300	1.0838360	-4.2178160
H	-6.7797160	1.6052940	-0.7622080
H	-6.5028200	1.5641300	-3.2289360
C	1.6395760	-0.7716910	2.1446730
C	2.0736070	0.3137090	2.9141430
C	1.0728010	-1.8772210	2.7842300
C	1.9953070	0.2659440	4.3016290
H	2.4711160	1.2046070	2.4294170
C	0.9779340	-1.9152100	4.1730240
H	0.6921100	-2.7046810	2.1881210
C	1.4509200	-0.8499010	4.9345310
H	2.3487470	1.1097290	4.8900280
H	0.5360870	-2.7825760	4.6586980
H	1.3852770	-0.8830780	6.0196320
C	3.3414210	-0.3021880	-0.2461980
C	3.5565050	-0.1937340	-1.6265460
C	4.4084750	-0.0966760	0.6323200
C	4.8240490	0.1017180	-2.1151450
H	2.7280850	-0.3370930	-2.3202230
C	5.6715970	0.2172520	0.1365270
H	4.2664300	-0.2017800	1.7057820
C	5.8830700	0.3155670	-1.2349950
H	4.9812830	0.1762490	-3.1887860
H	6.4942150	0.3754220	0.8302130
H	6.8712820	0.5582670	-1.6187570
C	-0.1411460	3.2611480	-0.8938730

H	-0.9309440	3.6175670	-0.2319100
H	-0.3575080	3.2768910	-1.9642110
C	2.2777870	3.0884850	-1.4286550
H	1.9627480	2.6712540	-2.3884940
H	3.1493280	2.5494010	-1.0450000
C	1.5492890	3.5995140	0.9528410
H	1.7533170	4.6793040	1.0020710
H	0.7505920	3.3741770	1.6707950
H	2.4664590	3.0899710	1.2782470
C	1.1708000	3.1897550	-0.4434560
Cl	2.9477230	4.7795280	-1.8448910
Pd	0.1935010	1.1224230	-0.4572500

1 – TS2

Lowest Frequency Vibration = -211.2227 cm**-1
Electronic Energy = -3755.59748135
Electronic and Zero-Point Energy = -3754.871770
Enthalpy = -3754.821472
Free Energy = -3754.952792
E large = -4548.82239108

Ti	-0.4475410	-1.6541080	-0.9001100
Cl	-1.2872260	-3.5218440	-1.8826750
Cl	0.1147090	-0.7876180	-3.0311020
N	-1.9099230	-1.2947740	0.3740020
N	1.1854350	-2.1951840	-0.0588730
C	-2.9044280	-2.1689280	1.0815420
C	-4.0254450	-2.5711290	0.1250560
H	-4.6314910	-1.7052940	-0.1669530
H	-3.6273460	-3.0363520	-0.7821990
H	-4.6878300	-3.2939090	0.6189890
C	-3.5138790	-1.4640300	2.2883800
H	-4.2583610	-2.1304280	2.7413980
H	-2.7591270	-1.2369390	3.0499620
H	-4.0292200	-0.5350510	2.0174340
C	-2.1680030	-3.4048400	1.5821160
H	-1.7882770	-4.0118210	0.7545020
H	-1.3262860	-3.1173930	2.2271240
H	-2.8510660	-4.0294810	2.1713400
C	1.9711890	-3.4860680	-0.0364000
C	1.1043330	-4.5867190	0.5650350
H	0.1860850	-4.7418070	-0.0099150
H	1.6664210	-5.5290140	0.5576740
H	0.8378980	-4.3639390	1.6057030
C	2.3470100	-3.8414730	-1.4728330
H	2.9755370	-3.0602990	-1.9171530
H	2.9118490	-4.7826790	-1.4880490

H	1.4562380	-3.9688950	-2.0986310
C	3.2444790	-3.3689650	0.7968060
H	3.0418990	-3.0422900	1.8232000
H	3.7104020	-4.3600480	0.8533280
H	3.9756580	-2.6910980	0.3466270
P	-2.0152800	0.3371040	0.0272000
P	1.6995770	-0.6274740	0.3229230
C	-2.1346290	1.4097780	1.5020950
C	-1.4474600	1.0676310	2.6702210
C	-2.7753780	2.6515400	1.4219860
C	-1.4343590	1.9352940	3.7562280
H	-0.9268410	0.1130240	2.7260310
C	-2.7569180	3.5183610	2.5116830
H	-3.2960750	2.9473690	0.5132330
C	-2.0902280	3.1622210	3.6802220
H	-0.9051850	1.6505870	4.6630970
H	-3.2672150	4.4763360	2.4429480
H	-2.0793690	3.8400480	4.5304870
C	-3.4732570	0.6884820	-1.0116320
C	-3.3097510	0.5751650	-2.3958740
C	-4.7427880	0.9638470	-0.4882340
C	-4.4010620	0.7268940	-3.2462920
H	-2.3228010	0.3640110	-2.8081010
C	-5.8294760	1.1179820	-1.3420660
H	-4.8883610	1.0565230	0.5868110
C	-5.6604480	0.9971070	-2.7199570
H	-4.2636710	0.6386290	-4.3212950
H	-6.8128340	1.3297420	-0.9285610
H	-6.5129650	1.1181640	-3.3841490
C	1.7686980	-0.4509590	2.1359890
C	2.2253710	0.7462950	2.6993600
C	1.2387820	-1.4420870	2.9659390
C	2.1901730	0.9284240	4.0772740
H	2.6129080	1.5405670	2.0608490
C	1.1902900	-1.2498080	4.3445090
H	0.8524370	-2.3630680	2.5307190
C	1.6734870	-0.0694710	4.9021050
H	2.5600730	1.8565410	4.5068150
H	0.7784130	-2.0281320	4.9829230
H	1.6420710	0.0774720	5.9791890
C	3.3736710	-0.3203350	-0.3466760
C	3.5320930	-0.3023730	-1.7377880
C	4.4698230	-0.0432960	0.4745450
C	4.7695030	-0.0037810	-2.2952810
H	2.6807120	-0.5105730	-2.3842770
C	5.7034780	0.2681040	-0.0910850

H	4.3711160	-0.0778420	1.5573520
C	5.8547970	0.2931870	-1.4737740
H	4.8821400	0.0093840	-3.3767280
H	6.5493570	0.4891150	0.5556590
H	6.8179530	0.5420200	-1.9129620
C	-0.4062760	2.9994170	-1.3947730
H	-1.3410630	3.3884250	-0.9917370
H	-0.3900870	2.7875820	-2.4658400
C	1.9955740	2.7346880	-1.2804380
H	1.9855340	2.2996890	-2.2757380
H	2.8673990	2.5360050	-0.6643830
C	0.8272170	3.9107590	0.6236820
H	1.1078860	4.9617050	0.4719480
H	-0.1524420	3.8844050	1.1157030
H	1.5705570	3.4695130	1.2982220
C	0.7942940	3.2095110	-0.6992850
Cl	3.1500810	4.6883950	-2.0935510
Pd	0.1719300	1.0258850	-0.6277750

2 - Ground

Lowest Frequency Vibration = 5.4219 cm**-1
Electronic Energy = -2395.20077790
Electronic and Zero-Point Energy = -2394.420275
Enthalpy = -2394.375109
Free Energy = -2394.496196
E large = -2396.98764723

C	2.3344230	2.2479610	1.7602010
C	3.2432900	3.3247900	1.1596510
H	3.8647550	2.9169870	0.3530210
H	2.6896720	4.1839720	0.7675200
H	3.9141220	3.7046350	1.9396890
C	3.2208630	1.2465880	2.4894960
H	3.7880290	1.7963120	3.2496850
H	2.6415080	0.4757930	3.0055730
H	3.9517700	0.7580300	1.8379560
C	1.4207980	2.8626200	2.8227430
H	0.7433510	3.6285110	2.4285990
H	0.8205520	2.0820070	3.3078620
H	2.0346570	3.3447470	3.5936720
C	-2.6753760	2.8933150	0.2308170
C	-2.0019440	4.1279970	0.8307060
H	-1.3259230	4.6318000	0.1313720
H	-2.7754760	4.8537100	1.1094520
H	-1.4418760	3.8681000	1.7384060
C	-3.4213250	3.2842120	-1.0468750
H	-4.0455220	2.4598420	-1.4106060

H	-4.0786040	4.1392060	-0.8447400
H	-2.7396730	3.5795470	-1.8535020
C	-3.6925830	2.4039480	1.2551180
H	-3.2354720	2.2021190	2.2283140
H	-4.4376720	3.1954890	1.3979090
H	-4.2372440	1.5135840	0.9288630
P	1.8019630	0.1834550	-0.1951910
P	-1.8398150	0.1693100	-0.0510530
C	2.3515800	-1.1595610	0.9143900
C	1.5116110	-1.5273700	1.9745020
C	3.4571310	-1.9601750	0.6154490
C	1.7957260	-2.6478490	2.7443130
H	0.6357620	-0.9232370	2.2082770
C	3.7334810	-3.0896230	1.3849070
H	4.1100060	-1.7104170	-0.2181010
C	2.9100560	-3.4332210	2.4518700
H	1.1371600	-2.9081370	3.5709840
H	4.6025430	-3.6986110	1.1461380
H	3.1328000	-4.3130460	3.0510700
C	3.1616910	0.5514380	-1.3706850
C	2.7899020	0.7699580	-2.7018530
C	4.5035920	0.7313710	-1.0079420
C	3.7312370	1.1594300	-3.6511470
H	1.7480290	0.6334290	-2.9945220
C	5.4455760	1.1103570	-1.9579800
H	4.8248870	0.5684240	0.0191390
C	5.0605970	1.3280950	-3.2794710
H	3.4247500	1.3291290	-4.6807350
H	6.4852820	1.2363550	-1.6647640
H	5.7993700	1.6304080	-4.0180560
C	-1.9171600	-0.4060100	1.6774940
C	-2.2160280	-1.7493090	1.9374420
C	-1.4811160	0.4092520	2.7244900
C	-2.1213890	-2.2525190	3.2304090
H	-2.5147270	-2.4089400	1.1227500
C	-1.3792960	-0.0978920	4.0171080
H	-1.2013090	1.4409930	2.5175980
C	-1.7051970	-1.4267830	4.2737710
H	-2.3665910	-3.2944220	3.4234840
H	-1.0405440	0.5487080	4.8241650
H	-1.6279620	-1.8228930	5.2836490
C	-3.4513710	-0.2332240	-0.8311660
C	-3.5361740	0.0001850	-2.2098550
C	-4.5586410	-0.7600020	-0.1627840
C	-4.7082640	-0.2727970	-2.9033620
H	-2.6753460	0.4093080	-2.7417990

C	-5.7302220	-1.0446230	-0.8614350
H	-4.5173380	-0.9407330	0.9102810
C	-5.8079620	-0.8004910	-2.2284170
H	-4.7635220	-0.0781940	-3.9719600
H	-6.5864070	-1.4545890	-0.3305870
H	-6.7245190	-1.0214290	-2.7706400
C	1.1234800	-2.3669370	-2.3876170
H	2.1457510	-2.6213750	-2.1104970
H	0.9960660	-1.8424930	-3.3356020
C	-1.2449030	-2.5603200	-2.0720190
H	-1.4574700	-2.0630130	-3.0194080
H	-2.1054290	-2.9778350	-1.5495570
C	0.2733570	-4.1317170	-0.7865730
H	0.1485780	-5.1264550	-1.2329210
H	1.2874730	-4.0773160	-0.3752680
H	-0.4495680	-4.0465390	0.0330760
C	0.0461870	-3.0843450	-1.8315080
Pd	-0.0547300	-0.9758460	-1.1161560
N	1.4498860	1.6040490	0.7029170
N	-1.6210960	1.8514190	-0.0620950
C	0.8026580	2.6352250	-0.1449140
H	1.5048750	3.0084600	-0.9129610
H	0.5888390	3.4863710	0.5054550
C	-0.4883390	2.3023040	-0.8846120
H	-0.7661550	3.2276690	-1.4048240
H	-0.3020710	1.5795090	-1.6897830

2 – TS1

Lowest Frequency Vibration = -366.9381 cm**-1
Electronic Energy = -2608.82036856
Electronic and Zero-Point Energy = -2607.887578
Enthalpy = -2607.835670
Free Energy = -2607.969955
E large = -2610.67498234

C	-3.8353120	-0.7517870	-1.8019000
C	-4.3579770	0.2931580	-2.7947770
H	-4.5979450	1.2414660	-2.3000360
H	-3.6522270	0.4992850	-3.6077950
H	-5.2805670	-0.0802300	-3.2573710
C	-4.8329020	-0.8464480	-0.6534550
H	-5.8317160	-0.9976750	-1.0800140
H	-4.6222260	-1.6942140	0.0053170
H	-4.8797450	0.0654380	-0.0503480
C	-3.7992950	-2.1244070	-2.4740260
H	-3.2571450	-2.1159930	-3.4267400
H	-3.3336790	-2.8632140	-1.8067380

H	-4.8240020	-2.4521820	-2.6879630
C	0.6016490	-3.7860500	-1.9124390
C	-0.6118660	-4.7202950	-1.9505670
H	-1.3995210	-4.3706520	-2.6271800
H	-0.2969780	-5.7071840	-2.3122680
H	-1.0554170	-4.8574520	-0.9575320
C	1.2417500	-3.7544050	-3.3070400
H	2.0609230	-3.0254760	-3.3511610
H	1.6661250	-4.7430990	-3.5203700
H	0.5298920	-3.5332080	-4.1089450
C	1.6467810	-4.4027710	-0.9841530
H	1.3726050	-4.3742290	0.0732090
H	1.7552270	-5.4583160	-1.2592920
H	2.6288150	-3.9364880	-1.1050580
P	-2.0616850	0.6867820	-0.0664820
P	0.8641450	-1.4232080	-0.2725500
C	-2.5645480	0.0499810	1.5677180
C	-2.7965460	-1.3025480	1.8201100
C	-2.5057710	0.9405630	2.6505640
C	-3.0365990	-1.7453310	3.1179300
H	-2.7850050	-2.0172560	0.9986040
C	-2.7339570	0.4935840	3.9465430
H	-2.2867060	1.9953310	2.4809830
C	-3.0143200	-0.8506300	4.1824060
H	-3.2337010	-2.8000860	3.2972240
H	-2.6975860	1.1993340	4.7735790
H	-3.2006210	-1.2008550	5.1952310
C	-3.0629680	2.2044150	-0.3375460
C	-2.6268520	3.0348250	-1.3788580
C	-4.2210350	2.5537030	0.3630820
C	-3.3468780	4.1698020	-1.7327760
H	-1.7174570	2.7798560	-1.9257420
C	-4.9357860	3.6977150	0.0171290
H	-4.5761440	1.9309050	1.1825740
C	-4.5056130	4.5020540	-1.0340930
H	-3.0023870	4.7991060	-2.5504110
H	-5.8355400	3.9572800	0.5707200
H	-5.0698170	5.3918820	-1.3043620
C	0.5381730	-2.2002270	1.3587150
C	1.0349180	-1.5444250	2.4943410
C	-0.2552640	-3.3342220	1.5405790
C	0.7922720	-2.0444310	3.7691120
H	1.6223710	-0.6329910	2.3794450
C	-0.4892560	-3.8428870	2.8153620
H	-0.7060400	-3.8201190	0.6794270
C	0.0394330	-3.2052270	3.9323390

H	1.1957300	-1.5264690	4.6365720
H	-1.0995910	-4.7359690	2.9330790
H	-0.1464380	-3.6005770	4.9285540
C	2.6890900	-1.5220170	-0.4987220
C	3.1730240	-1.0526770	-1.7271940
C	3.6025400	-1.9574920	0.4638250
C	4.5352610	-1.0512870	-2.0017720
H	2.4694570	-0.6806740	-2.4749490
C	4.9698420	-1.9427530	0.1939930
H	3.2492760	-2.3388350	1.4205070
C	5.4393660	-1.4988570	-1.0389620
H	4.8939660	-0.6962650	-2.9657400
H	5.6700700	-2.2939920	0.9490840
H	6.5067630	-1.4955260	-1.2486310
C	0.5811900	2.9782890	0.5445930
H	-0.0518760	3.3550610	1.3493230
H	0.4865490	3.5109410	-0.4037560
C	2.7134330	1.9907390	-0.1616060
H	2.4426880	2.1774970	-1.1987730
H	3.4165540	1.1783710	0.0026360
C	2.1602480	2.0591440	2.3061100
H	2.6169760	2.9398810	2.7800380
H	1.2655410	1.8065520	2.8910290
H	2.8764040	1.2303630	2.3906360
C	1.8060740	2.3354610	0.8703270
Pd	0.2923720	0.9157250	0.0544920
N	4.2506390	3.3772500	-0.2274890
H	4.6667100	3.2436420	-1.1514890
C	3.6531670	4.7112640	-0.1376310
H	2.9291550	4.6936850	0.6922950
H	4.4281180	5.4460140	0.1317130
C	5.2686470	3.1306320	0.8028010
H	4.7681270	3.1812040	1.7792350
H	6.0042850	3.9511170	0.7827590
C	5.9713490	1.8041520	0.6168420
H	6.3682060	1.7091790	-0.4024530
H	6.8165790	1.7283250	1.3084350
H	5.3152860	0.9462290	0.8062380
C	2.9779380	5.1147060	-1.4288890
H	2.5263060	6.1066850	-1.3270060
H	3.7006950	5.1601730	-2.2529650
H	2.1833240	4.4142490	-1.7117990
N	-2.4456680	-0.4328210	-1.3079480
N	0.1458460	-2.3977050	-1.4822130
C	-1.3948720	-0.4630390	-2.3468430
H	-0.6961900	0.3656630	-2.1736430

H	-1.8418710	-0.2481720	-3.3280930
C	-0.5850800	-1.7329900	-2.5779860
H	-1.2474160	-2.4872030	-3.0104300
H	0.1104510	-1.4460380	-3.3861220

2 – Int 1

Lowest Frequency Vibration = 18.2918 cm**-1
Electronic Energy = -2608.8759903
Electronic and Zero-Point Energy = -2607.899902
Enthalpy = -2607.848572
Free Energy = -2607.980496
E large = -2610.69016220

C	-3.6541440	-0.8185800	-1.9736620
C	-4.1831600	0.2685050	-2.9172170
H	-4.5185020	1.1544480	-2.3661600
H	-3.4421250	0.5871140	-3.6596470
H	-5.0462860	-0.1226920	-3.4711160
C	-4.7143670	-1.0669340	-0.9080630
H	-5.6677540	-1.2680570	-1.4116480
H	-4.4767710	-1.9372600	-0.2886810
H	-4.8728780	-0.2035380	-0.2548790
C	-3.4901130	-2.1280360	-2.7479050
H	-2.9128870	-2.0056070	-3.6715390
H	-2.9988930	-2.8837600	-2.1187910
H	-4.4781420	-2.5081650	-3.0353850
C	0.8567970	-3.6250910	-2.0392080
C	-0.3356190	-4.5725560	-2.2149300
H	-1.1286630	-4.1535190	-2.8442650
H	0.0056770	-5.4970120	-2.6981860
H	-0.7784800	-4.8506110	-1.2515800
C	1.5791980	-3.4859060	-3.3861130
H	2.3842580	-2.7430400	-3.3269680
H	2.0345970	-4.4495910	-3.6451650
H	0.9115380	-3.2154410	-4.2108210
C	1.8488290	-4.3007350	-1.0936420
H	1.5039650	-4.3500740	-0.0575270
H	1.9871440	-5.3325970	-1.4381030
H	2.8312100	-3.8205740	-1.1151570
P	-2.0688720	0.6125820	-0.0341550
P	0.9928370	-1.3551950	-0.2389120
C	-2.7456720	-0.0781650	1.5164170
C	-2.9035690	-1.4454940	1.7471850
C	-2.8958850	0.8076770	2.5941920
C	-3.2560370	-1.9128750	3.0104070
H	-2.7406080	-2.1534060	0.9366800
C	-3.2430350	0.3394270	3.8558440

H	-2.7386040	1.8760420	2.4444920
C	-3.4333820	-1.0246210	4.0662230
H	-3.3852670	-2.9814760	3.1692540
H	-3.3661140	1.0436480	4.6758730
H	-3.7109620	-1.3928260	5.0513720
C	-3.0969270	2.1112540	-0.3568500
C	-2.5548440	3.0196780	-1.2757930
C	-4.3628600	2.3739390	0.1764000
C	-3.2718400	4.1403300	-1.6808670
H	-1.5581300	2.8391830	-1.6826060
C	-5.0763790	3.5030190	-0.2169690
H	-4.8004740	1.6942360	0.9061650
C	-4.5376960	4.3824180	-1.1524470
H	-2.8410040	4.8302810	-2.4033920
H	-6.0603180	3.6924550	0.2069470
H	-5.1004610	5.2605660	-1.4613990
C	0.5788030	-2.2867140	1.2904350
C	1.0536350	-1.8202910	2.5245350
C	-0.3055750	-3.3673980	1.2850060
C	0.7016410	-2.4614470	3.7084740
H	1.7105360	-0.9514820	2.5631720
C	-0.6496610	-4.0161270	2.4674140
H	-0.7338810	-3.6954210	0.3402150
C	-0.1413290	-3.5697900	3.6828370
H	1.0898080	-2.0923240	4.6555180
H	-1.3297820	-4.8653300	2.4371420
H	-0.4103780	-4.0738540	4.6085740
C	2.8314680	-1.4361110	-0.3764490
C	3.3751340	-0.8604950	-1.5338560
C	3.7026630	-1.9746460	0.5744160
C	4.7478800	-0.8655390	-1.7572750
H	2.7090530	-0.4116620	-2.2747160
C	5.0799310	-1.9600860	0.3616880
H	3.3076170	-2.4406010	1.4756630
C	5.6063190	-1.4171550	-0.8070180
H	5.1501210	-0.4332070	-2.6715370
H	5.7433880	-2.3914700	1.1084210
H	6.6807840	-1.4193240	-0.9764950
C	0.6841810	2.8637230	1.0741310
H	0.2226340	2.9601530	2.0592120
H	0.3679470	3.6132770	0.3465880
C	2.7756160	2.4690360	-0.2576700
H	2.1530180	2.7303150	-1.1192650
H	3.3826050	1.5995670	-0.5327860
C	2.5959170	1.6350960	2.1805960
H	3.1988390	2.3722410	2.7333730

H	1.8380820	1.2672790	2.8828410
H	3.2573890	0.7950500	1.9257070
C	1.9334010	2.2145010	0.9541320
Pd	0.2865420	0.9106770	0.2764390
N	3.7912390	3.6363540	-0.1630740
H	4.1591230	3.7268460	-1.1181540
C	3.1459550	4.9485300	0.1798270
H	2.5595220	4.7775150	1.0890620
H	3.9608250	5.6372600	0.4243960
C	4.9929810	3.3900940	0.7106670
H	4.6467160	3.4154300	1.7474400
H	5.6400940	4.2595420	0.5548290
C	5.7264640	2.1162100	0.3748990
H	5.9704620	2.0640200	-0.6937140
H	6.6695610	2.1016970	0.9299610
H	5.1675780	1.2160940	0.6525050
C	2.3132070	5.4923280	-0.9552010
H	1.9255170	6.4752040	-0.6708150
H	2.9173950	5.6237730	-1.8612080
H	1.4546100	4.8588130	-1.2004360
N	-2.3241090	-0.4656240	-1.3602250
N	0.3561990	-2.2771670	-1.5425900
C	-1.2180710	-0.3450720	-2.3337640
H	-0.5801350	0.4998370	-2.0446160
H	-1.6212160	-0.0632570	-3.3175490
C	-0.3197540	-1.5435200	-2.6270660
H	-0.9037820	-2.2809810	-3.1837290
H	0.4165670	-1.1448880	-3.3489060

2 – Int 2

Lowest Frequency Vibration = 20.4038 cm**-1
Electronic Energy = -2855.51146946
Electronic and Zero-Point Energy = -2854.729432
Enthalpy = -2854.682546
Free Energy = -2854.806550
E large = -2857.32830726

C	-3.2498930	-2.0335590	-1.6920440
C	-3.8887980	-1.3545460	-2.9067520
H	-4.3403840	-0.3936840	-2.6341990
H	-3.1613400	-1.1749310	-3.7080710
H	-4.6805350	-1.9923340	-3.3205050
C	-4.3054330	-2.1662390	-0.5990220
H	-5.1538800	-2.7283080	-1.0076370
H	-3.9292770	-2.7142580	0.2709280
H	-4.6947760	-1.2009760	-0.2637770
C	-2.8296110	-3.4545870	-2.0722940

H	-2.1524380	-3.4846740	-2.9329220
H	-2.3468450	-3.9610790	-1.2262990
H	-3.7216670	-4.0322950	-2.3451300
C	1.6077640	-3.4910040	-0.1565870
C	0.5025200	-4.4708540	0.2483910
H	-0.2406190	-4.6460090	-0.5375710
H	0.9480830	-5.4445620	0.4886990
H	-0.0185040	-4.1060920	1.1429510
C	2.3999780	-4.0622520	-1.3392360
H	3.1691620	-3.3586660	-1.6802460
H	2.9060740	-4.9837900	-1.0259900
H	1.7690850	-4.3194350	-2.1961530
C	2.5538190	-3.4213470	1.0369490
H	2.0469350	-3.0954710	1.9496210
H	2.9405400	-4.4316460	1.2167900
H	3.4186260	-2.7727030	0.8711280
P	-2.0184140	0.0533390	-0.1260740
P	1.6212930	-0.5729340	-0.2420050
C	-2.2260010	-0.6361630	1.5569590
C	-1.9908320	-1.9899010	1.8133280
C	-2.3826180	0.2376330	2.6419770
C	-1.9538410	-2.4697970	3.1205900
H	-1.8086830	-2.6645930	0.9772490
C	-2.3535130	-0.2429760	3.9467640
H	-2.5181070	1.3057830	2.4678450
C	-2.1430540	-1.5993620	4.1905270
H	-1.7712660	-3.5277400	3.3011240
H	-2.4872730	0.4469740	4.7772110
H	-2.1160140	-1.9727720	5.2118580
C	-3.5045480	1.1015940	-0.4228570
C	-3.4473820	1.9053870	-1.5695390
C	-4.6282570	1.1930420	0.4031190
C	-4.4985460	2.7512130	-1.9024510
H	-2.5649120	1.8575580	-2.2110960
C	-5.6747510	2.0547790	0.0813730
H	-4.6960020	0.5823090	1.3026280
C	-5.6161360	2.8294080	-1.0728630
H	-4.4428360	3.3583100	-2.8033900
H	-6.5424980	2.1139850	0.7349850
H	-6.4371340	3.4973070	-1.3239660
C	2.2877950	-0.4681020	1.4585900
C	3.5390970	0.0925190	1.7319500
C	1.4284400	-0.7511420	2.5305440
C	3.9382910	0.3264560	3.0475970
H	4.2126110	0.3538510	0.9180550
C	1.8321040	-0.5248220	3.8397000

H	0.4394000	-1.1675450	2.3339840
C	3.0919690	0.0125870	4.1047070
H	4.9190750	0.7563970	3.2406450
H	1.1583850	-0.7662200	4.6595090
H	3.4055850	0.1919920	5.1306740
C	3.0719660	-0.4148470	-1.3783930
C	2.8464780	0.3479140	-2.5305800
C	4.3173660	-1.0415370	-1.2313520
C	3.8289270	0.4838450	-3.5089130
H	1.8839330	0.8478100	-2.6528350
C	5.3046660	-0.8989690	-2.2004320
H	4.5310680	-1.6409030	-0.3482920
C	5.0606350	-0.1398630	-3.3436670
H	3.6300180	1.0795510	-4.3971400
H	6.2688670	-1.3842770	-2.0640010
H	5.8333920	-0.0329140	-4.1018890
C	-0.4211880	3.3480860	0.1789740
H	-1.1528120	3.4892240	0.9767670
H	-0.7126040	3.7505100	-0.7942210
C	1.9726070	3.4742080	-0.5216500
H	1.6132070	3.4210930	-1.5509370
H	2.8896050	2.8943950	-0.3879660
C	1.3947290	3.1469070	1.9246650
H	1.6467620	4.1551180	2.2882700
H	0.6054370	2.7479090	2.5745430
H	2.2908400	2.5244770	2.0534440
C	0.9422010	3.1874500	0.4894630
Pd	0.0474970	1.2591270	-0.1169270
N	-2.0483920	-1.2651970	-1.2180260
N	0.9570740	-2.1616010	-0.4876920
Cl	2.6145580	5.2754270	-0.3900280
C	-0.8859140	-1.2778180	-2.1186760
H	-0.4929880	-0.2583590	-2.2235540
H	-1.2095810	-1.5606310	-3.1296380
C	0.2496310	-2.2452790	-1.7887000
H	-0.1594600	-3.2558190	-1.8642060
H	0.9654610	-2.1508100	-2.6278800

2 – TS2

Lowest Frequency Vibration = -278.2949 cm**-1
Electronic Energy = -2855.50900161
Electronic and Zero-Point Energy = -2854.727295
Enthalpy = -2854.680928
Free Energy = -2854.803683
E large = -2857.32525743

C	-3.2214760	-2.0189440	-1.7446900

C	-3.8413320	-1.3230430	-2.9594070
H	-4.2822440	-0.3578530	-2.6847760
H	-3.1068420	-1.1489660	-3.7553920
H	-4.6383820	-1.9481710	-3.3818750
C	-4.2893280	-2.1554750	-0.6646100
H	-5.1319400	-2.7174850	-1.0847500
H	-3.9224390	-2.7054880	0.2077890
H	-4.6848710	-1.1919700	-0.3311950
C	-2.8029470	-3.4377380	-2.1344200
H	-2.1154480	-3.4617940	-2.9869610
H	-2.3327500	-3.9551280	-1.2880060
H	-3.6941420	-4.0082420	-2.4243760
C	1.6218050	-3.4917900	-0.1750090
C	0.5121950	-4.4738730	0.2100930
H	-0.2278880	-4.6342910	-0.5818010
H	0.9545270	-5.4522740	0.4365170
H	-0.0114520	-4.1225400	1.1082890
C	2.4273120	-4.0541080	-1.3521980
H	3.1989180	-3.3474880	-1.6809340
H	2.9312190	-4.9766490	-1.0386730
H	1.8053880	-4.3071250	-2.2169250
C	2.5523800	-3.4254560	1.0305680
H	2.0329100	-3.1033940	1.9375970
H	2.9373360	-4.4360980	1.2119300
H	3.4190700	-2.7757200	0.8786960
P	-2.0010790	0.0258800	-0.1271090
P	1.6371540	-0.5796980	-0.2432530
C	-2.2230770	-0.6857020	1.5425160
C	-1.9948250	-2.0431530	1.7840210
C	-2.3885710	0.1761710	2.6353080
C	-1.9721230	-2.5380330	3.0859970
H	-1.8082580	-2.7094000	0.9423440
C	-2.3740250	-0.3197180	3.9343710
H	-2.5191290	1.2464490	2.4730820
C	-2.1693630	-1.6794100	4.1638340
H	-1.7949840	-3.5985290	3.2558520
H	-2.5147810	0.3605370	4.7714640
H	-2.1534920	-2.0650160	5.1807640
C	-3.4654330	1.0983970	-0.4289330
C	-3.3867260	1.9091370	-1.5692040
C	-4.5955500	1.1944000	0.3872390
C	-4.4235030	2.7717610	-1.9035220
H	-2.4990230	1.8552980	-2.2029390
C	-5.6278710	2.0720760	0.0628660
H	-4.6795020	0.5755040	1.2796190
C	-5.5474820	2.8565650	-1.0832990

H	-4.3517860	3.3861520	-2.7982250
H	-6.5014600	2.1359250	0.7080060
H	-6.3571550	3.5375210	-1.3357920
C	2.2764210	-0.4667780	1.4665920
C	3.5187100	0.1068810	1.7529400
C	1.4049210	-0.7546660	2.5272770
C	3.8968950	0.3519110	3.0725430
H	4.2005010	0.3706110	0.9468740
C	1.7890660	-0.5183090	3.8407640
H	0.4233580	-1.1826170	2.3188510
C	3.0391870	0.0340890	4.1194260
H	4.8703960	0.7926700	3.2769740
H	1.1078600	-0.7632950	4.6531450
H	3.3368390	0.2219950	5.1485560
C	3.0925330	-0.3888300	-1.3623950
C	2.8864830	0.4197870	-2.4862130
C	4.3304300	-1.0318840	-1.2230880
C	3.8819330	0.5833790	-3.4468730
H	1.9303340	0.9329440	-2.6009420
C	5.3297760	-0.8624150	-2.1750500
H	4.5284370	-1.6654450	-0.3606550
C	5.1058550	-0.0575660	-3.2907670
H	3.6996090	1.2149180	-4.3134420
H	6.2882340	-1.3606090	-2.0456450
H	5.8881950	0.0706280	-4.0356350
C	-0.5564140	3.2695270	0.2589250
H	-1.2998770	3.3875370	1.0485350
H	-0.8547740	3.6512720	-0.7202570
C	1.8051390	3.3149330	-0.4273440
H	1.4795720	3.3240780	-1.4644100
H	2.7806460	2.8680860	-0.2479820
C	1.2596750	3.1724220	2.0286050
H	1.4972960	4.1905480	2.3702330
H	0.4750740	2.7712090	2.6826600
H	2.1643510	2.5646250	2.1632180
C	0.8137320	3.1961480	0.5947550
Pd	0.0541990	1.2349560	-0.1067140
N	-2.0187540	-1.2637490	-1.2476740
N	0.9745140	-2.1604080	-0.5066780
Cl	2.5877770	5.3712070	-0.4353630
C	-0.8515410	-1.2620420	-2.1428170
H	-0.4617500	-0.2403920	-2.2372090
H	-1.1705520	-1.5342770	-3.1576010
C	0.2817720	-2.2320830	-1.8164880
H	-0.1260690	-3.2420230	-1.9059860
H	1.0063120	-2.1277230	-2.6465790

6 - Ground

Lowest Frequency Vibration = 40.1011 cm**-1
Electronic Energy = -3337.85593275
Electronic and Zero-Point Energy = -3337.127149
Enthalpy = -3337.079818
Free Energy = -3337.201253
E large = -5468.82140424

Ti	-0.0613550	-1.7690820	0.3155610
Cl	-0.3922500	-3.8757850	0.9937380
Cl	0.1422540	-2.4251390	-1.9259290
N	-1.5306540	-0.8085860	1.1593660
N	1.6561600	-1.2457500	0.9385170
C	-2.4257630	-1.1399080	2.3292840
C	-3.4026450	-2.2520470	1.9505330
H	-4.1296820	-1.9093240	1.2048070
H	-2.8853910	-3.1315980	1.5538200
H	-3.9610240	-2.5614030	2.8432790
C	-3.2252420	0.0716550	2.7949590
H	-3.8599270	-0.2424540	3.6327560
H	-2.5814910	0.8818680	3.1514740
H	-3.8938620	0.4634790	2.0203500
C	-1.5252810	-1.5799070	3.4765060
H	-0.9783830	-2.4983800	3.2413120
H	-0.8033820	-0.7896870	3.7229410
H	-2.1353950	-1.7739810	4.3669700
C	2.6970840	-1.9518240	1.7913150
C	2.0463480	-2.3332840	3.1166360
H	1.2063150	-3.0209740	2.9777200
H	2.7886140	-2.8396920	3.7454790
H	1.6924880	-1.4484330	3.6601060
C	3.1639840	-3.2015310	1.0506250
H	3.6698580	-2.9362110	0.1155650
H	3.8764960	-3.7527730	1.6769200
H	2.3304610	-3.8721170	0.8167930
C	3.9124630	-1.0779750	2.0872610
H	3.6519720	-0.1543510	2.6142700
H	4.5793070	-1.6513700	2.7421340
H	4.4819580	-0.8292010	1.1873590
P	-1.8643600	0.1873450	-0.1478360
P	1.8345080	0.1164140	-0.0542190
C	-2.0408610	1.9369240	0.3344640
C	-1.3631460	2.4115500	1.4599320
C	-2.7654320	2.8328300	-0.4605120
C	-1.4341030	3.7561780	1.8053380
H	-0.7801860	1.7261590	2.0721180

C	-2.8315150	4.1780220	-0.1116060
H	-3.2835710	2.4917960	-1.3544070
C	-2.1684910	4.6416900	1.0206210
H	-0.9148560	4.1104050	2.6930250
H	-3.4057020	4.8637770	-0.7301560
H	-2.2243540	5.6929660	1.2926600
C	-3.4277930	-0.3609420	-0.9128780
C	-3.3806390	-1.5198850	-1.6962610
C	-4.6625200	0.2400160	-0.6477880
C	-4.5508930	-2.0694460	-2.2062910
H	-2.4253190	-2.0023770	-1.8995400
C	-5.8308380	-0.3113920	-1.1660340
H	-4.7252230	1.1335070	-0.0300990
C	-5.7774460	-1.4646250	-1.9430940
H	-4.5036070	-2.9711240	-2.8119880
H	-6.7864350	0.1630390	-0.9557790
H	-6.6931540	-1.8929920	-2.3437050
C	1.9725240	1.6199920	0.9627070
C	2.2024920	2.8489630	0.3337510
C	1.7940620	1.5770670	2.3473850
C	2.2906640	4.0138860	1.0873040
H	2.3205970	2.8989560	-0.7477690
C	1.8803550	2.7462340	3.0983010
H	1.5785920	0.6291890	2.8391680
C	2.1357270	3.9623080	2.4710020
H	2.4795530	4.9633180	0.5920180
H	1.7475640	2.7039580	4.1767460
H	2.2062410	4.8737680	3.0599310
C	3.3973370	-0.0640070	-0.9927190
C	3.5092900	-1.1299630	-1.8928290
C	4.4640210	0.8268240	-0.8439950
C	4.6769950	-1.3041570	-2.6266580
H	2.6845180	-1.8288440	-2.0183530
C	5.6273530	0.6511120	-1.5883460
H	4.4039780	1.6488830	-0.1342260
C	5.7355340	-0.4109350	-2.4799020
H	4.7561660	-2.1383090	-3.3196570
H	6.4519950	1.3487450	-1.4637080
H	6.6465440	-0.5462330	-3.0579820
C	-1.1471380	0.8227910	-3.0002950
H	-2.1631590	1.2054990	-2.9241830
H	-1.0342240	-0.1543440	-3.4730160
C	1.2010280	1.0802470	-2.8542790
H	1.3692590	0.1221200	-3.3492320
H	2.0896290	1.6785320	-2.6553030
C	-0.2156800	3.1696920	-2.6835930

H	0.2943500	3.7380350	-3.4702270
H	-1.2681120	3.4657690	-2.6741820
H	0.2344570	3.4609350	-1.7259030
C	-0.0551460	1.7055100	-2.9493400
Ni	0.0072990	0.3218210	-1.3706710

6 – TS1

Lowest Frequency Vibration = -295.8651 cm**-1
Electronic Energy = -3551.49439920
Electronic and Zero-Point Energy = -3550.616549
Enthalpy = -3550.561279
Free Energy = -3550.701705
E large = -5682.52522733

Ti	-0.9505860	-1.1267030	-1.4333960
Cl	-1.9936980	-2.1055130	-3.1855370
Cl	0.1689140	0.3923880	-2.8755340
N	-2.4304080	-0.8355150	-0.1842060
N	0.3309940	-2.3799690	-0.7921710
C	-3.7707070	-1.4918440	-0.0093890
C	-4.7206430	-1.0612160	-1.1263040
H	-4.9768280	0.0019950	-1.0483750
H	-4.2846270	-1.2404280	-2.1147760
H	-5.6524590	-1.6369250	-1.0553060
C	-4.3962460	-1.1402680	1.3359080
H	-5.3853040	-1.6112250	1.3949080
H	-3.7983500	-1.5123700	2.1747540
H	-4.5438230	-0.0614720	1.4622780
C	-3.5533130	-2.9988050	-0.0527390
H	-3.1906050	-3.3288240	-1.0319170
H	-2.8313410	-3.3063410	0.7159200
H	-4.5017050	-3.5144930	0.1423340
C	0.7295240	-3.7807430	-1.2020570
C	-0.4986840	-4.6790850	-1.1116570
H	-1.3062570	-4.3261180	-1.7605320
H	-0.2270140	-5.6911330	-1.4362530
H	-0.8735840	-4.7455040	-0.0830050
C	1.2389470	-3.7427800	-2.6412750
H	2.1512830	-3.1397570	-2.7207190
H	1.4783300	-4.7619450	-2.9707160
H	0.4864740	-3.3325140	-3.3250410
C	1.8200970	-4.3607700	-0.3059430
H	1.5299110	-4.3729410	0.7501750
H	1.9938750	-5.3993540	-0.6120600
H	2.7715470	-3.8298340	-0.4071940
P	-1.9605250	0.7205520	0.2225980
P	1.1669710	-1.2502230	0.1564050

C	-1.9981130	1.0388670	2.0211260
C	-1.7389940	-0.0008460	2.9170070
C	-2.1602340	2.3406710	2.5125700
C	-1.6709620	0.2498310	4.2833510
H	-1.5908130	-1.0130640	2.5450740
C	-2.0907270	2.5868890	3.8803550
H	-2.3483520	3.1711830	1.8353630
C	-1.8484210	1.5427440	4.7684860
H	-1.4752000	-0.5716840	4.9692220
H	-2.2302930	3.5998290	4.2506330
H	-1.7983220	1.7368000	5.8372820
C	-3.1037040	1.9050840	-0.5683530
C	-2.8888900	2.1869920	-1.9219360
C	-4.2454510	2.4107260	0.0639160
C	-3.8060600	2.9517420	-2.6350070
H	-2.0050330	1.7931930	-2.4234560
C	-5.1578670	3.1794210	-0.6519360
H	-4.4388280	2.1980360	1.1138470
C	-4.9423590	3.4469700	-2.0011880
H	-3.6303480	3.1609520	-3.6875790
H	-6.0442610	3.5645300	-0.1534130
H	-5.6606110	4.0432410	-2.5589930
C	1.0459400	-1.7439430	1.9060550
C	1.7257310	-1.0072970	2.8818490
C	0.2053200	-2.7897500	2.2949900
C	1.6015630	-1.3432430	4.2254110
H	2.3628050	-0.1718610	2.5911180
C	0.0776070	-3.1193660	3.6415720
H	-0.3599830	-3.3379450	1.5425200
C	0.7815950	-2.4034620	4.6059310
H	2.1429450	-0.7736370	4.9770070
H	-0.5719880	-3.9403970	3.9357260
H	0.6859580	-2.6662620	5.6569360
C	2.9381700	-1.3019560	-0.3181770
C	3.2644780	-0.9928500	-1.6442380
C	3.9614950	-1.5812760	0.5916430
C	4.5934590	-0.9562480	-2.0493100
H	2.4769460	-0.7686660	-2.3616500
C	5.2925630	-1.5376560	0.1806820
H	3.7312960	-1.8516980	1.6195740
C	5.6117160	-1.2216020	-1.1357550
H	4.8332770	-0.7193900	-3.0834170
H	6.0805320	-1.7579310	0.8971490
H	6.6517120	-1.1880890	-1.4516410
C	0.1742200	2.8103390	-0.1887140
H	-0.5875640	3.3311380	0.3903840

H	0.1606470	2.9989830	-1.2636820
C	2.3833890	1.8351320	-0.3389920
H	2.2607840	1.7290840	-1.4128720
H	3.1572440	1.2326830	0.1248550
C	1.5582970	2.6055480	1.9258560
H	1.7732380	3.6589700	2.1516190
H	0.6535320	2.3341450	2.4840840
H	2.3949410	2.0098410	2.3081370
C	1.3734410	2.4225960	0.4459250
Ni	0.2216670	0.8052200	-0.1750940
N	3.9256580	3.3789060	-0.6893510
H	4.5047810	3.0150890	-1.4479800
C	3.2301530	4.5865010	-1.1240340
H	2.4193510	4.7830690	-0.4036990
H	3.9098530	5.4542080	-1.0735210
C	4.7427740	3.5738120	0.5088150
H	4.0634670	3.8169730	1.3388540
H	5.3987280	4.4512430	0.3748290
C	5.5773520	2.3542860	0.8362350
H	6.1955400	2.0597500	-0.0219130
H	6.2512340	2.5706560	1.6714920
H	4.9647540	1.4895590	1.1233310
C	2.6761810	4.4430360	-2.5244410
H	2.1708010	5.3639630	-2.8324800
H	3.4795050	4.2470420	-3.2459310
H	1.9495380	3.6240950	-2.5981090

6 – Int 1

Lowest Frequency Vibration = 29.2188 cm**-1
Electronic Energy = -3551.52197140
Electronic and Zero-Point Energy = -3550.639467
Enthalpy = -3550.584565
Free Energy = -3550.722801
E large = -5682.54890263

Ti	-0.8107750	-0.8603280	-1.5680590
Cl	-1.7218580	-1.5545240	-3.5559700
Cl	0.2767430	0.9620080	-2.6924840
N	-2.4086400	-0.8909760	-0.4286170
N	0.5125800	-2.1654180	-1.1222690
C	-3.7163260	-1.6175320	-0.4533630
C	-4.6173940	-1.0350310	-1.5423080
H	-4.9091020	-0.0037530	-1.3069930
H	-4.1185660	-1.0408490	-2.5171720
H	-5.5348340	-1.6331570	-1.6210380
C	-4.4425540	-1.5224080	0.8844480
H	-5.4047830	-2.0430900	0.8001970

H	-3.8759200	-1.9945400	1.6940770
H	-4.6598320	-0.4853740	1.1674420
C	-3.4203000	-3.0853820	-0.7355860
H	-2.9558000	-3.2203560	-1.7184790
H	-2.7464760	-3.4955150	0.0296320
H	-4.3514970	-3.6655440	-0.7182990
C	0.9721220	-3.4566290	-1.7495120
C	-0.2241650	-4.3948890	-1.8740120
H	-1.0115210	-3.9575930	-2.4968690
H	0.0979260	-5.3310750	-2.3472060
H	-0.6487870	-4.6432910	-0.8933160
C	1.5259290	-3.1502760	-3.1399860
H	2.4221020	-2.5226170	-3.0754200
H	1.8036980	-4.0860790	-3.6421730
H	0.7835250	-2.6371390	-3.7611360
C	2.0602150	-4.1538160	-0.9374220
H	1.7406400	-4.3870510	0.0836510
H	2.3000730	-5.1022140	-1.4333950
H	2.9834530	-3.5670600	-0.8936970
P	-2.0050250	0.5640620	0.2931380
P	1.2276590	-1.1927140	0.0710620
C	-2.1045790	0.5170630	2.1181220
C	-1.8807350	-0.6819360	2.7972160
C	-2.2521270	1.7005580	2.8538710
C	-1.8235210	-0.7047700	4.1868300
H	-1.7481270	-1.6023770	2.2325410
C	-2.1873460	1.6753450	4.2435260
H	-2.4243820	2.6494050	2.3488560
C	-1.9721450	0.4738250	4.9131990
H	-1.6590590	-1.6494200	4.7011440
H	-2.3120170	2.5998920	4.8028120
H	-1.9253920	0.4552260	5.9995440
C	-3.1695410	1.8563050	-0.2680120
C	-2.9331440	2.4176370	-1.5281070
C	-4.3266140	2.2116710	0.4334360
C	-3.8450420	3.3100830	-2.0826050
H	-2.0329750	2.1452040	-2.0806630
C	-5.2328720	3.1102670	-0.1210280
H	-4.5328640	1.7800420	1.4113470
C	-4.9958960	3.6570300	-1.3793970
H	-3.6549610	3.7372520	-3.0646060
H	-6.1308300	3.3776310	0.4314510
H	-5.7088050	4.3558350	-1.8110490
C	1.0524000	-2.0621600	1.6721640
C	1.6631060	-1.5614570	2.8269150
C	0.2317150	-3.1894020	1.7743850

C	1.5018210	-2.2084010	4.0480590
H	2.2771900	-0.6647990	2.7759750
C	0.0651170	-3.8318300	2.9978330
H	-0.2885110	-3.5590540	0.8922750
C	0.7093280	-3.3501130	4.1344550
H	1.9950010	-1.8158350	4.9343560
H	-0.5686830	-4.7135460	3.0598440
H	0.5850580	-3.8574330	5.0884830
C	3.0243070	-1.0963890	-0.2974160
C	3.4001530	-0.5730750	-1.5418080
C	4.0179480	-1.5244120	0.5879360
C	4.7423080	-0.5011810	-1.8996470
H	2.6367530	-0.2196080	-2.2346040
C	5.3618930	-1.4372130	0.2300120
H	3.7541900	-1.9575530	1.5499610
C	5.7276220	-0.9312630	-1.0131620
H	5.0180120	-0.1076460	-2.8756110
H	6.1232330	-1.7833480	0.9254200
H	6.7769780	-0.8756800	-1.2932340
C	0.1913350	2.7559860	0.4939090
H	-0.4541470	2.9461150	1.3520380
H	-0.0697670	3.2858620	-0.4229460
C	2.5208950	2.4576420	-0.3652570
H	2.0503130	2.5193760	-1.3504640
H	3.2430450	1.6372790	-0.3937670
C	1.9413030	1.9721300	2.1115630
H	2.2232520	2.8862920	2.6559120
H	1.1382150	1.4990320	2.6901140
H	2.8109570	1.3028110	2.1277380
C	1.4856980	2.2698950	0.7037790
Ni	0.1775910	0.8089130	0.0102450
N	3.3832080	3.7258840	-0.2617780
H	3.9189940	3.7331480	-1.1394030
C	2.5840370	4.9987980	-0.2451760
H	1.8713750	4.9151480	0.5824890
H	3.2921480	5.7983800	-0.0059900
C	4.4146770	3.7183580	0.8375850
H	3.8762550	3.7964700	1.7861230
H	4.9841880	4.6431320	0.7008530
C	5.3297800	2.5206050	0.7817380
H	5.7672930	2.3992830	-0.2172210
H	6.1528900	2.6785360	1.4853280
H	4.8330190	1.5858560	1.0624820
C	1.9108000	5.2666410	-1.5689520
H	1.4132390	6.2398810	-1.5217790
H	2.6441600	5.3071740	-2.3830510

H	1.1511330	4.5204340	-1.8220580

6 – Int 2

Lowest Frequency Vibration = 18.0511 cm**-1
Electronic Energy = -3798.18879499
Electronic and Zero-Point Energy = -3797.461044
Enthalpy = -3797.411070
Free Energy = -3797.541123
E large = -5929.18134707

Ti	-0.3403490	-1.2740920	-1.2293190
Cl	-0.9635200	-2.8419210	-2.7843240
Cl	0.2198280	0.2557410	-2.9926880
N	-1.8784180	-1.3564650	-0.0079860
N	1.2813840	-1.9124100	-0.4518250
C	-2.9138400	-2.3803770	0.3303940
C	-3.9336340	-2.4971650	-0.8030970
H	-4.5121550	-1.5722960	-0.9194370
H	-3.4419220	-2.7227240	-1.7554810
H	-4.6385920	-3.3092620	-0.5813510
C	-3.6504020	-2.0334130	1.6202470
H	-4.3978550	-2.8114880	1.8205040
H	-2.9733360	-1.9879230	2.4801030
H	-4.1885130	-1.0804560	1.5494730
C	-2.1998940	-3.7123880	0.5267150
H	-1.7128790	-4.0439400	-0.3969500
H	-1.4405260	-3.6319370	1.3166720
H	-2.9219880	-4.4834360	0.8240320
C	2.1309060	-3.1414000	-0.6465830
C	1.2701320	-4.3743980	-0.3900780
H	0.4197970	-4.4198290	-1.0789480
H	1.8745620	-5.2776940	-0.5415580
H	0.8906300	-4.3933760	0.6392400
C	2.6368890	-3.1632070	-2.0880910
H	3.3068430	-2.3175100	-2.2818450
H	3.1987550	-4.0889280	-2.2686660
H	1.8065210	-3.1233230	-2.8022800
C	3.3338010	-3.1833880	0.2919220
H	3.0445450	-3.1788960	1.3479320
H	3.8811610	-4.1150270	0.1027600
H	4.0284910	-2.3567670	0.1123560
P	-1.9396590	0.3114490	0.1216210
P	1.6539350	-0.4134340	0.2595040
C	-2.0540410	0.9121030	1.8471810
C	-1.4992700	0.1751650	2.8965080
C	-2.5672890	2.1894200	2.1111270
C	-1.4800620	0.6928120	4.1876760

H	-1.0696050	-0.8072300	2.7074600
C	-2.5428500	2.7052250	3.4030490
H	-2.9966420	2.7877700	1.3099280
C	-2.0000250	1.9584250	4.4448450
H	-1.0496270	0.1026860	4.9942710
H	-2.9530950	3.6945700	3.5928040
H	-1.9830390	2.3616950	5.4547310
C	-3.4288670	0.9133270	-0.7499340
C	-3.3473980	1.0079270	-2.1436270
C	-4.6550680	1.1457010	-0.1181000
C	-4.4772110	1.3172340	-2.8941360
H	-2.3935130	0.8287140	-2.6416120
C	-5.7817050	1.4609470	-0.8713080
H	-4.7409860	1.0718120	0.9645710
C	-5.6954540	1.5429650	-2.2586590
H	-4.4036580	1.3847430	-3.9770830
H	-6.7317020	1.6365880	-0.3714210
H	-6.5787870	1.7858110	-2.8450320
C	1.7017320	-0.6794200	2.0700990
C	2.0951300	0.3428070	2.9403060
C	1.2403760	-1.8850510	2.6070710
C	2.0800860	0.1422610	4.3169730
H	2.4247510	1.3021290	2.5468590
C	1.2175020	-2.0818540	3.9847940
H	0.8854180	-2.6685460	1.9397380
C	1.6488510	-1.0731900	4.8422290
H	2.4026150	0.9419530	4.9797880
H	0.8625950	-3.0281330	4.3871260
H	1.6391600	-1.2302250	5.9184460
C	3.3444410	0.0605330	-0.2738160
C	3.5724040	0.2134890	-1.6474510
C	4.3912970	0.2949740	0.6213390
C	4.8280430	0.5852340	-2.1136550
H	2.7602050	0.0534660	-2.3548600
C	5.6433990	0.6828210	0.1497330
H	4.2458700	0.1556460	1.6899720
C	5.8654100	0.8276070	-1.2157360
H	4.9925490	0.6950450	-3.1832040
H	6.4493490	0.8619700	0.8577230
H	6.8447060	1.1284810	-1.5807620
C	-0.4822110	2.9626700	-0.6836840
H	-1.2478350	3.2595500	0.0333010
H	-0.7558180	3.0384080	-1.7381560
C	1.9059920	3.0836260	-1.3569540
H	1.5931060	2.6773250	-2.3214400
H	2.8702760	2.6621520	-1.0599720

C	1.2711320	3.3572660	1.0847760
H	1.3500610	4.4507220	1.1790180
H	0.5437980	3.0095670	1.8293980
H	2.2578200	2.9462380	1.3353720
C	0.8619590	2.9675760	-0.3089780
Cl	2.3014130	4.8762440	-1.7091810
Ni	0.0731580	1.0464840	-0.4171430

6 – TS2

Lowest Frequency Vibration = -209.9454 cm**-1
Electronic Energy = -3798.17628713
Electronic and Zero-Point Energy = -3797.450035
Enthalpy = -3797.399858
Free Energy = -3797.530735
E large = -5929.16948806

Ti	0.3651240	1.6541460	-0.7610630
Cl	1.0328950	3.6068320	-1.7142110
Cl	-0.1969920	0.7761340	-2.8992040
N	1.8669330	1.2540490	0.4305850
N	-1.2558560	2.0154470	0.1716040
C	2.8951820	2.0973300	1.1226060
C	3.9389240	2.5919180	0.1219560
H	4.5203860	1.7615660	-0.2956630
H	3.4734790	3.1401030	-0.7037840
H	4.6382230	3.2694160	0.6290200
C	3.6014710	1.3235110	2.2304980
H	4.3497660	1.9788940	2.6932510
H	2.9062010	1.0018410	3.0134000
H	4.1318900	0.4417920	1.8515760
C	2.1688370	3.2799570	1.7499170
H	1.6787510	3.8990930	0.9905040
H	1.4117200	2.9306750	2.4644110
H	2.8835000	3.9123650	2.2912180
C	-2.0948270	3.2561800	0.3690610
C	-1.2272490	4.3273500	1.0195550
H	-0.3687120	4.5900290	0.3924640
H	-1.8252000	5.2357520	1.1635590
H	-0.8646780	4.0023200	2.0026470
C	-2.5799310	3.7387800	-0.9959640
H	-3.2333540	2.9958500	-1.4685030
H	-3.1519030	4.6678410	-0.8754560
H	-1.7387050	3.9429010	-1.6682910
C	-3.3029150	3.0075270	1.2672470
H	-3.0153480	2.6577220	2.2641760
H	-3.8356110	3.9582890	1.3913970
H	-4.0090540	2.2939750	0.8319130

P	1.9423110	-0.3577170	-0.0154600
P	-1.6827020	0.3797810	0.3332920
C	2.0818900	-1.4944880	1.4086810
C	1.4462340	-1.1736850	2.6108030
C	2.7035690	-2.7423200	1.2751800
C	1.4593620	-2.0704760	3.6734810
H	0.9407840	-0.2152220	2.7169390
C	2.7127820	-3.6371310	2.3412830
H	3.1895980	-3.0249870	0.3434610
C	2.0926920	-3.3036970	3.5417820
H	0.9677510	-1.8020840	4.6061700
H	3.2069880	-4.5993360	2.2285550
H	2.1016510	-4.0043750	4.3734080
C	3.4184700	-0.6034480	-1.0626440
C	3.3053750	-0.2419640	-2.4093320
C	4.6666430	-0.9849500	-0.5578380
C	4.4237710	-0.2531130	-3.2361730
H	2.3375740	0.0618590	-2.8079870
C	5.7813060	-1.0029470	-1.3902090
H	4.7801400	-1.2566760	0.4897290
C	5.6623890	-0.6341640	-2.7275500
H	4.3250250	0.0331700	-4.2805310
H	6.7472320	-1.3010560	-0.9891270
H	6.5368500	-0.6447710	-3.3740150
C	-1.7655540	-0.0220850	2.1114380
C	-2.1859600	-1.2939030	2.5150270
C	-1.3130580	0.8862320	3.0716870
C	-2.1927310	-1.6361120	3.8628670
H	-2.5256980	-2.0196740	1.7766070
C	-1.3127110	0.5382050	4.4200480
H	-0.9478000	1.8645880	2.7632370
C	-1.7596620	-0.7188680	4.8177800
H	-2.5347330	-2.6227350	4.1664850
H	-0.9626160	1.2542320	5.1601160
H	-1.7646370	-0.9869600	5.8718190
C	-3.3635040	0.1461150	-0.3623420
C	-3.5422960	0.3651200	-1.7337140
C	-4.4458850	-0.2838710	0.4095980
C	-4.7819750	0.1470720	-2.3221480
H	-2.7039800	0.6941670	-2.3448630
C	-5.6844610	-0.5063890	-0.1868820
H	-4.3360430	-0.4339850	1.4812390
C	-5.8539810	-0.2969970	-1.5515060
H	-4.9073110	0.3177810	-3.3887740
H	-6.5200990	-0.8411840	0.4232620
H	-6.8210720	-0.4761050	-2.0155160

C	0.6049580	-2.5265980	-1.6298960
H	1.5186340	-2.9834560	-1.2515750
H	0.6350100	-2.1910520	-2.6686300
C	-1.8119740	-2.4032440	-1.6523870
H	-1.7660040	-1.8134040	-2.5625100
H	-2.7395600	-2.3738400	-1.0894650
C	-0.7085160	-3.7613480	0.1568300
H	-0.6776340	-4.8099860	-0.1688570
H	0.1262560	-3.6003640	0.8501750
H	-1.6504890	-3.6214310	0.6981560
C	-0.6279140	-2.8664950	-1.0429260
Cl	-2.7486520	-4.2652210	-2.8610220
Ni	-0.0945480	-0.8705670	-0.7344370

7 - Ground

Lowest Frequency Vibration = 27.3166 cm**-1
Electronic Energy = -3287.66813107
Electronic and Zero-Point Energy = -3286.940983
Enthalpy = -3286.893086
Free Energy = -3287.017880
E large = -4079.91553943

Cl	-0.3452300	-4.0816770	0.8358280
Cl	0.2323660	-2.5433990	-1.9853280
N	-1.5397070	-1.0589460	1.1626460
N	1.6701650	-1.4294600	0.9529770
C	-2.4606080	-1.5615730	2.2561660
C	-3.3793420	-2.6546020	1.7113920
H	-4.1025850	-2.2435870	0.9956940
H	-2.8202420	-3.4544130	1.2173900
H	-3.9440220	-3.0992330	2.5406480
C	-3.3418800	-0.4523870	2.8263360
H	-4.0337950	-0.9089500	3.5441190
H	-2.7660390	0.3075800	3.3618870
H	-3.9548210	0.0397460	2.0637760
C	-1.5890870	-2.0809060	3.3941770
H	-1.0074000	-2.9614980	3.1081950
H	-0.9009470	-1.2964600	3.7372200
H	-2.2263640	-2.3657170	4.2403440
C	2.7323180	-2.2214900	1.7065390
C	2.1232930	-2.7136990	3.0144630
H	1.2381860	-3.3344210	2.8475760
H	2.8626840	-3.3267790	3.5440100
H	1.8509560	-1.8773630	3.6701810
C	3.1712920	-3.3993880	0.8424160
H	3.6005740	-3.0518760	-0.1049500
H	3.9414860	-3.9713370	1.3748420

H	2.3416310	-4.0778780	0.6205730
C	3.9642020	-1.3832570	2.0387070
H	3.7176880	-0.4582480	2.5707660
H	4.6013110	-1.9802100	2.7017940
H	4.5590990	-1.1427050	1.1533460
P	-1.8905920	0.1588430	0.0687710
P	1.8518580	0.0701870	0.1907250
C	-2.1042240	1.8015260	0.8260080
C	-1.4988850	2.1067130	2.0464980
C	-2.7584130	2.8084480	0.1061960
C	-1.5866830	3.3937150	2.5654170
H	-0.9491370	1.3384030	2.5880820
C	-2.8384940	4.0955900	0.6274560
H	-3.2069800	2.5937260	-0.8628600
C	-2.2585210	4.3879880	1.8595280
H	-1.1213310	3.6194010	3.5223890
H	-3.3574970	4.8709880	0.0689490
H	-2.3264940	5.3936060	2.2675230
C	-3.4260190	-0.2851290	-0.8088970
C	-3.3360860	-1.3181790	-1.7489510
C	-4.6760860	0.2582350	-0.4979840
C	-4.4829960	-1.8111790	-2.3588730
H	-2.3637080	-1.7493870	-1.9897350
C	-5.8215900	-0.2368610	-1.1149060
H	-4.7698020	1.0588100	0.2330700
C	-5.7275030	-1.2716480	-2.0404960
H	-4.4040340	-2.6165010	-3.0851220
H	-6.7910740	0.1877300	-0.8658210
H	-6.6254380	-1.6588020	-2.5162670
C	1.9144520	1.4189910	1.4102700
C	2.0725960	2.7308920	0.9461320
C	1.7391530	1.1854520	2.7752660
C	2.1030820	3.7901670	1.8450560
H	2.1824040	2.9264930	-0.1207940
C	1.7605090	2.2513600	3.6716590
H	1.5793270	0.1725010	3.1414700
C	1.9506230	3.5499960	3.2093270
H	2.2401430	4.8046190	1.4787550
H	1.6289880	2.0626410	4.7345510
H	1.9724000	4.3791320	3.9126920
C	3.4163040	0.0700820	-0.7506160
C	3.5609460	-0.8806060	-1.7676510
C	4.4428400	0.9847170	-0.5055380
C	4.7271030	-0.9201810	-2.5220370
H	2.7571080	-1.5862230	-1.9732950
C	5.6019070	0.9487550	-1.2763480

H	4.3560390	1.7170200	0.2943130
C	5.7475670	-0.0026460	-2.2807630
H	4.8357650	-1.6667850	-3.3050840
H	6.3966840	1.6647520	-1.0815720
H	6.6565620	-0.0298200	-2.8768410
C	-1.1398860	1.3185250	-2.9459610
H	-2.1085320	1.7840940	-2.7664540
H	-1.1421300	0.4498900	-3.6078390
C	1.2510780	1.3933110	-2.8853490
H	1.3281730	0.5059280	-3.5170200
H	2.1864660	1.9040280	-2.6583490
C	-0.0186020	3.5423650	-2.4246870
H	-0.0480890	4.1775020	-3.3192670
H	-0.9169040	3.7580090	-1.8355850
H	0.8688130	3.8241550	-1.8480270
C	0.0342190	2.1140170	-2.8521350
Pt	0.0165550	0.4994400	-1.2475720
Ti	-0.0332460	-1.9441750	0.2529140

7 – TS1

Lowest Frequency Vibration = -310.0893 cm**-1
Electronic Energy = -3501.30267892
Electronic and Zero-Point Energy = -3500.424564
Enthalpy = -3500.369238
Free Energy = -3500.509920
E large = -4293.61656127

Ti	1.1258840	1.1608360	-1.4794780
Cl	2.3443680	2.1539190	-3.1002940
Cl	-0.0723400	-0.0473830	-3.1290830
N	2.5697090	0.6776210	-0.1984650
N	-0.0286350	2.5250990	-0.7974060
C	3.9736420	1.1978670	-0.0247950
C	4.8682060	0.7242560	-1.1697990
H	4.9928060	-0.3652770	-1.1542640
H	4.4664130	1.0123200	-2.1455030
H	5.8631180	1.1762740	-1.0663110
C	4.5862190	0.7248150	1.2902850
H	5.6131150	1.1055450	1.3506420
H	4.0388450	1.1034070	2.1598580
H	4.6444750	-0.3679130	1.3603250
C	3.9054140	2.7201950	0.0130030
H	3.5609340	3.1415730	-0.9368550
H	3.2320280	3.0557910	0.8136440
H	4.9035540	3.1280140	0.2158990
C	-0.2768410	3.9693320	-1.1865560
C	1.0293020	4.7454090	-1.0605140

H	1.8045500	4.3425500	-1.7189690
H	0.8540660	5.7886660	-1.3505970
H	1.4047880	4.7417680	-0.0297890
C	-0.7660890	4.0000240	-2.6310810
H	-1.7101140	3.4522530	-2.7354720
H	-0.9391720	5.0396040	-2.9372020
H	-0.0306180	3.5622980	-3.3145460
C	-1.3252290	4.6376930	-0.3004120
H	-1.0758440	4.5810860	0.7650310
H	-1.3673250	5.6993650	-0.5707020
H	-2.3265870	4.2246570	-0.4547480
P	1.9963790	-0.8243400	0.2522950
P	-0.9694590	1.5261560	0.1946180
C	2.0440680	-1.1719150	2.0427760
C	1.8780860	-0.1351380	2.9639380
C	2.0578220	-2.4974570	2.4935670
C	1.7732120	-0.4162000	4.3216280
H	1.8164230	0.8951390	2.6161370
C	1.9486350	-2.7732800	3.8531670
H	2.1516690	-3.3201730	1.7873380
C	1.8113120	-1.7342970	4.7694850
H	1.6516090	0.4012120	5.0293720
H	1.9719110	-3.8056570	4.1941490
H	1.7301200	-1.9522080	5.8318150
C	2.9542860	-2.1197770	-0.6025960
C	2.6444930	-2.3521940	-1.9472210
C	4.0488300	-2.7723000	-0.0254110
C	3.4255190	-3.2151800	-2.7077170
H	1.7930000	-1.8457460	-2.4040290
C	4.8217470	-3.6425770	-0.7879800
H	4.3102340	-2.5967460	1.0161740
C	4.5149880	-3.8610350	-2.1282030
H	3.1793210	-3.3864950	-3.7529880
H	5.6713460	-4.1456000	-0.3322050
H	5.1255330	-4.5367090	-2.7226840
C	-0.7439450	1.9924380	1.9403770
C	-1.4434570	1.2910230	2.9294730
C	0.2032470	2.9482520	2.3123890
C	-1.2272890	1.5782680	4.2720090
H	-2.1591850	0.5171840	2.6494610
C	0.4243430	3.2263560	3.6591910
H	0.7774510	3.4670330	1.5468580
C	-0.2964740	2.5491190	4.6382140
H	-1.7810800	1.0374760	5.0357870
H	1.1608980	3.9750210	3.9409550
H	-0.1265750	2.7696050	5.6896560

C	-2.7344400	1.7372300	-0.2318810
C	-3.1376260	1.4164240	-1.5338810
C	-3.6828340	2.1657230	0.7002210
C	-4.4743540	1.5312230	-1.8966810
H	-2.4048090	1.0672370	-2.2610910
C	-5.0226280	2.2682400	0.3324920
H	-3.3814140	2.4428120	1.7081030
C	-5.4197130	1.9545890	-0.9634770
H	-4.7782160	1.2882990	-2.9123050
H	-5.7537820	2.6080240	1.0623000
H	-6.4659110	2.0397780	-1.2479770
C	-0.6175150	-2.8839830	-0.0813930
H	0.0339000	-3.4713190	0.5670760
H	-0.6088590	-3.1788810	-1.1340520
C	-2.7339410	-1.6777690	-0.3673660
H	-2.5604440	-1.6280420	-1.4391470
H	-3.4271390	-0.9528980	0.0489400
C	-2.0821320	-2.4381260	1.9570360
H	-2.5235010	-3.4162530	2.1929520
H	-1.1559800	-2.3476310	2.5397160
H	-2.7844470	-1.6660190	2.2956770
C	-1.8117360	-2.3293790	0.4823340
Pt	-0.3018740	-0.7555340	-0.0813160
N	-4.4127930	-3.0168690	-0.7095140
H	-4.8815410	-2.6429040	-1.5366150
C	-3.8520230	-4.3336780	-1.0036080
H	-3.0962200	-4.5558310	-0.2327670
H	-4.6335780	-5.1059700	-0.9077850
C	-5.3389750	-3.0106670	0.4253850
H	-4.7627750	-3.2595720	1.3279970
H	-6.0844860	-3.8144590	0.2997400
C	-6.0435050	-1.6805100	0.5803830
H	-6.5714680	-1.4073600	-0.3425730
H	-6.7883510	-1.7381180	1.3806870
H	-5.3547820	-0.8636930	0.8297920
C	-3.2374680	-4.3863030	-2.3849610
H	-2.8110770	-5.3763410	-2.5754590
H	-3.9926470	-4.1943690	-3.1576090
H	-2.4346570	-3.6481290	-2.5081730

7 – Int 1

Lowest Frequency Vibration = 18.2149 cm**-1
Electronic Energy = -3501.32799619
Electronic and Zero-Point Energy = -3500.446177
Enthalpy = -3500.390886
Free Energy = -3500.532349

E large = -4293.63899784

Ti	-1.0076150	-1.0825480	-1.5137430
Cl	-2.1487400	-2.0442580	-3.2459550
Cl	0.1725780	0.2488920	-3.1008840
N	-2.5501990	-0.8057670	-0.2792710
N	0.1953750	-2.4363940	-0.8847210
C	-3.9189950	-1.4115230	-0.1606910
C	-4.8211420	-0.9243980	-1.2942950
H	-5.0078280	0.1543400	-1.2220180
H	-4.3816950	-1.1342980	-2.2737810
H	-5.7904570	-1.4367390	-1.2378260
C	-4.5782660	-1.0535010	1.1682690
H	-5.5857810	-1.4871020	1.1867440
H	-4.0244190	-1.4570340	2.0224760
H	-4.6905410	0.0285370	1.3044550
C	-3.7696280	-2.9271980	-0.2131860
H	-3.3808290	-3.2636460	-1.1789050
H	-3.0954270	-3.2765150	0.5811670
H	-4.7479090	-3.4009710	-0.0621970
C	0.5191760	-3.8354900	-1.3613970
C	-0.7453700	-4.6861040	-1.2983420
H	-1.5386190	-4.2773050	-1.9314840
H	-0.5161270	-5.6966470	-1.6590000
H	-1.1243630	-4.7738060	-0.2727670
C	1.0158930	-3.7568830	-2.8034030
H	1.9383040	-3.1676330	-2.8685290
H	1.2320580	-4.7676870	-3.1727060
H	0.2670090	-3.3063460	-3.4639820
C	1.5973380	-4.5066800	-0.5129100
H	1.3478820	-4.5172070	0.5540900
H	1.6860220	-5.5496620	-0.8398050
H	2.5786310	-4.0396980	-0.6434040
P	-2.0582180	0.6989980	0.2456690
P	1.0510460	-1.4376400	0.1845530
C	-2.1260090	0.9489950	2.0553070
C	-1.9469380	-0.1236960	2.9323250
C	-2.1628090	2.2524320	2.5667220
C	-1.8481680	0.0998740	4.3016260
H	-1.8661670	-1.1368120	2.5408520
C	-2.0594320	2.4713660	3.9368260
H	-2.2644980	3.1051890	1.8974710
C	-1.9076090	1.3957760	4.8079140
H	-1.7151280	-0.7461300	4.9728480
H	-2.1000590	3.4873080	4.3229710
H	-1.8305970	1.5675790	5.8789970
C	-3.0999660	1.9847060	-0.5246980

C	-2.8133590	2.3134780	-1.8541890
C	-4.2231330	2.5431590	0.0949770
C	-3.6475840	3.1745660	-2.5594050
H	-1.9381370	1.8799720	-2.3419240
C	-5.0505480	3.4104640	-0.6117230
H	-4.4647000	2.2964680	1.1276490
C	-4.7676010	3.7225480	-1.9388030
H	-3.4199270	3.4194040	-3.5943070
H	-5.9236290	3.8383930	-0.1243840
H	-5.4196540	4.3960490	-2.4902400
C	0.7983400	-2.0339150	1.8892990
C	1.4332990	-1.3788780	2.9501660
C	-0.1018660	-3.0660230	2.1612080
C	1.2034720	-1.7837970	4.2602220
H	2.1122090	-0.5497130	2.7518200
C	-0.3383540	-3.4630530	3.4750920
H	-0.6279430	-3.5519490	1.3417750
C	0.3213350	-2.8297430	4.5243570
H	1.7100540	-1.2767680	5.0782300
H	-1.0386620	-4.2705600	3.6759020
H	0.1411280	-3.1433460	5.5501630
C	2.8334770	-1.5805680	-0.2045120
C	3.2439980	-1.2303840	-1.4973330
C	3.7785020	-2.0395000	0.7169240
C	4.5758350	-1.3754800	-1.8704020
H	2.5147770	-0.8519530	-2.2143930
C	5.1145400	-2.1643060	0.3425730
H	3.4734080	-2.3356130	1.7185940
C	5.5137470	-1.8436840	-0.9513390
H	4.8811990	-1.1202950	-2.8828400
H	5.8407330	-2.5324690	1.0637250
H	6.5550630	-1.9564870	-1.2443050
C	0.6254550	2.9182240	0.1564350
H	0.0440250	3.3684710	0.9638610
H	0.4852030	3.3789980	-0.8240440
C	2.9010860	2.1528500	-0.6035810
H	2.4415020	2.2317600	-1.5946590
H	3.4381720	1.1998880	-0.5637140
C	2.2843290	2.1913580	1.9159350
H	2.7081220	3.1461210	2.2645630
H	1.4242880	1.9740460	2.5621640
H	3.0410920	1.4121930	2.0834940
C	1.8549200	2.2661440	0.4683980
Pt	0.2690690	0.8087400	-0.0130920
N	4.0055400	3.2251280	-0.5916490
H	4.4737640	3.1155350	-1.5000980

C	3.4676800	4.6300100	-0.5565740
H	2.7577730	4.6766530	0.2755880
H	4.3155390	5.2792630	-0.3187230
C	5.0893750	3.0193960	0.4384870
H	4.6449860	3.1941000	1.4216530
H	5.8164140	3.8168030	0.2536080
C	5.7533690	1.6685110	0.3345950
H	6.0730950	1.4614510	-0.6943870
H	6.6498460	1.6720380	0.9622170
H	5.1167270	0.8456460	0.6790170
C	2.8439440	5.0299350	-1.8708260
H	2.5330440	6.0772930	-1.8123720
H	3.5660020	4.9443860	-2.6916840
H	1.9585340	4.4369940	-2.1219540

7 – Int 2

Lowest Frequency Vibration = 18.9506 cm**-1
Electronic Energy = -3747.99647670
Electronic and Zero-Point Energy = -3747.270523
Enthalpy = -3747.219731
Free Energy = -3747.353506
E large = -4540.27374980

Cl	-1.0169690	-2.7041760	-3.0775700
Cl	0.1816120	0.3173590	-3.1718330
N	-2.0199630	-1.3894160	-0.3269620
N	1.1915830	-2.0425450	-0.7114830
C	-3.1596830	-2.3662990	-0.2555950
C	-4.0638680	-2.2102400	-1.4787040
H	-4.5735950	-1.2380870	-1.4706620
H	-3.4998470	-2.2982660	-2.4114980
H	-4.8344660	-2.9922740	-1.4682640
C	-4.0201840	-2.1600990	0.9894080
H	-4.8518650	-2.8746640	0.9545580
H	-3.4645290	-2.3412670	1.9144300
H	-4.4609940	-1.1575590	1.0350390
C	-2.5759050	-3.7734690	-0.1843680
H	-2.0230310	-4.0338420	-1.0915300
H	-1.9012240	-3.8646300	0.6783050
H	-3.3855590	-4.5038340	-0.0603450
C	1.9695330	-3.2978000	-1.0286010
C	1.0564590	-4.5067150	-0.8554380
H	0.1911000	-4.4557330	-1.5219520
H	1.6144640	-5.4198370	-1.0983280
H	0.6979520	-4.5973150	0.1776470
C	2.4615730	-3.2131920	-2.4718100
H	3.1288070	-2.3532120	-2.6034970

H	3.0227810	-4.1217730	-2.7260860
H	1.6296930	-3.1179340	-3.1772840
C	3.1843690	-3.4778330	-0.1197270
H	2.9191020	-3.4969370	0.9427360
H	3.6489160	-4.4421940	-0.3585170
H	3.9419920	-2.7047110	-0.2809680
P	-2.0130620	0.1962710	0.1955290
P	1.6580180	-0.7178260	0.2293670
C	-2.1667560	0.3687350	2.0056660
C	-1.7688990	-0.6676160	2.8517890
C	-2.5275790	1.6051270	2.5553100
C	-1.7776060	-0.4882290	4.2311380
H	-1.4370620	-1.6140970	2.4269790
C	-2.5286580	1.7825320	3.9348650
H	-2.8078500	2.4340770	1.9068790
C	-2.1600140	0.7349840	4.7752250
H	-1.4722440	-1.3057270	4.8812450
H	-2.8209070	2.7431880	4.3528600
H	-2.1648020	0.8746160	5.8537190
C	-3.4016020	1.1002870	-0.5727520
C	-3.2474120	1.4636710	-1.9158500
C	-4.6185760	1.3488960	0.0694790
C	-4.2997650	2.0504900	-2.6096970
H	-2.2983770	1.2758960	-2.4208140
C	-5.6670850	1.9434090	-0.6266700
H	-4.7587660	1.0751460	1.1138460
C	-5.5115680	2.2900380	-1.9656830
H	-4.1707500	2.3248860	-3.6540970
H	-6.6107430	2.1312970	-0.1194510
H	-6.3338170	2.7526380	-2.5067840
C	1.6476940	-1.1814210	1.9943180
C	2.0649940	-0.2496800	2.9520040
C	1.1365840	-2.4112310	2.4146020
C	2.0209730	-0.5674560	4.3050750
H	2.4256100	0.7286460	2.6375480
C	1.0881550	-2.7249980	3.7702420
H	0.7634850	-3.1218230	1.6787440
C	1.5390970	-1.8084270	4.7157070
H	2.3612240	0.1586720	5.0397370
H	0.6951340	-3.6886570	4.0869340
H	1.5058840	-2.0564250	5.7742500
C	3.3634490	-0.2282210	-0.2192380
C	3.5873830	0.1874890	-1.5375750
C	4.4222970	-0.2249110	0.6924840
C	4.8575630	0.5839230	-1.9393840
H	2.7598050	0.2132130	-2.2467530

C	5.6880960	0.1923500	0.2885230
H	4.2718780	-0.5630820	1.7156480
C	5.9094990	0.5930440	-1.0252300
H	5.0225370	0.8987400	-2.9673120
H	6.5055950	0.1939140	1.0060170
H	6.9004220	0.9141020	-1.3378030
C	-0.2344440	3.2011390	-0.0566550
H	-0.8935560	3.4882580	0.7649190
H	-0.5606230	3.5291330	-1.0475650
C	2.1100940	3.2277100	-0.9282150
H	1.6866270	2.9872490	-1.9067380
H	3.0602470	2.7039240	-0.7858420
C	1.7202680	3.2302070	1.5737400
H	1.9433680	4.2937870	1.7451790
H	1.0170660	2.9059680	2.3508910
H	2.6623160	2.6793340	1.7028990
C	1.1559950	3.0236730	0.1928840
Cl	2.6108900	5.0231480	-1.0665640
Pt	0.1398220	1.0841610	-0.0951120
Ti	-0.3883680	-1.2135070	-1.4509410

7 – TS2

Lowest Frequency Vibration = -236.3892 cm**-1
Electronic Energy = -3747.98527824
Electronic and Zero-Point Energy = -3747.259696
Enthalpy = -3747.209441
Free Energy = -3747.341404
E large = -4540.26185944

Cl	1.1896520	3.4457900	-2.2081160
Cl	-0.2308490	0.6447890	-3.1154190
N	1.9207530	1.4014260	0.1952630
N	-1.1966570	2.1945310	-0.1856330
C	2.9788090	2.3437780	0.7034440
C	4.0239840	2.6104390	-0.3790740
H	4.5970350	1.7040790	-0.6112430
H	3.5668680	2.9755580	-1.3036970
H	4.7314080	3.3715990	-0.0245950
C	3.6914060	1.7868870	1.9328990
H	4.4780650	2.4932450	2.2254160
H	3.0111530	1.6729280	2.7834960
H	4.1777750	0.8229980	1.7444830
C	2.2884450	3.6376530	1.1210610
H	1.8779020	4.1783590	0.2636920
H	1.4743900	3.4251020	1.8283400
H	3.0107560	4.2982860	1.6165530
C	-2.0063900	3.4742300	-0.2363710

C	-1.1410730	4.6150990	0.2876800
H	-0.2322740	4.7357830	-0.3092800
H	-1.7065690	5.5535910	0.2320950
H	-0.8551020	4.4563530	1.3347980
C	-2.4046240	3.7442480	-1.6852310
H	-3.0451610	2.9423670	-2.0716220
H	-2.9694410	4.6838140	-1.7398410
H	-1.5282720	3.8373260	-2.3361200
C	-3.2770450	3.3996730	0.6071720
H	-3.0779940	3.1164890	1.6469540
H	-3.7313760	4.3975390	0.6205170
H	-4.0167500	2.7120780	0.1866500
P	1.9983640	-0.2647010	0.1376860
P	-1.6589650	0.6599760	0.3687570
C	2.1777070	-1.0805770	1.7613670
C	1.5917890	-0.5142050	2.8967620
C	2.7375250	-2.3612310	1.8429520
C	1.6053310	-1.2004570	4.1055120
H	1.1168500	0.4640370	2.8312300
C	2.7426940	-3.0463020	3.0543120
H	3.1694760	-2.8332030	0.9622970
C	2.1815100	-2.4660540	4.1881210
H	1.1590840	-0.7439250	4.9862570
H	3.1880750	-4.0369180	3.1087010
H	2.1882830	-3.0011860	5.1348180
C	3.4035620	-0.7695920	-0.9099160
C	3.2081880	-0.7167590	-2.2943950
C	4.6748490	-1.0631610	-0.4044600
C	4.2729760	-0.9364370	-3.1614340
H	2.2174330	-0.4951760	-2.6936120
C	5.7352980	-1.2900700	-1.2763790
H	4.8482880	-1.1068460	0.6693760
C	5.5375980	-1.2211510	-2.6528180
H	4.1116820	-0.8902710	-4.2357290
H	6.7210460	-1.5158060	-0.8763150
H	6.3697720	-1.3949440	-3.3309320
C	-1.6665840	0.6319290	2.1903740
C	-1.9898380	-0.5671650	2.8362320
C	-1.2726860	1.7365980	2.9475500
C	-1.9655480	-0.6431940	4.2235860
H	-2.2643140	-1.4443240	2.2492410
C	-1.2355010	1.6527100	4.3376700
H	-0.9843180	2.6626390	2.4536260
C	-1.5927140	0.4691990	4.9764110
H	-2.2292390	-1.5753560	4.7177790
H	-0.9323070	2.5190220	4.9210670

H	-1.5707310	0.4082980	6.0620620
C	-3.3577450	0.3060330	-0.2049930
C	-3.5888830	0.2682400	-1.5855710
C	-4.4072020	0.0454950	0.6788940
C	-4.8589090	-0.0185170	-2.0708510
H	-2.7728230	0.4547770	-2.2830770
C	-5.6745090	-0.2540290	0.1845140
H	-4.2484970	0.0906560	1.7542250
C	-5.9028760	-0.2852230	-1.1869930
H	-5.0309870	-0.0435630	-3.1442670
H	-6.4860630	-0.4567680	0.8794130
H	-6.8936310	-0.5194020	-1.5692450
C	0.4501500	-2.9777320	-1.0357490
H	1.3018760	-3.4070970	-0.5066130
H	0.5505820	-2.9447500	-2.1240280
C	-1.9793310	-2.7805740	-1.2549060
H	-1.8451570	-2.3921370	-2.2605840
H	-2.9283490	-2.5719880	-0.7684840
C	-1.0563470	-3.7621480	0.8715260
H	-1.0710960	-4.8552600	0.7627710
H	-0.2517890	-3.4995930	1.5701380
H	-2.0172020	-3.4671780	1.3099910
C	-0.8540070	-3.1283540	-0.4724420
Cl	-2.8805500	-4.8161410	-2.0756770
Pt	-0.1283460	-0.9947350	-0.4436840
Ti	0.4055730	1.6457320	-1.0707060

8 – Ground

Lowest Frequency Vibration = 32.7815 cm**-1
Electronic Energy = -2437.77940286
Electronic and Zero-Point Energy = -2436.994893
Enthalpy = -2436.951235
Free Energy = -2437.064920
E large = -3777.33808460

C	-2.3854070	-0.8170650	2.5989120
C	-3.2619670	-2.0691420	2.7119920
H	-3.8472990	-2.2303500	1.7977240
H	-2.6898240	-2.9789030	2.9191110
H	-3.9682950	-1.9399140	3.5409560
C	-3.3156430	0.3902170	2.5816250
H	-3.9025510	0.3660540	3.5073060
H	-2.7716560	1.3383420	2.5678640
H	-4.0304770	0.3827360	1.7523430
C	-1.5152170	-0.6673980	3.8482790
H	-0.7936090	-1.4819830	3.9763380
H	-0.9631780	0.2807920	3.8168250

H	-2.1523990	-0.6595580	4.7414350
C	2.6654750	-2.1036130	1.7870770
C	2.0095590	-2.8381280	2.9564720
H	1.4120330	-3.7014540	2.6429010
H	2.7951060	-3.2162220	3.6219460
H	1.3736070	-2.1606470	3.5410590
C	3.4927420	-3.0957050	0.9650000
H	4.1490720	-2.5809700	0.2539030
H	4.1266410	-3.6916910	1.6334910
H	2.8601740	-3.7959020	0.4051240
C	3.6047050	-1.0651360	2.3899630
H	3.0977480	-0.4261990	3.1199480
H	4.4094500	-1.5948290	2.9134770
H	4.0786530	-0.4279090	1.6375210
P	-1.7198740	-0.2515640	-0.1705160
P	1.7849280	-0.1015710	-0.0552930
C	-2.3622300	1.4535110	-0.0466430
C	-1.5933550	2.3983650	0.6455510
C	-3.4847450	1.8820290	-0.7603030
C	-1.9697910	3.7358700	0.6630190
H	-0.7057640	2.0828570	1.1940620
C	-3.8507750	3.2265760	-0.7510520
H	-4.0831970	1.1722200	-1.3271760
C	-3.1011230	4.1540830	-0.0345850
H	-1.3747910	4.4548210	1.2219910
H	-4.7315000	3.5445740	-1.3043590
H	-3.3938390	5.2013340	-0.0235600
C	-2.9898520	-1.3061400	-0.9691880
C	-2.5272850	-2.2643700	-1.8779390
C	-4.3480260	-1.2993200	-0.6271190
C	-3.4015110	-3.1875750	-2.4445200
H	-1.4686300	-2.2854470	-2.1387570
C	-5.2238000	-2.2138880	-1.2018890
H	-4.7302800	-0.5765960	0.0908270
C	-4.7515210	-3.1588740	-2.1103980
H	-3.0267750	-3.9281350	-3.1473030
H	-6.2781500	-2.1910880	-0.9364600
H	-5.4384730	-3.8760740	-2.5537190
C	1.9006920	1.3918180	0.9809660
C	2.2757740	2.6055950	0.3915310
C	1.4274920	1.3889680	2.2957130
C	2.2176030	3.7878050	1.1217240
H	2.6126590	2.6307600	-0.6448490
C	1.3686260	2.5741810	3.0239460
H	1.0805520	0.4551580	2.7370550
C	1.7690230	3.7735950	2.4408580

H	2.5222450	4.7233650	0.6581310
H	1.0041250	2.5589610	4.0489740
H	1.7251040	4.6987590	3.0108820
C	3.3803590	-0.2905610	-0.9416480
C	3.4038500	-1.2808220	-1.9323830
C	4.5421330	0.4396150	-0.6855260
C	4.5691700	-1.5500290	-2.6385420
H	2.4995750	-1.8548610	-2.1428810
C	5.7096590	0.1738850	-1.3984000
H	4.5495500	1.2128230	0.0809390
C	5.7269270	-0.8214510	-2.3696700
H	4.5759070	-2.3271630	-3.3994320
H	6.6101300	0.7458930	-1.1864610
H	6.6409660	-1.0289890	-2.9213420
C	-1.1057170	0.5296780	-3.0576630
H	-2.1455520	0.8464370	-2.9909230
H	-0.9265750	-0.4376690	-3.5322490
C	1.2258590	0.9548980	-2.8980710
H	1.4737690	0.0140880	-3.3942440
H	2.0655720	1.6181350	-2.6913490
C	-0.3523280	2.9314420	-2.7622010
H	-0.2723940	3.4877890	-3.7050100
H	-1.3634220	3.0875020	-2.3690440
H	0.3763230	3.3636300	-2.0658050
C	-0.0744400	1.4848090	-3.0217420
Ni	0.0627730	0.2068550	-1.4182250
N	-1.4492810	-0.8906550	1.4022350
N	1.5909230	-1.4591500	0.9454330
C	-0.7920150	-2.2164600	1.3293170
H	-1.4845290	-2.9779020	0.9270700
H	-0.5642660	-2.5215260	2.3537650
C	0.4920520	-2.3378740	0.5243840
H	0.8044130	-3.3862060	0.6109490
H	0.2894070	-2.1954480	-0.5463170

8 – TS1
Lowest Frequency Vibration = -377.5366 cm**-1
Electronic Energy = -2651.39551031
Electronic and Zero-Point Energy = -2650.461360
Enthalpy = -2650.410154
Free Energy = -2650.541241
E large = -3991.02021141

8 – Int 1
Lowest Frequency Vibration = 22.4682 cm**-1
Electronic Energy = -2651.41658483

Electronic and Zero-Point Energy = -2650.479430
Enthalpy = -2650.428442
Free Energy = -2650.558081
E large = -3991.03815922

8 – Int 2

Lowest Frequency Vibration = 19.5355 cm**-1
Electronic Energy = -2898.08449212
Electronic and Zero-Point Energy = -2897.302334
Enthalpy = -2897.255741
Free Energy = -3897.378253
E large = -4237.67159544

C	-3.0717660	-1.8097260	-1.9989280
C	-3.6780880	-1.0146090	-3.1586650
H	-4.1190850	-0.0757630	-2.8045480
H	-2.9352520	-0.7753610	-3.9293590
H	-4.4721430	-1.5983930	-3.6421690
C	-4.1685980	-2.0788320	-0.9744760
H	-4.9756840	-2.6321230	-1.4697120
H	-3.8121010	-2.6891180	-0.1388950
H	-4.6096790	-1.1609420	-0.5763950
C	-2.5981930	-3.1713670	-2.5140210
H	-1.8793720	-3.0905360	-3.3378820
H	-2.1399450	-3.7596700	-1.7077520
H	-3.4601560	-3.7334750	-2.8944570
C	1.8215260	-3.2481160	-0.4702130
C	0.7802810	-4.3364840	-0.1901620
H	0.0492400	-4.4595510	-0.9977930
H	1.2821380	-5.3039060	-0.0610480
H	0.2351750	-4.1077500	0.7347810
C	2.6577900	-3.6334870	-1.6974810
H	3.3622010	-2.8368420	-1.9667530
H	3.2433550	-4.5324270	-1.4681560
H	2.0494300	-3.8658700	-2.5774170
C	2.7567740	-3.2454210	0.7339120
H	2.2264030	-3.0523020	1.6706130
H	3.2068370	-4.2425660	0.8110140
H	3.5777040	-2.5274490	0.6445690
P	-1.9046200	0.0558240	-0.1139610
P	1.5878130	-0.3382950	-0.2034750
C	-2.1176260	-0.8724760	1.4519250
C	-1.8881000	-2.2496080	1.5111650
C	-2.2953150	-0.1680700	2.6506160
C	-1.8804410	-2.9180800	2.7329610
H	-1.6904030	-2.7960510	0.5894120
C	-2.2951050	-0.8366630	3.8710880

H	-2.4291010	0.9136480	2.6333580
C	-2.0935690	-2.2149920	3.9155500
H	-1.7042140	-3.9920460	2.7582910
H	-2.4473770	-0.2774970	4.7919010
H	-2.0923780	-2.7362840	4.8703560
C	-3.4164000	1.0985230	-0.2682580
C	-3.4135390	2.0236470	-1.3212400
C	-4.5094330	1.0812630	0.6018000
C	-4.4820290	2.8918130	-1.5122380
H	-2.5600230	2.0581350	-2.0013900
C	-5.5741210	1.9621360	0.4223400
H	-4.5408260	0.3693770	1.4253950
C	-5.5653910	2.8652230	-0.6354940
H	-4.4653420	3.5973720	-2.3401940
H	-6.4164580	1.9357860	1.1105330
H	-6.3971240	3.5520360	-0.7757070
C	2.2671500	-0.4066910	1.4927790
C	3.4992030	0.1546510	1.8406500
C	1.4139660	-0.8409900	2.5172910
C	3.8868090	0.2402620	3.1774410
H	4.1680740	0.5370830	1.0727460
C	1.8030600	-0.7574280	3.8480370
H	0.4440550	-1.2693330	2.2630240
C	3.0442580	-0.2175990	4.1840200
H	4.8537190	0.6718910	3.4276520
H	1.1324730	-1.1141850	4.6273570
H	3.3480620	-0.1511240	5.2262700
C	2.9936710	0.0631340	-1.3359960
C	2.6719180	0.8864500	-2.4221420
C	4.2888570	-0.4693740	-1.2701870
C	3.6089240	1.1753700	-3.4110250
H	1.6672880	1.3069280	-2.4908190
C	5.2315180	-0.1719130	-2.2490620
H	4.5754710	-1.1215220	-0.4474370
C	4.8928020	0.6482020	-3.3232770
H	3.3351560	1.8143420	-4.2477670
H	6.2346120	-0.5864450	-2.1740710
H	5.6306350	0.8737480	-4.0900070
C	-0.6741440	2.9687700	0.4426280
H	-1.3971890	3.0293450	1.2600410
H	-1.0224740	3.4050450	-0.4991910
C	1.6836850	3.3851500	-0.2699020
H	1.3309130	3.3248730	-1.3013270
H	2.6774330	2.9398710	-0.1668890
C	1.1828300	2.8824820	2.1566580
H	1.3373950	3.9011290	2.5462550

H	0.4462570	2.3918570	2.8058510
H	2.1336770	2.3439720	2.2647880
C	0.7131050	2.9167610	0.7259650
Ni	-0.0191610	1.1704990	0.0548720
N	-1.9106310	-1.0737430	-1.3962680
N	1.0771760	-1.9420310	-0.6620870
Cl	2.0747280	5.2627780	-0.0835150
C	-0.7226970	-0.9456960	-2.2496230
H	-0.3565610	0.0897540	-2.2101670
H	-1.0062670	-1.1114150	-3.2974970
C	0.4201010	-1.9194440	-1.9882090
H	0.0321470	-2.9246730	-2.1746720
H	1.1596670	-1.7258870	-2.7887020

8 – TS2

Lowest Frequency Vibration = -275.0099 cm**-1
Electronic Energy = -2898.08276465
Electronic and Zero-Point Energy = -2897.300768
Enthalpy = -2897.254690
Free Energy = -2897.375758
E large = -4237.66927647

C	-3.0605550	-1.8330610	-1.9830020
C	-3.6615080	-1.0598140	-3.1599320
H	-4.1067070	-0.1157720	-2.8256680
H	-2.9162850	-0.8334950	-3.9321030
H	-4.4516990	-1.6551620	-3.6352610
C	-4.1620580	-2.0795800	-0.9578930
H	-4.9658470	-2.6440240	-1.4454800
H	-3.8103310	-2.6707080	-0.1067480
H	-4.6065590	-1.1536200	-0.5829240
C	-2.5868770	-3.2048950	-2.4698990
H	-1.8679990	-3.1413260	-3.2951180
H	-2.1296070	-3.7778530	-1.6522120
H	-3.4492060	-3.7734840	-2.8395660
C	1.8268590	-3.2528870	-0.4243310
C	0.7835100	-4.3349500	-0.1300480
H	0.0520890	-4.4677400	-0.9358290
H	1.2839890	-5.3011920	0.0117620
H	0.2391670	-4.0935690	0.7919490
C	2.6661650	-3.6569060	-1.6429950
H	3.3752720	-2.8667050	-1.9191750
H	3.2469090	-4.5552130	-1.3996220
H	2.0602530	-3.8977820	-2.5223240
C	2.7584000	-3.2306090	0.7825030
H	2.2258770	-3.0230150	1.7149250
H	3.2073730	-4.2267490	0.8764160

H	3.5811500	-2.5158380	0.6837680
P	-1.9013960	0.0512560	-0.1200620
P	1.5991620	-0.3446190	-0.2116910
C	-2.1133750	-0.8560450	1.4563700
C	-1.8877420	-2.2332100	1.5265650
C	-2.2925410	-0.1403340	2.6480530
C	-1.8863840	-2.8913540	2.7539070
H	-1.6881220	-2.7878960	0.6103590
C	-2.2992510	-0.7993280	3.8736970
H	-2.4223030	0.9417210	2.6226010
C	-2.1022920	-2.1778350	3.9295780
H	-1.7132010	-3.9654330	2.7889650
H	-2.4533130	-0.2323880	4.7893250
H	-2.1063890	-2.6913160	4.8885290
C	-3.4033020	1.0994090	-0.3009670
C	-3.4032040	1.9878330	-1.3848620
C	-4.4898240	1.1145310	0.5768250
C	-4.4683250	2.8553970	-1.5955380
H	-2.5563640	1.9944910	-2.0742190
C	-5.5516270	1.9940520	0.3754570
H	-4.5192950	0.4292480	1.4225810
C	-5.5453390	2.8629330	-0.7106180
H	-4.4543910	3.5329930	-2.4464440
H	-6.3897860	1.9933290	1.0690880
H	-6.3747110	3.5488790	-0.8675320
C	2.2601060	-0.3741120	1.4925610
C	3.4884950	0.1957890	1.8395280
C	1.4012400	-0.7968180	2.5170110
C	3.8658180	0.3040160	3.1773640
H	4.1635810	0.5640800	1.0705070
C	1.7813630	-0.6918480	3.8489920
H	0.4352320	-1.2339030	2.2635330
C	3.0178330	-0.1419440	4.1848530
H	4.8296220	0.7423560	3.4274140
H	1.1080810	-1.0403030	4.6296160
H	3.3143670	-0.0586740	5.2279410
C	3.0051450	0.0464510	-1.3425510
C	2.6879690	0.8550670	-2.4405830
C	4.2997020	-0.4847820	-1.2604250
C	3.6310140	1.1311090	-3.4272060
H	1.6836100	1.2733870	-2.5210300
C	5.2478550	-0.1997250	-2.2375920
H	4.5810020	-1.1249260	-0.4265170
C	4.9145290	0.6058910	-3.3243140
H	3.3624030	1.7592650	-4.2736170
H	6.2508430	-0.6120430	-2.1510060

H	5.6568230	0.8220190	-4.0893800
C	-0.7641240	2.9209490	0.4808520
H	-1.4983170	2.9572990	1.2885870
H	-1.1115710	3.3471310	-0.4650520
C	1.5718830	3.2234720	-0.2369050
H	1.2207800	3.2360210	-1.2663460
H	2.5879930	2.8546900	-0.1087170
C	1.0912400	2.9084990	2.2152580
H	1.2292600	3.9334070	2.5912430
H	0.3633670	2.4101220	2.8677650
H	2.0526720	2.3895240	2.3194890
C	0.6208100	2.9367420	0.7891260
Ni	-0.0168160	1.1687850	0.0390480
N	-1.8980280	-1.0872390	-1.3902190
N	1.0833360	-1.9490200	-0.6412660
Cl	2.1494830	5.3162140	-0.1762350
C	-0.7093720	-0.9730870	-2.2447570
H	-0.3406980	0.0618160	-2.2208870
H	-0.9939220	-1.1517730	-3.2899360
C	0.4295350	-1.9466390	-1.9695990
H	0.0391580	-2.9535490	-2.1400450
H	1.1711100	-1.7679720	-2.7711240

9 – Ground

Lowest Frequency Vibration = 23.5639 cm**-1
Electronic Energy = -2387.59777847
Electronic and Zero-Point Energy = -2386.816120
Enthalpy = -2386.771295
Free Energy = -2386.889516
E large = -2388.43576723

C	2.3428580	2.8055630	0.9678730
C	3.2316560	3.6378030	0.0383600
H	3.8505040	2.9992620	-0.6038020
H	2.6616360	4.3200730	-0.6008100
H	3.9042000	4.2545230	0.6463080
C	3.2501640	2.1094830	1.9742280
H	3.8059050	2.8890700	2.5083680
H	2.6886880	1.5405050	2.7198020
H	3.9926280	1.4487700	1.5150030
C	1.4342070	3.7301780	1.7816230
H	0.7193870	4.2896100	1.1676740
H	0.8757100	3.1577300	2.5328400
H	2.0499940	4.4689340	2.3096820
C	-2.6704780	2.9072690	-0.6967190
C	-2.0062870	4.2780390	-0.5618280
H	-1.3283130	4.5110450	-1.3908100

H	-2.7850220	5.0502500	-0.5579320
H	-1.4509260	4.3566640	0.3816570
C	-3.4189250	2.8311300	-2.0292080
H	-4.0371390	1.9284070	-2.0869850
H	-4.0825730	3.6990610	-2.1291460
H	-2.7403080	2.8387910	-2.8906980
C	-3.6849120	2.7883030	0.4345880
H	-3.2273340	2.9219610	1.4194050
H	-4.4315700	3.5807900	0.3066120
H	-4.2275910	1.8387490	0.4233890
P	1.7786430	0.2064540	-0.1782600
P	-1.8133450	0.2635940	-0.0216560
C	2.3913630	-0.6821650	1.2953330
C	1.5890120	-0.6979060	2.4451050
C	3.5104190	-1.5156130	1.2352650
C	1.9291080	-1.4974500	3.5283290
H	0.6996580	-0.0695930	2.4962190
C	3.8406860	-2.3258150	2.3207640
H	4.1338020	-1.5413440	0.3442200
C	3.0570400	-2.3154850	3.4691760
H	1.3063360	-1.4868900	4.4205300
H	4.7193820	-2.9641840	2.2645830
H	3.3199950	-2.9445600	4.3163650
C	3.0834490	0.1558520	-1.4655670
C	2.6822070	-0.1395150	-2.7726530
C	4.4228480	0.4966700	-1.2312980
C	3.5955730	-0.1040580	-3.8229350
H	1.6413550	-0.4022660	-2.9648900
C	5.3370700	0.5214570	-2.2783810
H	4.7618290	0.7397470	-0.2260010
C	4.9245970	0.2225260	-3.5752770
H	3.2678750	-0.3346800	-4.8339090
H	6.3758230	0.7753680	-2.0801570
H	5.6420650	0.2461680	-4.3923020
C	-1.8859790	0.3083860	1.7992740
C	-2.1818600	-0.8695510	2.4967860
C	-1.4629860	1.4335920	2.5094750
C	-2.0919000	-0.9046790	3.8837640
H	-2.4752620	-1.7673810	1.9531160
C	-1.3665100	1.3944240	3.8981420
H	-1.1930160	2.3390620	1.9689980
C	-1.6862470	0.2283680	4.5873310
H	-2.3332230	-1.8213030	4.4171660
H	-1.0397330	2.2791840	4.4407390
H	-1.6133670	0.1981090	5.6719240
C	-3.4156100	-0.3996940	-0.6200450

C	-3.5042870	-0.6281340	-1.9992170
C	-4.5085180	-0.7080560	0.1918630
C	-4.6647830	-1.1493770	-2.5563740
H	-2.6549880	-0.3864090	-2.6403680
C	-5.6690690	-1.2398410	-0.3669500
H	-4.4652880	-0.5264700	1.2644630
C	-5.7494450	-1.4605130	-1.7375730
H	-4.7232820	-1.3162760	-3.6294280
H	-6.5145290	-1.4774080	0.2745710
H	-6.6572040	-1.8742700	-2.1706360
C	1.1142730	-2.9045640	-1.4026240
H	2.1323110	-3.0663250	-1.0496230
H	0.9983220	-2.7791110	-2.4803570
C	-1.2642120	-2.9869940	-1.0454020
H	-1.4819120	-2.8892560	-2.1105920
H	-2.1203840	-3.2245010	-0.4133860
C	0.2616420	-4.0545530	0.6892690
H	0.1410150	-5.1407050	0.5859660
H	1.2749380	-3.8632710	1.0596960
H	-0.4630870	-3.7109030	1.4358840
C	0.0324410	-3.4077660	-0.6381800
Pt	-0.0658130	-1.1819920	-0.6440400
N	1.4489240	1.8495260	0.1886620
N	-1.6064490	1.8367440	-0.6157260
C	0.8105650	2.5431850	-0.9565660
H	1.5150860	2.6358930	-1.8026460
H	0.5979180	3.5621800	-0.6255280
C	-0.4789100	1.9873520	-1.5455390
H	-0.7595200	2.6907830	-2.3386540
H	-0.2957430	1.0400780	-2.0684850

9 – TS1

Lowest Frequency Vibration = -400.4051 cm**-1
Electronic Energy = -2601.21921568
Electronic and Zero-Point Energy = -2600.285080
Enthalpy = -2600.233307
Free Energy = -2600.366550
E large = -2602.12348896

C	-4.1273050	-0.6378940	-1.6517540
C	-4.4345290	0.3299710	-2.7969810
H	-4.4291570	1.3703750	-2.4523330
H	-3.7167100	0.2374970	-3.6210430
H	-5.4310970	0.1188080	-3.2052590
C	-5.1063400	-0.3676870	-0.5141870
H	-6.1238500	-0.4515110	-0.9142090
H	-5.0095010	-1.0969640	0.2958660

H	-5.0126080	0.6394330	-0.0977590
C	-4.3766900	-2.0731980	-2.1173560
H	-3.8022190	-2.3407500	-3.0115310
H	-4.1423080	-2.7913290	-1.3209210
H	-5.4378220	-2.1866540	-2.3704080
C	-0.3656790	-4.1373320	-0.3722250
C	-1.7710580	-4.5581890	0.0654670
H	-2.0390420	-4.0612380	1.0065620
H	-2.5453100	-4.3330070	-0.6764320
H	-1.7933040	-5.6420240	0.2351340
C	0.0525040	-4.9267020	-1.6191120
H	1.0249650	-4.5894030	-1.9983180
H	0.1433740	-5.9883790	-1.3599030
H	-0.6749140	-4.8579860	-2.4344000
C	0.5679530	-4.5445980	0.7607510
H	0.2902410	-4.0889560	1.7150740
H	0.4882470	-5.6312740	0.8811340
H	1.6203420	-4.3206310	0.5608510
P	-2.0880410	0.5907750	-0.0534570
P	0.8599280	-1.4967020	-0.3079360
C	-2.5308960	-0.0164820	1.6119980
C	-2.9235180	-1.3423000	1.8075550
C	-2.2576650	0.7846630	2.7283530
C	-3.0780210	-1.8502040	3.0953150
H	-3.0839760	-1.9819030	0.9410180
C	-2.4183180	0.2786410	4.0133790
H	-1.8990260	1.8054600	2.5944820
C	-2.8321500	-1.0397770	4.1999490
H	-3.3853660	-2.8851180	3.2328370
H	-2.2094410	0.9118250	4.8727610
H	-2.9520350	-1.4365140	5.2055890
C	-2.9186070	2.2131760	-0.2732000
C	-2.5439630	2.9431640	-1.4089590
C	-3.8552490	2.7619030	0.6050470
C	-3.1077630	4.1856670	-1.6702220
H	-1.8074630	2.5254290	-2.0982190
C	-4.4109120	4.0139690	0.3500720
H	-4.1634330	2.2094360	1.4911560
C	-4.0421440	4.7250420	-0.7869720
H	-2.8160270	4.7383230	-2.5604980
H	-5.1386760	4.4296430	1.0434270
H	-4.4798400	5.7009460	-0.9845890
C	1.5725040	-1.8019550	1.3471260
C	2.9490370	-1.8948810	1.5680160
C	0.7121920	-1.7259680	2.4516570
C	3.4515330	-1.9422390	2.8682960

H	3.6407840	-1.9355930	0.7283970
C	1.2149510	-1.7848070	3.7444050
H	-0.3630550	-1.6375790	2.2945720
C	2.5888810	-1.8936740	3.9579960
H	4.5252600	-2.0231160	3.0242720
H	0.5295400	-1.7406750	4.5885830
H	2.9838400	-1.9361870	4.9703390
C	2.1965760	-1.7855610	-1.5432980
C	2.3073620	-0.8396050	-2.5687500
C	3.0342620	-2.9087560	-1.5764250
C	3.2345640	-1.0000610	-3.5953030
H	1.6583250	0.0378780	-2.5513320
C	3.9667980	-3.0667270	-2.5962170
H	2.9717640	-3.6646370	-0.7954320
C	4.0683350	-2.1132590	-3.6075340
H	3.3044030	-0.2552430	-4.3851290
H	4.6171700	-3.9385750	-2.6005800
H	4.7972680	-2.2417190	-4.4045140
C	0.5757490	2.8285070	0.4553150
H	0.0121200	3.2454720	1.2932090
H	0.5277210	3.4372420	-0.4520500
C	2.7225060	1.8339800	-0.2919960
H	2.4630220	2.0873860	-1.3174510
H	3.4039480	0.9952770	-0.1761670
C	2.1608820	1.8069850	2.1769160
H	2.6661360	2.6589550	2.6549990
H	1.2638730	1.5895250	2.7705600
H	2.8281480	0.9377360	2.2424510
C	1.8004950	2.1203640	0.7487860
Pt	0.2366840	0.7877950	-0.0378820
N	4.2742490	3.1732670	-0.2602910
H	4.7187360	3.0632000	-1.1743370
C	3.7103930	4.5219560	-0.1458470
H	2.9732100	4.5034620	0.6715620
H	4.5017720	5.2267770	0.1543060
C	5.2583000	2.8734940	0.7909710
H	4.7356320	2.9232940	1.7552440
H	6.0204260	3.6695340	0.8030210
C	5.9240260	1.5277900	0.6028980
H	6.3394090	1.4306800	-0.4084050
H	6.7520730	1.4204040	1.3108430
H	5.2390160	0.6893070	0.7730730
C	3.0696840	4.9791570	-1.4368570
H	2.6664410	5.9902970	-1.3212860
H	3.8030040	5.0045370	-2.2525080
H	2.2429520	4.3263660	-1.7415170

N	-2.6933620	-0.5069450	-1.2036930
N	-0.3944750	-2.6398330	-0.6289550
C	-1.6811900	-0.9707120	-2.1641590
H	-0.8923010	-0.2152270	-2.2668700
H	-2.1348260	-1.0372060	-3.1611830
C	-1.0781530	-2.3481230	-1.9120540
H	-1.8902710	-3.0732180	-2.0093960
H	-0.4001970	-2.5328630	-2.7662310

9 – Int 1

Lowest Frequency Vibration = 15.9605 cm**-1
Electronic Energy = -2601.23486847
Electronic and Zero-Point Energy = -2600.296370
Enthalpy = -2600.245198
Free Energy = -2600.376690
E large = -2602.13767029

C	-4.0688340	-0.5904890	-1.8021190
C	-4.3253180	0.4138340	-2.9286960
H	-4.2958140	1.4431620	-2.5539600
H	-3.5912950	0.3233430	-3.7385780
H	-5.3174820	0.2432080	-3.3662850
C	-5.0980390	-0.3558460	-0.7010930
H	-6.0977970	-0.4370350	-1.1441970
H	-5.0289460	-1.1055410	0.0930570
H	-5.0270610	0.6401110	-0.2544900
C	-4.2970580	-2.0090500	-2.3270700
H	-3.6738010	-2.2489600	-3.1958220
H	-4.1089030	-2.7550980	-1.5439910
H	-5.3424850	-2.1098480	-2.6437670
C	-0.3249300	-4.1087550	-0.5009150
C	-1.7436610	-4.5521220	-0.1326530
H	-2.0400610	-4.1031330	0.8236940
H	-2.4947640	-4.2859790	-0.8848810
H	-1.7717360	-5.6433630	-0.0205430
C	0.1459470	-4.8500850	-1.7585200
H	1.1299200	-4.4935630	-2.0868890
H	0.2351710	-5.9201210	-1.5354120
H	-0.5494550	-4.7552500	-2.5987380
C	0.5638620	-4.5599690	0.6513990
H	0.2464250	-4.1427760	1.6109950
H	0.4827070	-5.6508890	0.7246750
H	1.6221730	-4.3259480	0.5033790
P	-2.0890550	0.5645240	-0.0552610
P	0.8896430	-1.4601690	-0.2973980
C	-2.5880830	-0.1440430	1.5567810
C	-2.9990720	-1.4744340	1.6637720

C	-2.3351590	0.5808330	2.7296500
C	-3.1935840	-2.0599890	2.9126510
H	-3.1450470	-2.0598140	0.7570310
C	-2.5353380	-0.0018930	3.9766890
H	-1.9656420	1.6052050	2.6693950
C	-2.9681480	-1.3238030	4.0721770
H	-3.5168970	-3.0974210	2.9760370
H	-2.3423950	0.5753770	4.8783890
H	-3.1187600	-1.7800610	5.0481750
C	-2.9533640	2.1836560	-0.1919620
C	-2.5819200	2.9816770	-1.2826210
C	-3.8934490	2.6796370	0.7139430
C	-3.1533140	4.2334760	-1.4753220
H	-1.8408180	2.6079430	-1.9922050
C	-4.4534940	3.9426650	0.5318230
H	-4.2018250	2.0753870	1.5658550
C	-4.0896080	4.7190010	-0.5634590
H	-2.8647610	4.8349970	-2.3347150
H	-5.1832470	4.3158600	1.2472160
H	-4.5322560	5.7023250	-0.7065510
C	1.5521050	-1.8484680	1.3617870
C	2.9217170	-1.9511300	1.6163960
C	0.6634380	-1.8148380	2.4458900
C	3.3916610	-2.0440500	2.9262490
H	3.6347290	-1.9619930	0.7942900
C	1.1332870	-1.9165110	3.7484690
H	-0.4074600	-1.7210110	2.2621070
C	2.5018890	-2.0293080	3.9944410
H	4.4613170	-2.1299920	3.1069970
H	0.4267750	-1.9019030	4.5761660
H	2.8701500	-2.1033070	5.0151370
C	2.2670830	-1.7282870	-1.5002910
C	2.4045680	-0.7577610	-2.4997650
C	3.1089560	-2.8486300	-1.5415280
C	3.3551450	-0.8938070	-3.5090340
H	1.7554070	0.1199350	-2.4767390
C	4.0660550	-2.9821150	-2.5420730
H	3.0285310	-3.6248630	-0.7825150
C	4.1903350	-2.0056610	-3.5286910
H	3.4419320	-0.1309320	-4.2799670
H	4.7173600	-3.8533870	-2.5511510
H	4.9371670	-2.1157650	-4.3119050
C	0.6936890	2.8151370	0.5567090
H	0.2137320	3.1715890	1.4733810
H	0.5644730	3.4956270	-0.2894330
C	2.9480020	2.1262010	-0.4039780

H	2.4870970	2.3541330	-1.3707140
H	3.5073470	1.1909420	-0.5126850
C	2.3644200	1.6750650	2.0697490
H	2.8529450	2.5128780	2.5930350
H	1.4998980	1.3918020	2.6838650
H	3.0596180	0.8250790	2.0736500
C	1.9111480	2.0420480	0.6727110
Pt	0.2546110	0.8135720	0.0352800
N	4.0470130	3.2072560	-0.2432250
H	4.5335370	3.2079560	-1.1482470
C	3.4928150	4.5900840	-0.0514520
H	2.7844910	4.5308980	0.7815950
H	4.3327320	5.2197150	0.2593500
C	5.1108810	2.9105240	0.7825170
H	4.6587770	3.0553480	1.7669800
H	5.8660250	3.6917010	0.6439160
C	5.7319260	1.5444390	0.6296020
H	6.0399620	1.3567190	-0.4064320
H	6.6302020	1.5000290	1.2531040
H	5.0687540	0.7344850	0.9506520
C	2.8585690	5.1334350	-1.3085950
H	2.5409680	6.1647270	-1.1270360
H	3.5735930	5.1485530	-2.1396630
H	1.9747060	4.5664760	-1.6178750
N	-2.6596930	-0.4697740	-1.2877110
N	-0.3524930	-2.6034530	-0.6997130
C	-1.6025610	-0.8903510	-2.2185590
H	-0.8158290	-0.1263550	-2.2545040
H	-2.0096400	-0.9242330	-3.2375390
C	-0.9940970	-2.2705800	-1.9939280
H	-1.7935220	-3.0002520	-2.1487010
H	-0.2840050	-2.4173050	-2.8298380

9 – Int 2

Lowest Frequency Vibration = 20.6165 cm**-1
Electronic Energy = -2847.90331221
Electronic and Zero-Point Energy = -2847.121134
Enthalpy = -2847.074555
Free Energy = -2847.197728
E large = -2848.77125073

C	-3.2604950	-2.0152160	-1.7937100
C	-3.8887930	-1.2601120	-2.9680180
H	-4.2960790	-0.2940300	-2.6479270
H	-3.1677040	-1.0767970	-3.7739400
H	-4.7124500	-1.8473210	-3.3940530
C	-4.3140650	-2.1843120	-0.7043830

H	-5.1611490	-2.7369350	-1.1279430
H	-3.9337740	-2.7556290	0.1481050
H	-4.7069130	-1.2309310	-0.3406820
C	-2.8653570	-3.4219760	-2.2484490
H	-2.1854400	-3.4201050	-3.1074990
H	-2.3936380	-3.9799560	-1.4292370
H	-3.7663840	-3.9687090	-2.5533460
C	1.5931330	-3.5935310	-0.3699170
C	0.4865410	-4.5847900	0.0006550
H	-0.2829530	-4.6892380	-0.7723160
H	0.9228760	-5.5798050	0.1561220
H	-0.0010270	-4.2768250	0.9345530
C	2.3571510	-4.1035450	-1.5987100
H	3.1014670	-3.3725520	-1.9363800
H	2.8898190	-5.0262330	-1.3374670
H	1.7050810	-4.3412240	-2.4454390
C	2.5646360	-3.5995090	0.8050340
H	2.0799740	-3.3284330	1.7469380
H	2.9445990	-4.6221870	0.9155110
H	3.4322870	-2.9491140	0.6598310
P	-1.9832410	-0.0652570	-0.1003990
P	1.5793060	-0.6708460	-0.2483220
C	-2.1930710	-0.8482030	1.5397830
C	-1.9743720	-2.2157870	1.7253090
C	-2.3361540	-0.0280350	2.6675760
C	-1.9340330	-2.7598960	3.0074460
H	-1.8076330	-2.8519930	0.8567920
C	-2.3029560	-0.5726160	3.9465840
H	-2.4582380	1.0487220	2.5478270
C	-2.1040950	-1.9414100	4.1205770
H	-1.7636160	-3.8275700	3.1337560
H	-2.4236340	0.0759300	4.8114620
H	-2.0730190	-2.3661650	5.1214910
C	-3.4330330	1.0449660	-0.3312840
C	-3.3546070	1.9171060	-1.4255110
C	-4.5549240	1.1087380	0.4988130
C	-4.3817370	2.8121650	-1.6983570
H	-2.4731080	1.8873210	-2.0690940
C	-5.5767990	2.0192300	0.2375510
H	-4.6406590	0.4409630	1.3548390
C	-5.4959230	2.8671480	-0.8622110
H	-4.3094040	3.4757540	-2.5572170
H	-6.4424910	2.0587090	0.8952420
H	-6.2963260	3.5751420	-1.0652490
C	2.3110360	-0.7022950	1.4274440
C	3.5964120	-0.2254840	1.6947740

C	1.4683630	-1.0186820	2.5025900
C	4.0426260	-0.1033320	3.0104490
H	4.2575230	0.0594950	0.8785880
C	1.9176160	-0.9026300	3.8111290
H	0.4562110	-1.3746830	2.3076370
C	3.2099620	-0.4454190	4.0699420
H	5.0489300	0.2629780	3.2028030
H	1.2530520	-1.1652940	4.6320400
H	3.5615380	-0.3506890	5.0948980
C	2.9635570	-0.3625200	-1.4297500
C	2.7108500	0.5824010	-2.4304130
C	4.1892800	-1.0426310	-1.4494390
C	3.6533690	0.8514860	-3.4199980
H	1.7580360	1.1151990	-2.4195490
C	5.1353440	-0.7708390	-2.4319050
H	4.4179460	-1.7851960	-0.6871110
C	4.8694050	0.1767780	-3.4188820
H	3.4381070	1.5906690	-4.1884700
H	6.0858840	-1.2998830	-2.4254970
H	5.6118150	0.3853170	-4.1860250
C	-0.4170370	3.1401390	0.4790950
H	-1.0290500	3.2722570	1.3760390
H	-0.7830550	3.7031570	-0.3850440
C	1.9122480	3.4529780	-0.4212560
H	1.4693490	3.4615510	-1.4195150
H	2.8865350	2.9540390	-0.4334470
C	1.5919850	2.8828180	2.0180150
H	1.7718050	3.8911270	2.4232830
H	0.9168220	2.3594860	2.7074590
H	2.5535290	2.3515570	2.0254110
C	1.0056850	2.9553940	0.6304910
Pt	0.0436760	1.1301390	-0.0028260
N	-2.0413660	-1.2984670	-1.2825040
N	0.9421940	-2.2449280	-0.6184090
Cl	2.3869700	5.2807780	-0.1516360
C	-0.8916760	-1.2648870	-2.1989720
H	-0.5039700	-0.2411170	-2.2691500
H	-1.2305560	-1.5053780	-3.2151320
C	0.2422740	-2.2483090	-1.9247510
H	-0.1695500	-3.2517640	-2.0599000
H	0.9625890	-2.1046730	-2.7525990

9 – TS2

Lowest Frequency Vibration = -276.9643 cm**-1
Electronic Energy = -2847.90051961
Electronic and Zero-Point Energy = -2847.117958

Enthalpy = -2847.071977
Free Energy = -2847.193518
E large = -2648.76778832

C	-3.2805370	-2.0579890	-1.6882920
C	-3.9200250	-1.3523740	-2.8867800
H	-4.3515030	-0.3867850	-2.5988260
H	-3.2004610	-1.1777170	-3.6959880
H	-4.7285340	-1.9714880	-3.2958390
C	-4.3224220	-2.1737420	-0.5804500
H	-5.1887300	-2.7133520	-0.9815510
H	-3.9475010	-2.7366680	0.2800790
H	-4.6862670	-1.2024580	-0.2336500
C	-2.8970340	-3.4848670	-2.0842160
H	-2.2314320	-3.5234210	-2.9534830
H	-2.4146120	-4.0079630	-1.2483320
H	-3.8050510	-4.0402110	-2.3496690
C	1.5729050	-3.6149780	-0.2387080
C	0.4646120	-4.5872280	0.1736090
H	-0.3023880	-4.7291650	-0.5961330
H	0.9011610	-5.5734420	0.3763160
H	-0.0256450	-4.2371370	1.0911090
C	2.3342130	-4.1748410	-1.4469130
H	3.0837670	-3.4616990	-1.8101340
H	2.8602500	-5.0906050	-1.1507400
H	1.6812970	-4.4390260	-2.2848140
C	2.5468910	-3.5724990	0.9330950
H	2.0673000	-3.2546160	1.8629440
H	2.9217620	-4.5910180	1.0891260
H	3.4184560	-2.9354060	0.7548980
P	-1.9810350	-0.0443440	-0.1046130
P	1.5749340	-0.6988200	-0.2423910
C	-2.1813740	-0.7504160	1.5697460
C	-1.9756730	-2.1124340	1.8039330
C	-2.3123310	0.1141940	2.6645790
C	-1.9365220	-2.6084690	3.1051740
H	-1.8175960	-2.7811300	0.9585090
C	-2.2805460	-0.3831540	3.9627280
H	-2.4233890	1.1867240	2.5043910
C	-2.0950740	-1.7464360	4.1867060
H	-1.7756910	-3.6720390	3.2713110
H	-2.3914990	0.2986510	4.8029250
H	-2.0648260	-2.1330950	5.2029210
C	-3.4139130	1.0698660	-0.3887980
C	-3.3388000	1.8694380	-1.5369990
C	-4.5263950	1.1923670	0.4472740
C	-4.3633040	2.7517740	-1.8565010

H	-2.4644220	1.7927100	-2.1861450
C	-5.5462110	2.0892730	0.1360450
H	-4.6070020	0.5806130	1.3446640
C	-5.4699940	2.8647630	-1.0161710
H	-4.2958200	3.3588120	-2.7564350
H	-6.4058140	2.1754930	0.7970240
H	-6.2696790	3.5611630	-1.2580740
C	2.3044210	-0.6434830	1.4330400
C	3.5793080	-0.1256550	1.6743240
C	1.4681540	-0.9242450	2.5227680
C	4.0222870	0.0720370	2.9818660
H	4.2346130	0.1319740	0.8445620
C	1.9151590	-0.7332470	3.8231370
H	0.4626690	-1.3082430	2.3475520
C	3.1971090	-0.2357690	4.0576520
H	5.0199030	0.4703890	3.1541070
H	1.2567670	-0.9690290	4.6569530
H	3.5461990	-0.0822650	5.0762750
C	2.9481710	-0.4440350	-1.4463850
C	2.6806700	0.4262780	-2.5088960
C	4.1823450	-1.1083900	-1.4214750
C	3.6177860	0.6366360	-3.5173350
H	1.7243900	0.9513290	-2.5337490
C	5.1239650	-0.8918850	-2.4219890
H	4.4216420	-1.7935400	-0.6103520
C	4.8426530	-0.0201320	-3.4721220
H	3.3907930	1.3171300	-4.3348960
H	6.0821180	-1.4051810	-2.3802480
H	5.5809660	0.1453420	-4.2535370
C	-0.4791880	3.1392280	0.3431780
H	-1.1778280	3.3150980	1.1645120
H	-0.7548250	3.6463930	-0.5861200
C	1.8995420	3.1864610	-0.3680650
H	1.5677430	3.2409290	-1.4016460
H	2.8795720	2.7380580	-0.2157440
C	1.3808500	2.9604730	2.0839840
H	1.6025350	3.9789400	2.4364820
H	0.6073000	2.5389590	2.7385640
H	2.2954260	2.3641590	2.2052740
C	0.9208200	2.9968680	0.6532350
Pt	0.0480830	1.1201080	-0.0590060
N	-2.0484570	-1.3256010	-1.2262290
N	0.9241630	-2.2754760	-0.5421790
Cl	2.6550740	5.2519580	-0.2988640
C	-0.9077520	-1.3489510	-2.1541130
H	-0.5087670	-0.3346370	-2.2776020

H	-1.2604730	-1.6336690	-3.1538530
C	0.2178310	-2.3309390	-1.8440590
H	-0.2023780	-3.3359330	-1.9321420
H	0.9347890	-2.2296560	-2.6806020

10 – Ground

Lowest Frequency Vibration = 40.1688 cm**-1
Electronic Energy = -1247.72441010
Electronic and Zero-Point Energy = -1247.395819
Enthalpy = -1247.374112
Free Energy = -1247.443084
E large = -2586.88721091

C	-1.1464780	2.1027360	-0.6865670
H	-2.0571860	2.3178890	-0.1278500
H	-1.2646050	1.9761410	-1.7655350
C	1.2350480	2.0079190	-0.8209660
H	1.2034540	1.8457210	-1.9014670
H	2.2232720	2.1560970	-0.3883080
C	0.1963640	3.0586510	1.2283980
H	0.2189610	4.1552210	1.1964830
H	-0.6676210	2.7657710	1.8367430
H	1.1121370	2.7246230	1.7293420
C	0.0974660	2.5057830	-0.1588380
Ni	0.0001560	0.4785010	-0.3057880
P	1.7361340	-0.8400760	0.0152690
P	-1.8068600	-0.7404760	0.0181540
C	2.9027150	-0.9289590	-1.3865740
H	3.2811490	0.0685870	-1.6316590
H	3.7491140	-1.5782250	-1.1312320
H	2.3954660	-1.3348740	-2.2682120
C	2.7722600	-0.2446550	1.4001210
H	3.6087120	-0.9342630	1.5690120
H	3.1704280	0.7511150	1.1811490
H	2.1700770	-0.1852080	2.3139440
C	1.5290210	-2.6005900	0.4591260
H	2.5158610	-3.0542010	0.6150490
H	0.9530180	-2.6840440	1.3877260
H	1.0117710	-3.1456540	-0.3366240
C	-1.7747660	-2.5641510	-0.1038380
H	-1.4215350	-2.8718700	-1.0940330
H	-1.1171030	-2.9941820	0.6567030
H	-2.7891160	-2.9537780	0.0466360
C	-3.2493840	-0.3426160	-1.0310820
H	-4.0911550	-0.9953950	-0.7707310
H	-3.5543590	0.6990680	-0.8944720
H	-2.9953310	-0.4971640	-2.0854940

C	-2.4036140	-0.4532260	1.7190460
H	-2.6246840	0.6114450	1.8548200
H	-3.3065330	-1.0411900	1.9247970
H	-1.6194650	-0.7367440	2.4309700

10 – TS1

Lowest Frequency Vibration = -377.7175 cm**-1
Electronic Energy = -1461.34547812
Electronic and Zero-Point Energy = -1460.866952
Enthalpy = -1460.837554
Free Energy = -1460.924651
E large = -2800.57339816

C	-0.1884110	-1.7851720	0.6307280
H	0.1961770	-2.3599270	1.4763750
H	-0.3409300	-2.3709000	-0.2800310
C	-1.7110960	-0.0178370	-0.1646970
H	-1.5450030	-0.3508370	-1.1892500
H	-1.9881570	1.0291630	-0.0542160
C	-1.1890870	-0.1549500	2.3031580
H	-2.0736310	-0.6053120	2.7794830
H	-0.3201340	-0.4159120	2.9207310
H	-1.3171340	0.9345220	2.3441260
C	-1.0096830	-0.6488020	0.8935050
Ni	0.7695690	-0.1601070	0.1152810
P	0.9876920	1.9823290	-0.3737150
P	2.7276330	-1.1308080	0.0143530
C	0.3636380	2.4289100	-2.0399280
H	-0.7098380	2.2197050	-2.1051960
H	0.5332660	3.4928090	-2.2496360
H	0.8779810	1.8296330	-2.7997140
C	0.0870970	3.1749480	0.6941450
H	0.2197940	4.2008800	0.3272130
H	-0.9839530	2.9419500	0.7069210
H	0.4669750	3.1145870	1.7203290
C	2.6523580	2.7514030	-0.4053680
H	2.5733240	3.8342630	-0.5647610
H	3.1727110	2.5688460	0.5423690
H	3.2432150	2.3210120	-1.2210940
C	4.1545580	-0.4232860	-0.8955890
H	3.8889460	-0.2460980	-1.9439370
H	4.4504420	0.5289180	-0.4430670
H	5.0107980	-1.1087440	-0.8575010
C	2.7779320	-2.8713450	-0.5576710
H	3.7977220	-3.2703000	-0.4903360
H	2.1151110	-3.4904060	0.0563840
H	2.4396840	-2.9307400	-1.5981580

C	3.3994710	-1.2550810	1.7155760
H	2.6877730	-1.7956140	2.3505020
H	4.3645150	-1.7780070	1.7281990
H	3.5306110	-0.2484100	2.1301340
C	-4.5185770	0.6328200	-0.0901820
H	-4.1743150	1.3393410	-0.8601330
H	-5.5575910	0.3703140	-0.3442470
C	-4.4628360	1.2548550	1.2864340
H	-5.1205000	2.1285070	1.3333110
H	-4.8003370	0.5439210	2.0511820
H	-3.4511630	1.5839930	1.5515340
C	-3.9749670	-1.3708790	-1.3769830
H	-3.7188130	-0.7638820	-2.2578210
H	-5.0603420	-1.5522520	-1.4234710
C	-3.2256890	-2.6840450	-1.3832930
H	-3.5809090	-3.3165530	-2.2030000
H	-2.1475460	-2.5430530	-1.5152010
H	-3.3844920	-3.2312670	-0.4449790
N	-3.6733690	-0.5637150	-0.1885730
H	-3.7867270	-1.1371730	0.6505290

10 – Int 1

Lowest Frequency Vibration = 24.5613 cm**-1
Electronic Energy = -1461.35952657
Electronic and Zero-Point Energy = -1460.876595
Enthalpy = -1460.847799
Free Energy = -1460.932768
E large = -2800.58597320

C	-0.3796400	-1.5979140	0.7967300
H	-0.0711440	-2.0401510	1.7486080
H	-0.5096620	-2.3240850	-0.0086680
C	-2.0197550	-0.0373590	-0.3319580
H	-1.6526640	-0.4395410	-1.2818620
H	-2.1503060	1.0451140	-0.4497630
C	-1.3834070	0.3120160	2.1213810
H	-2.3376640	-0.0050270	2.5758410
H	-0.5933950	0.0805060	2.8459980
H	-1.4233720	1.4045230	2.0167860
C	-1.1041560	-0.3702300	0.8027100
Ni	0.7642760	-0.1290030	0.2173170
P	1.0243410	1.9660660	-0.3798270
P	2.6898170	-1.1746390	0.0660830
C	0.7337000	2.2477050	-2.1745350
H	-0.3042600	2.0054860	-2.4308620
H	0.9326730	3.2919820	-2.4488220
H	1.3894520	1.5947930	-2.7628280

C	-0.0455540	3.2744100	0.3500860
H	0.1533230	4.2503210	-0.1119010
H	-1.1040200	3.0271970	0.2031920
H	0.1435100	3.3499380	1.4272450
C	2.6738360	2.7546450	-0.1816980
H	2.6451490	3.8192190	-0.4481060
H	3.0166930	2.6562410	0.8547960
H	3.3977090	2.2520390	-0.8334610
C	4.0561460	-0.6547410	-1.0514760
H	3.6815610	-0.5445300	-2.0758930
H	4.4556580	0.3117940	-0.7239600
H	4.8726870	-1.3882090	-1.0458230
C	2.6144780	-2.9725550	-0.3065400
H	3.6092000	-3.4337340	-0.2577310
H	1.9571250	-3.4660420	0.4185740
H	2.1967930	-3.1300570	-1.3077420
C	3.5521620	-1.1937000	1.6886370
H	2.8927380	-1.6366410	2.4444660
H	4.4854320	-1.7700450	1.6427060
H	3.7810880	-0.1669030	1.9969230
C	-4.5103450	0.4898030	-0.1448370
H	-4.3551380	1.0771610	-1.0569810
H	-5.4812040	-0.0085180	-0.2262150
C	-4.4592060	1.3357390	1.1005440
H	-5.2827430	2.0556680	1.0663130
H	-4.5884780	0.7260380	2.0024220
H	-3.5284570	1.9037210	1.1936880
C	-3.8279550	-1.5895210	-1.2507300
H	-3.7355440	-1.0497480	-2.2003780
H	-4.8847080	-1.8314560	-1.0997200
C	-2.9929680	-2.8429720	-1.2243150
H	-3.4105880	-3.5522520	-1.9457880
H	-1.9514020	-2.6633400	-1.5062340
H	-3.0148860	-3.3201820	-0.2377880
N	-3.4694420	-0.5970030	-0.1774670
H	-3.5011610	-1.0935330	0.7225380

10 – Int 2

Lowest Frequency Vibration = 35.4515 cm**-1
Electronic Energy = -1708.02999110
Electronic and Zero-Point Energy = -1707.702387
Enthalpy = -1707.678283
Free Energy = -1707.753600
E large = -3047.22105660

C	-0.8794100	-1.8931300	0.2686040
H	-0.5722880	-2.5322050	1.1014290

H	-0.9474700	-2.4092270	-0.6943820
C	-2.5341510	-0.2309710	-0.5752890
H	-2.1334440	-0.4241050	-1.5732180
H	-2.8055420	0.8218140	-0.4570360
C	-2.1265660	-0.4058060	1.9165700
H	-3.0512110	-0.9284580	2.2098520
H	-1.3516350	-0.6787450	2.6437040
H	-2.3182690	0.6712710	2.0185990
C	-1.7062870	-0.7623930	0.5151680
Cl	-4.2673800	-1.0668930	-0.6607290
Ni	0.1554050	-0.2418660	0.0863660
P	0.2603680	1.9472360	-0.0261700
P	2.1690500	-1.0743970	-0.1322700
C	0.0184610	2.6019970	-1.7280090
H	-0.9759840	2.3315670	-2.1011460
H	0.1228400	3.6946760	-1.7530770
H	0.7642030	2.1575970	-2.3983420
C	-0.9417630	2.9698490	0.9198800
H	-0.7956090	4.0390950	0.7177150
H	-1.9685670	2.6961740	0.6503300
H	-0.8107650	2.7941680	1.9940790
C	1.8283570	2.7990540	0.4269950
H	1.7013920	3.8893630	0.4349340
H	2.1671980	2.4722880	1.4176800
H	2.6047260	2.5455780	-0.3039700
C	3.5938390	-0.1484190	-0.8391130
H	3.3399560	0.2338740	-1.8350020
H	3.8321550	0.7042820	-0.1930400
H	4.4845940	-0.7853160	-0.9179200
C	2.3197870	-2.6690320	-1.0321470
H	3.3461990	-3.0563200	-0.9917310
H	1.6426280	-3.4057950	-0.5853790
H	2.0314720	-2.5336940	-2.0808100
C	2.8473640	-1.5311310	1.5134060
H	2.1673080	-2.2363780	2.0054790
H	3.8406400	-1.9907100	1.4258450
H	2.9205290	-0.6340730	2.1397690

10 – TS2

Lowest Frequency Vibration = -271.8647 cm**-1
Electronic Energy = -1708.02795506
Electronic and Zero-Point Energy = -1707.701304
Enthalpy = -1707.677415
Free Energy = -1707.752624
E large = -3047.21856721

C	-0.8166060	-1.9306990	0.2765420

H	-0.4884900	-2.5897780	1.0840750
H	-0.8844880	-2.4139460	-0.7028040
C	-2.3683640	-0.1803580	-0.4895790
H	-2.0526000	-0.3917730	-1.5095860
H	-2.7164500	0.8365290	-0.3198180
C	-2.0801120	-0.5168750	1.9882460
H	-3.0193230	-1.0213060	2.2616970
H	-1.3111210	-0.8398070	2.7006160
H	-2.2391070	0.5612900	2.1240040
C	-1.6875940	-0.8433780	0.5753900
Cl	-4.3860470	-0.9814650	-0.7238590
Ni	0.1475010	-0.2392600	0.0758690
P	0.2845440	1.9581330	-0.0225360
P	2.1528430	-1.0857040	-0.1495050
C	-0.0399240	2.6575290	-1.6887490
H	-1.0606050	2.4166290	-2.0065750
H	0.0864920	3.7479140	-1.6901890
H	0.6574350	2.2165550	-2.4110660
C	-0.8625860	2.9423840	1.0236950
H	-0.7328240	4.0168210	0.8386070
H	-1.9024350	2.6693300	0.8108890
H	-0.6611110	2.7408160	2.0821070
C	1.8787080	2.7779990	0.3844790
H	1.7561140	3.8675470	0.4322300
H	2.2563920	2.4206390	1.3500480
H	2.6200780	2.5465770	-0.3882950
C	3.5460870	-0.1504350	-0.8988070
H	3.2558120	0.2364580	-1.8827060
H	3.8106150	0.6966500	-0.2564470
H	4.4304410	-0.7902880	-1.0133500
C	2.2670610	-2.6744110	-1.0594490
H	3.3003150	-3.0433950	-1.0831570
H	1.6327570	-3.4235130	-0.5728910
H	1.9114530	-2.5421420	-2.0875200
C	2.8656390	-1.5382750	1.4790240
H	2.1970340	-2.2416600	1.9885880
H	3.8557950	-1.9988830	1.3672790
H	2.9559250	-0.6403760	2.1014060

11 – Ground

Lowest Frequency Vibration = 32.1527 cm**-1
Electronic Energy = -1205.14669610
Electronic and Zero-Point Energy = -1204.819221
Enthalpy = -1204.797073
Free Energy = -1204.867432
E large = -1206.53661006

C	-0.9045570	2.4677700	-0.7070960
H	-1.8249810	2.7633350	-0.2069190
H	-0.9574110	2.3594740	-1.7915360
C	1.4811250	2.1355750	-0.6656070
H	1.5472380	2.0235580	-1.7491710
H	2.4282280	2.1716850	-0.1281220
C	0.3893240	3.2500450	1.3177790
H	0.6071580	4.3251790	1.2946870
H	-0.5652820	3.1157250	1.8379480
H	1.1830750	2.7657440	1.8981090
C	0.3339090	2.7132470	-0.0787780
Pd	0.0385250	0.5129100	-0.2676100
P	1.6820880	-1.1452260	0.0427790
P	-1.9169180	-0.7602530	0.0451890
C	3.1818700	-0.9395110	-0.9785350
H	3.6539480	0.0244200	-0.7622610
H	3.8967820	-1.7451390	-0.7704870
H	2.9127130	-0.9631730	-2.0399890
C	2.3091840	-1.0846200	1.7564220
H	3.1029460	-1.8259390	1.9124090
H	2.7026700	-0.0823900	1.9627360
H	1.4864340	-1.2828090	2.4529950
C	1.2866280	-2.9099440	-0.2049890
H	2.1657590	-3.5223590	0.0322410
H	0.4578220	-3.2187510	0.4409360
H	1.0079700	-3.0834170	-1.2500890
C	-2.2280940	-2.1290480	-1.1226140
H	-2.3212230	-1.7320110	-2.1390630
H	-1.4047060	-2.8506140	-1.1046380
H	-3.1588800	-2.6437360	-0.8530750
C	-3.4943100	0.1585210	-0.0071560
H	-4.3352250	-0.5270520	0.1567120
H	-3.5027090	0.9266390	0.7733940
H	-3.6130670	0.6432380	-0.9821450
C	-1.9798060	-1.5701860	1.6813980
H	-1.8620010	-0.8183340	2.4693690
H	-2.9395080	-2.0851640	1.8160280
H	-1.1690910	-2.3008810	1.7755610

11 – TS1

Lowest Frequency Vibration = -371.8417 cm**-1
Electronic Energy = -1418.77010138
Electronic and Zero-Point Energy = -1418.291548
Enthalpy = -1418.261974
Free Energy = -1418.349453
E large = -1420.22626493

C	-0.4820740	-1.8999610	0.5408160
H	-0.1166520	-2.5309350	1.3520460
H	-0.6047750	-2.4056000	-0.4193760
C	-1.9184110	-0.0274880	-0.1678600
H	-1.7626620	-0.3056860	-1.2091990
H	-2.1683920	1.0173000	0.0081580
C	-1.4731250	-0.3568150	2.2924860
H	-2.4447550	-0.7086410	2.6704240
H	-0.6957460	-0.7847310	2.9356810
H	-1.4505600	0.7334110	2.4155660
C	-1.2672630	-0.7621790	0.8595330
Pd	0.7129690	-0.1649500	0.0831780
P	1.0378100	2.1545640	-0.3563200
P	2.8356710	-1.2195390	0.0032360
C	0.3779840	2.7501470	-1.9608370
H	-0.6970550	2.5433090	-2.0191820
H	0.5416440	3.8293400	-2.0780170
H	0.8734200	2.2230860	-2.7838400
C	0.2224290	3.2995890	0.8238740
H	0.4421210	4.3465340	0.5766200
H	-0.8635180	3.1492620	0.7938220
H	0.5692420	3.0929050	1.8424840
C	2.7463880	2.8168640	-0.3954890
H	2.7445970	3.9026630	-0.5552460
H	3.2523630	2.5941340	0.5516150
H	3.3030020	2.3385780	-1.2096660
C	4.2324700	-0.5301280	-0.9635570
H	3.9439830	-0.4090280	-2.0133870
H	4.5094410	0.4507190	-0.5616710
H	5.1063080	-1.1923140	-0.9080420
C	2.8434280	-2.9733190	-0.5277470
H	3.8496530	-3.4036120	-0.4437070
H	2.1546940	-3.5507060	0.0992330
H	2.5068050	-3.0486760	-1.5676600
C	3.5608300	-1.3226090	1.6835820
H	2.8557780	-1.8273330	2.3545620
H	4.5107180	-1.8730400	1.6769130
H	3.7336570	-0.3106820	2.0688720
C	-4.7255720	0.6973610	-0.0049400

H	-4.3766040	1.4514680	-0.7260430
H	-5.7775830	0.4861460	-0.2547680
C	-4.6257420	1.2109790	1.4134120
H	-5.2653820	2.0900300	1.5400870
H	-4.9619480	0.4508000	2.1298770
H	-3.6024740	1.5005410	1.6802750
C	-4.2493760	-1.1943900	-1.4748540
H	-3.9466440	-0.5311030	-2.2983560
H	-5.3426270	-1.3091470	-1.5487160
C	-3.5756950	-2.5431080	-1.5865560
H	-3.9426030	-3.0743980	-2.4704060
H	-2.4879600	-2.4560060	-1.6797510
H	-3.7941070	-3.1649660	-0.7087200
N	-3.9205740	-0.5119240	-0.2180550
H	-4.0477940	-1.1574900	0.5647740

11 – Int 1

Lowest Frequency Vibration = 36.1458 cm**-1
Electronic Energy = -1418.78575969
Electronic and Zero-Point Energy = -1418.303441
Enthalpy = -1418.274140
Free Energy = -1418.360791
E large = -1420.24058574

C	-0.6663700	-1.7288690	0.7344880
H	-0.3477050	-2.2177530	1.6569240
H	-0.7838020	-2.3963120	-0.1196650
C	-2.2501310	-0.0691230	-0.3222380
H	-1.8862570	-0.4313490	-1.2884480
H	-2.3308130	1.0221030	-0.3766330
C	-1.6233420	0.1245350	2.1536530
H	-2.5964760	-0.1758730	2.5765840
H	-0.8539880	-0.1816170	2.8715580
H	-1.6167170	1.2216980	2.1083900
C	-1.3624780	-0.5019060	0.8047730
Pd	0.7060270	-0.1537120	0.1686050
P	1.0400130	2.1496750	-0.3763710
P	2.8254760	-1.2556630	0.0165870
C	0.4285750	2.6822020	-2.0271050
H	-0.6530280	2.5194040	-2.0972410
H	0.6409260	3.7439740	-2.2102280
H	0.9124220	2.0836790	-2.8073110
C	0.2525090	3.4111490	0.7059770
H	0.4867500	4.4316210	0.3750020
H	-0.8360980	3.2757310	0.6931360
H	0.5994310	3.2835660	1.7378790
C	2.7673240	2.7740430	-0.4503220

H	2.7987430	3.8522960	-0.6547740
H	3.2784150	2.5745810	0.4993170
H	3.3031860	2.2460190	-1.2484950
C	4.1807730	-0.6970770	-1.0941100
H	3.8255530	-0.6551450	-2.1299630
H	4.5049740	0.3080900	-0.8002750
H	5.0433440	-1.3743610	-1.0385080
C	2.7857070	-3.0552580	-0.3573770
H	3.7859200	-3.5034480	-0.2922580
H	2.1223150	-3.5577780	0.3567550
H	2.3856170	-3.2179760	-1.3647030
C	3.6932670	-1.2602010	1.6365060
H	3.0458540	-1.7159900	2.3946270
H	4.6378180	-1.8181100	1.5871990
H	3.9026490	-0.2288900	1.9443830
C	-4.7139410	0.5566300	-0.1516370
H	-4.5203080	1.1673330	-1.0408380
H	-5.7033270	0.1022620	-0.2631910
C	-4.6402770	1.3557080	1.1241280
H	-5.4391590	2.1034880	1.1127850
H	-4.7938900	0.7178620	2.0026300
H	-3.6908750	1.8881900	1.2404110
C	-4.1010780	-1.5093620	-1.3240570
H	-3.9847360	-0.9341940	-2.2500180
H	-5.1659750	-1.7213460	-1.1869880
C	-3.3074920	-2.7900110	-1.3442320
H	-3.7484600	-3.4566600	-2.0920270
H	-2.2599150	-2.6366680	-1.6198880
H	-3.3479220	-3.3037450	-0.3767910
N	-3.7198460	-0.5726400	-0.2085880
H	-3.7933870	-1.1003630	0.6710500

11 – Int 2

Lowest Frequency Vibration = 25.5177 cm**-1
Electronic Energy = -1665.45669557
Electronic and Zero-Point Energy = -1665.129947
Enthalpy = -1665.105255
Free Energy = -1665.183482
E large = -1666.87634766

C	-1.1174240	-2.0011390	0.3107040
H	-0.8357500	-2.6291920	1.1576250
H	-1.1339220	-2.5083190	-0.6566190
C	-2.6821610	-0.2988310	-0.6156250
H	-2.2423330	-0.5118370	-1.5926740
H	-2.9037570	0.7671250	-0.5141100
C	-2.3930810	-0.4812490	1.8957370

H	-3.3721230	-0.9327310	2.1203100
H	-1.6886650	-0.8219230	2.6634190
H	-2.5062290	0.6064290	1.9992720
C	-1.9202520	-0.8600340	0.5176050
Cl	-4.4228740	-1.0668520	-0.7484710
Pd	0.1460460	-0.2381600	0.1437940
P	0.2517100	2.1453340	-0.0114720
P	2.3531960	-1.1084210	-0.1297710
C	0.0058120	2.7353190	-1.7352350
H	-0.9725770	2.4038690	-2.1032870
H	0.0627140	3.8299100	-1.8019590
H	0.7753910	2.2967030	-2.3818760
C	-0.9698840	3.1840510	0.8909280
H	-0.8255380	4.2503800	0.6710890
H	-1.9894880	2.8997070	0.6046320
H	-0.8623170	3.0288780	1.9706400
C	1.8116340	3.0183780	0.4229570
H	1.7069470	4.1058530	0.3116810
H	2.0922550	2.7901620	1.4576990
H	2.6177850	2.6729730	-0.2351350
C	3.7749840	-0.0318040	-0.5799490
H	3.5643660	0.4879210	-1.5225870
H	3.9238760	0.7215650	0.2026860
H	4.7008840	-0.6119690	-0.6918700
C	2.5134730	-2.4411390	-1.3857050
H	3.5378210	-2.8347770	-1.4290990
H	1.8259910	-3.2578390	-1.1355210
H	2.2362180	-2.0561550	-2.3734750
C	3.0190450	-1.9538610	1.3597860
H	2.3179280	-2.7355310	1.6751180
H	4.0000330	-2.4071560	1.1645150
H	3.1147500	-1.2340410	2.1804240

11 – TS2

Lowest Frequency Vibration = -277.7453 cm**-1
Electronic Energy = -1665.45353371
Electronic and Zero-Point Energy = -1665.127061
Enthalpy = -1665.102879
Free Energy = -1665.179952
E large = -1666.87246787

C	-1.0617690	-2.0120790	0.1967710
H	-0.7559560	-2.7290190	0.9601460
H	-1.0913040	-2.4047580	-0.8220760
C	-2.5310330	-0.1542650	-0.4665880
H	-2.2226500	-0.3009240	-1.4988280
H	-2.8642520	0.8496880	-0.2152610

C	-2.3188470	-0.6987080	1.9791900
H	-3.3107230	-1.1346210	2.1689850
H	-1.6104990	-1.1545510	2.6802930
H	-2.3835480	0.3732090	2.2073370
C	-1.9061600	-0.9334340	0.5546010
Cl	-4.5963800	-0.8911830	-0.7776000
Pd	0.1292440	-0.2104590	0.0965260
P	0.3540780	2.1643720	0.0045510
P	2.2884400	-1.1745510	-0.1474210
C	0.0552400	2.8372960	-1.6765550
H	-0.9532530	2.5627180	-2.0077070
H	0.1549240	3.9304350	-1.6949260
H	0.7752180	2.3997670	-2.3783600
C	-0.7909190	3.1865760	1.0134750
H	-0.6156860	4.2571820	0.8432380
H	-1.8292710	2.9525320	0.7525490
H	-0.6458250	2.9675060	2.0772820
C	1.9652230	2.9412410	0.4167530
H	1.9032220	4.0357190	0.3587660
H	2.2710700	2.6551850	1.4297080
H	2.7285070	2.5918290	-0.2875370
C	3.7363670	-0.1469200	-0.6132450
H	3.5405210	0.3642780	-1.5634180
H	3.9115300	0.6107230	0.1591840
H	4.6411040	-0.7604610	-0.7175620
C	2.3876240	-2.5295090	-1.3802390
H	3.4044460	-2.9395250	-1.4390210
H	1.6955280	-3.3313080	-1.0972530
H	2.0936460	-2.1575520	-2.3679550
C	2.9060340	-2.0096650	1.3643890
H	2.1787610	-2.7645670	1.6846390
H	3.8745530	-2.4950870	1.1862540
H	3.0148510	-1.2776820	2.1722950

12 – Ground

Lowest Frequency Vibration = 30.6617 cm**-1
Electronic Energy = -1197.54643649
Electronic and Zero-Point Energy = -1197.218909
Enthalpy = -1197.196801
Free Energy = -1197.267515
E large = -1197.98786775

C	-0.7756440	2.4428090	-0.6306200
H	-1.6624210	2.8017300	-0.1108400
H	-0.8438050	2.4120310	-1.7196160
C	1.5973840	1.9712410	-0.6218320
H	1.6649400	1.9181030	-1.7101080

H	2.5467470	1.9606400	-0.0873410
C	0.5921290	3.1368500	1.3862670
H	0.8360930	4.2066050	1.3596790
H	-0.3535740	3.0240110	1.9278550
H	1.3878440	2.6289240	1.9434060
C	0.4892160	2.6147600	-0.0111770
Pt	0.0602800	0.4337890	-0.2034070
P	1.5573880	-1.3405620	0.0766550
P	-1.9371820	-0.7418740	0.0876960
C	3.1143480	-1.1560520	-0.8531590
H	3.6378630	-0.2526430	-0.5248750
H	3.7583960	-2.0267890	-0.6801880
H	2.9014340	-1.0706780	-1.9240460
C	2.1014320	-1.4408760	1.8123370
H	2.8540190	-2.2287990	1.9390000
H	2.5308970	-0.4751970	2.1043600
H	1.2445350	-1.6491320	2.4623560
C	1.0513220	-3.0421790	-0.3395850
H	1.8781270	-3.7306590	-0.1261300
H	0.1793100	-3.3480250	0.2472540
H	0.8032400	-3.1032600	-1.4049270
C	-2.3646840	-1.8902980	-1.2612070
H	-2.4156230	-1.3366000	-2.2049880
H	-1.6022080	-2.6699220	-1.3534930
H	-3.3370160	-2.3588240	-1.0655280
C	-3.4274410	0.2982350	0.2257510
H	-4.3092060	-0.3323130	0.3936300
H	-3.3203210	0.9974090	1.0617420
H	-3.5661590	0.8696970	-0.6982380
C	-2.0052710	-1.7580930	1.5989460
H	-1.8157710	-1.1252800	2.4728350
H	-2.9939820	-2.2227310	1.6990720
H	-1.2450430	-2.5456800	1.5652480

12 – TS1

Lowest Frequency Vibration = -379.5075 cm**-1
Electronic Energy = -1411.16643003
Electronic and Zero-Point Energy = -1410.686927
Enthalpy = -1410.657960
Free Energy = -1410.743436
E large = -1411.67370920

C	0.6539350	-1.8148030	-0.7764720
H	0.3892570	-2.3657850	-1.6810680
H	0.8483470	-2.4585380	0.0851920
C	2.0339070	0.0155690	0.1902360
H	1.8439680	-0.3758220	1.1885380

H	2.2616300	1.0791500	0.1408790
C	1.7199180	-0.0578780	-2.3078250
H	2.6752010	-0.4480740	-2.6908970
H	0.9401230	-0.3462640	-3.0220310
H	1.7889180	1.0377090	-2.3054900
C	1.4225480	-0.5979980	-0.9356760
Pt	-0.6015620	-0.1873210	-0.2159180
P	-1.0471010	2.0533010	0.3725840
P	-2.7091210	-1.1358940	0.0750080
C	-0.7566860	2.3896940	2.1477370
H	0.2839510	2.1471240	2.3939410
H	-0.9500020	3.4433700	2.3846650
H	-1.4093070	1.7563220	2.7599540
C	0.0156970	3.3026610	-0.4427840
H	-0.2286400	4.3125970	-0.0890490
H	1.0697990	3.0942960	-0.2238750
H	-0.1316420	3.2600250	-1.5275870
C	-2.7125260	2.7591430	0.0945540
H	-2.7402880	3.8095490	0.4111490
H	-2.9665200	2.7019110	-0.9699870
H	-3.4629090	2.2001390	0.6649000
C	-3.4785970	-0.8342500	1.7051150
H	-2.8026200	-1.1707910	2.4990230
H	-3.6645060	0.2375130	1.8373570
H	-4.4301410	-1.3746300	1.7883970
C	-2.7648530	-2.9566560	-0.0625720
H	-3.7800060	-3.3340380	0.1147970
H	-2.4391840	-3.2576810	-1.0646470
H	-2.0808220	-3.4005160	0.6695000
C	-4.0020670	-0.6039210	-1.1000830
H	-3.6938170	-0.8517300	-2.1216650
H	-4.9526030	-1.1062700	-0.8800120
H	-4.1431240	0.4807080	-1.0337780
C	4.8207600	0.8034400	0.3397860
H	4.3928260	1.4295070	1.1371550
H	5.8554070	0.5749040	0.6412410
C	4.8177990	1.5289820	-0.9867550
H	5.4259050	2.4368210	-0.9231800
H	5.2435540	0.8987830	-1.7777640
H	3.8082570	1.8245930	-1.2966760
C	4.3096010	-1.3128670	1.4401920
H	3.9888220	-0.7746550	2.3440570
H	5.3974950	-1.4615150	1.5314550
C	3.6083800	-2.6466060	1.3235790
H	3.9495190	-3.3226790	2.1139100
H	2.5212550	-2.5486620	1.4143770

H	3.8252700	-3.1235880	0.3589620
N	4.0381320	-0.4369340	0.2934830
H	4.2379790	-0.9423570	-0.5725800

12 – Int 1

Lowest Frequency Vibration = 22.4374 cm**-1
Electronic Energy = -1411.18226511
Electronic and Zero-Point Energy = -1410.699150
Enthalpy = -1410.670425
Free Energy = -1410.756138
E large = -1411.68787087

C	0.8302740	-1.6348750	-0.8385610
H	0.6492500	-2.0806250	-1.8201490
H	1.0168640	-2.3752930	-0.0586300
C	2.3539780	-0.0000520	0.3863230
H	1.9769760	-0.4458300	1.3120590
H	2.4240440	1.0833500	0.5370690
C	1.8320300	0.3356120	-2.0932160
H	2.8193680	0.0311960	-2.4812460
H	1.0946540	0.0802470	-2.8633060
H	1.8434710	1.4297210	-1.9986900
C	1.4818210	-0.3409580	-0.7861860
Pt	-0.5807800	-0.1626840	-0.2442510
P	-1.0880810	2.0406810	0.4131510
P	-2.6825340	-1.2000920	0.0217060
C	-0.8957750	2.3113980	2.2163990
H	0.1355630	2.0832420	2.5112640
H	-1.1284640	3.3484620	2.4899120
H	-1.5613790	1.6360500	2.7661610
C	-0.0383950	3.3814960	-0.2715790
H	-0.3394080	4.3615470	0.1210600
H	1.0115270	3.2010180	-0.0105430
H	-0.1246760	3.3943930	-1.3640380
C	-2.7628080	2.7234310	0.1067610
H	-2.8491720	3.7449150	0.4994280
H	-2.9622700	2.7390980	-0.9709350
H	-3.5190220	2.0928930	0.5896550
C	-3.5418310	-0.9618380	1.6238100
H	-2.8851730	-1.2727580	2.4444590
H	-3.7856340	0.0981750	1.7620840
H	-4.4694590	-1.5474440	1.6662970
C	-2.6588940	-3.0264680	-0.1224570
H	-3.6605880	-3.4579640	0.0023250
H	-2.2673850	-3.3031420	-1.1084360
H	-1.9885180	-3.4443200	0.6377400
C	-3.9898370	-0.7507550	-1.1810380

H	-3.6467650	-0.9781110	-2.1964880
H	-4.9144530	-1.3077640	-0.9816980
H	-4.1977440	0.3236390	-1.1223610
C	4.8178960	0.6524630	0.2808050
H	4.6475760	1.1732120	1.2302270
H	5.8095750	0.1911380	0.3221110
C	4.7182300	1.5799540	-0.9020600
H	5.5256910	2.3154860	-0.8300770
H	4.8444720	1.0421430	-1.8484150
H	3.7742500	2.1330620	-0.9355510
C	4.2108330	-1.4806080	1.3163760
H	4.0741460	-0.9655360	2.2743030
H	5.2805430	-1.6688010	1.1816940
C	3.4370360	-2.7713260	1.2478750
H	3.8794570	-3.4770480	1.9579760
H	2.3844380	-2.6498780	1.5206030
H	3.4955240	-3.2223530	0.2503390
N	3.8276960	-0.4823450	0.2566020
H	3.9115700	-0.9540050	-0.6531690

12 – Int 2

Lowest Frequency Vibration = 46.8025 cm**-1
Electronic Energy = -1657.85170051
Electronic and Zero-Point Energy = -1657.522473
Enthalpy = -1657.498869
Free Energy = -1657.573360
E large = -1658.32215141

C	-1.2323040	-1.8716900	0.2802290
H	-1.0678890	-2.5273960	1.1389020
H	-1.3531600	-2.4132730	-0.6630110
C	-2.7591200	-0.1048110	-0.6471690
H	-2.3375760	-0.3280190	-1.6300490
H	-2.9784350	0.9630840	-0.5547390
C	-2.4687110	-0.2868430	1.8561080
H	-3.4459100	-0.7515870	2.0624480
H	-1.7696810	-0.6254310	2.6300740
H	-2.5937100	0.7990120	1.9699270
C	-1.9723290	-0.6475540	0.4788850
Cl	-4.5031870	-0.8711910	-0.7470160
Pt	0.1019680	-0.2195010	0.1091810
P	0.4083120	2.1119050	-0.0422100
P	2.2579320	-1.1286870	-0.1522140
C	0.1190490	2.7533170	-1.7357140
H	-0.8935220	2.4881340	-2.0615300
H	0.2373730	3.8439240	-1.7760910
H	0.8318640	2.2895200	-2.4278390

C	-0.7351100	3.1507620	0.9476160
H	-0.5586990	4.2188420	0.7646970
H	-1.7716460	2.9100520	0.6840090
H	-0.5941480	2.9427940	2.0143360
C	2.0264240	2.8798720	0.3568280
H	1.9588770	3.9753720	0.3510070
H	2.3709380	2.5472840	1.3429490
H	2.7644820	2.5717120	-0.3922180
C	3.5394350	-0.2698560	-1.1457310
H	3.1221260	0.0427080	-2.1097930
H	3.8782770	0.6220150	-0.6060710
H	4.4050280	-0.9214600	-1.3216830
C	2.2784060	-2.8049950	-0.8927270
H	3.2965820	-3.2126320	-0.9430400
H	1.6512870	-3.4723450	-0.2900680
H	1.8587110	-2.7628250	-1.9043830
C	3.1450490	-1.4055670	1.4266700
H	2.5420170	-2.0534130	2.0728630
H	4.1245070	-1.8718560	1.2589100
H	3.2846010	-0.4469930	1.9399310

12 – TS2

Lowest Frequency Vibration = -284.6622 cm**-1
Electronic Energy = -1657.84844906
Electronic and Zero-Point Energy = -1657.520010
Enthalpy = -1657.496617
Free Energy = -1657.570834
E large = -1658.31838209

C	-1.1859570	-1.8993360	0.2324990
H	-0.9868840	-2.6124090	1.0354260
H	-1.3068150	-2.3673890	-0.7489750
C	-2.5871370	0.0066710	-0.5132190
H	-2.2768990	-0.1923990	-1.5362040
H	-2.8893500	1.0316290	-0.3096440
C	-2.4324580	-0.4650240	1.9514530
H	-3.4105180	-0.9352270	2.1328090
H	-1.7244600	-0.8692200	2.6843770
H	-2.5455830	0.6099670	2.1439030
C	-1.9767030	-0.7322070	0.5448540
Cl	-4.6633790	-0.6937930	-0.8160880
Pt	0.0949030	-0.2024970	0.0988700
P	0.5002690	2.1181570	-0.0234600
P	2.1975730	-1.1833640	-0.1740880
C	0.1830750	2.7980630	-1.6939870
H	-0.8535610	2.5904150	-1.9833850
H	0.3554400	3.8817240	-1.7205920

H	0.8455970	2.3102570	-2.4186050
C	-0.5687040	3.1711510	1.0291190
H	-0.3600870	4.2352490	0.8586120
H	-1.6212230	2.9722300	0.7984330
H	-0.3954090	2.9368670	2.0855570
C	2.1610740	2.7991820	0.3445080
H	2.1358570	3.8960360	0.3687540
H	2.5166660	2.4279110	1.3124300
H	2.8656620	2.4838610	-0.4329810
C	3.4843580	-0.3396750	-1.1667910
H	3.0657830	-0.0083520	-2.1238870
H	3.8503270	0.5369410	-0.6204910
H	4.3302440	-1.0127140	-1.3565610
C	2.1393310	-2.8404800	-0.9446220
H	3.1441890	-3.2724980	-1.0347640
H	1.5150850	-3.5014830	-0.3332320
H	1.6893410	-2.7665080	-1.9410920
C	3.0723660	-1.5118350	1.3974110
H	2.4520990	-2.1582050	2.0286080
H	4.0391910	-1.9994590	1.2180350
H	3.2372650	-0.5689340	1.9309890

Diethylamine

Lowest Frequency Vibration = 113.8485 cm**-1
Electronic Energy = -213.637198952
Electronic and Zero-Point Energy = -213.488693
Enthalpy = -213.480857
Free Energy = -213.518688
E large = -213.711192233

H	0.8178630	0.0000000	0.8831710
H	-0.8178630	0.0000000	0.8831710
C	0.0000000	2.4647200	0.3550640
H	0.0000000	3.3762500	-0.2492540
H	-0.8902880	2.4850040	0.9937230
H	0.8902880	2.4850040	0.9937230
C	0.0000000	-2.4647200	0.3550640
H	-0.8902880	-2.4850040	0.9937230
H	0.0000000	-3.3762500	-0.2492540
H	0.8902880	-2.4850040	0.9937230
N	0.0000000	0.0000000	0.2613200
C	0.0000000	-1.2591460	-0.5488910
H	0.8878840	-1.2151170	-1.1865090
H	-0.8878840	-1.2151170	-1.1865090
C	0.0000000	1.2591460	-0.5488910
H	-0.8878840	1.2151170	-1.1865090
H	0.8878840	1.2151170	-1.1865090

Protonated Diethylamine

Lowest Frequency Vibration = 71.4817 cm**-1
Electronic Energy = -214.103837908
Electronic and Zero-Point Energy = -213.940278
Enthalpy = -213.932281
Free Energy = -213.970163
E large = -214.170873954

H	0.8178630	0.0000000	0.8831710
H	-0.8178630	0.0000000	0.8831710
C	0.0000000	2.4647200	0.3550640
H	0.0000000	3.3762500	-0.2492540
H	-0.8902880	2.4850040	0.9937230
H	0.8902880	2.4850040	0.9937230
C	0.0000000	-2.4647200	0.3550640
H	-0.8902880	-2.4850040	0.9937230
H	0.0000000	-3.3762500	-0.2492540
H	0.8902880	-2.4850040	0.9937230
N	0.0000000	0.0000000	0.2613200
C	0.0000000	-1.2591460	-0.5488910
H	0.8878840	-1.2151170	-1.1865090
H	-0.8878840	-1.2151170	-1.1865090
C	0.0000000	1.2591460	-0.5488910
H	-0.8878840	1.2151170	-1.1865090
H	0.8878840	1.2151170	-1.1865090

Methallyl Chloride

Lowest Frequency Vibration = 76.5578 cm**-1
Electronic Energy = -616.664633428
Electronic and Zero-Point Energy = -616.565460
Enthalpy = -616.558393
Free Energy = -616.595583
E large = -616.750162646

C	-0.9725760	-0.0961360	0.0951880
C	0.3127640	-0.5225090	0.7163890
H	0.4612640	-0.0786920	1.7060310
H	0.4062030	-1.6085960	0.7826340
C	-1.2426670	1.3727330	0.0420970
H	-2.2407710	1.5818190	-0.3550800
H	-1.1620430	1.8242920	1.0403030
H	-0.5079390	1.8848720	-0.5928170
C	-1.8292150	-1.0182780	-0.3500280
H	-2.7944090	-0.7374720	-0.7684510
H	-1.5980100	-2.0811670	-0.3057940
Cl	1.7544630	0.0470640	-0.2663940

Methallyl Diethylamine
Lowest Frequency Vibration = 15.5122 cm**-1
Electronic Energy = -369.532876238
Electronic and Zero-Point Energy = -369.295874
Enthalpy = -369.283508
Free Energy = -369.333341
E large = -369.658787705

C	1.6236620	-0.0000260	0.0932930
C	0.3715500	-0.0000130	-0.7440040
H	0.4211890	0.8690890	-1.4253420
H	0.4211620	-0.8691290	-1.4253270
C	2.8877480	-0.0000700	-0.7082040
H	3.7773150	-0.0000060	-0.0698310
H	2.9382040	-0.8791730	-1.3664310
H	2.9381800	0.8789190	-1.3665860
C	1.6170160	-0.0000110	1.4270630
H	2.5473860	-0.0000190	1.9933770
H	0.6827150	0.0000160	1.9840580
N	-0.8925280	0.0000140	-0.0179600
C	-1.6704540	1.2102220	-0.2579520
H	-1.8594170	1.3594640	-1.3426800
H	-2.6550490	1.0706900	0.2091590
C	-1.6705170	-1.2101530	-0.2579560
H	-2.6551090	-1.0705600	0.2091410
H	-1.8594770	-1.3593960	-1.3426840
C	-1.0216110	2.4497730	0.3245110
H	-0.0402010	2.6533400	-0.1213430
H	-1.6493730	3.3301060	0.1450020
H	-0.8818120	2.3426000	1.4068850
C	-1.0217530	-2.4497360	0.3245310
H	-1.6496010	-3.3300230	0.1451000
H	-0.0403860	-2.6534120	-0.1213670
H	-0.8818830	-2.3425200	1.4068920

Protonated Diethylamine – Chloride Complex
Lowest Frequency Vibration = 56.0727 cm**-1
Electronic Energy = -674.453290682
Electronic and Zero-Point Energy = -674.289635
Enthalpy = -674.279715
Free Energy = -674.324426
E large = -374.553768922

H	-0.0004770	-1.1553900	-1.1817860
H	0.0001330	0.3146830	-0.3396370
C	-2.4597740	-0.7791670	-0.3610530
H	-3.3722980	-1.0383740	0.1838910
H	-2.4904730	0.2931750	-0.5848780

H	-2.4621150	-1.3345280	-1.3063270
C	2.4591690	-0.7808600	-0.3610240
H	2.4906850	0.2915010	-0.5846360
H	3.3715040	-1.0408570	0.1838480
H	2.4610890	-1.3360370	-1.3064030
N	-0.0003040	-0.7446770	-0.2425580
C	1.2498280	-1.1224150	0.4734280
H	1.1893830	-2.1921800	0.7005860
H	1.2364960	-0.5656500	1.4169750
C	-1.2507060	-1.1214260	0.4734850
H	-1.2370010	-0.5644710	1.4169210
H	-1.1910110	-2.1911820	0.7008620
Cl	0.0008890	2.2679560	0.0617340

6 – Constrained Ni-Ti Distance TS1

Lowest Frequency Vibration = -316.1936 cm**-1
Electronic Energy = -3551.49236420
Electronic and Zero-Point Energy = -3550.614411
Enthalpy = -3550.559181
Free Energy = -3550.699228
E large = -5682.52312552

Ti	-1.0259620	-1.2072580	-1.4588160
Cl	-2.0785340	-2.2385490	-3.1617720
Cl	0.0922420	0.2613800	-2.9151240
N	-2.4450840	-0.7911950	-0.1779320
N	0.2781880	-2.3914960	-0.7483750
C	-3.7953680	-1.4212200	0.0239670
C	-4.7444810	-1.0174270	-1.1035990
H	-4.9733460	0.0544330	-1.0701440
H	-4.3242740	-1.2506180	-2.0875020
H	-5.6896760	-1.5656100	-0.9997210
C	-4.4153010	-1.0153340	1.3568540
H	-5.4051470	-1.4818270	1.4353890
H	-3.8172950	-1.3559300	2.2085180
H	-4.5617540	0.0677220	1.4411580
C	-3.5940690	-2.9326060	0.0354950
H	-3.2379540	-3.3059410	-0.9312150
H	-2.8711920	-3.2172230	0.8124610
H	-4.5464040	-3.4316090	0.2532480
C	0.6785680	-3.8025370	-1.1307480
C	-0.5487060	-4.6999010	-1.0073160
H	-1.3627650	-4.3699310	-1.6601890
H	-0.2772170	-5.7201840	-1.3050890
H	-0.9179390	-4.7380690	0.0248390
C	1.1781880	-3.8005520	-2.5740240
H	2.0871800	-3.1959010	-2.6744640

H	1.4205340	-4.8272310	-2.8766640
H	0.4216440	-3.4134060	-3.2665660
C	1.7770480	-4.3654900	-0.2329870
H	1.5015300	-4.3526670	0.8267310
H	1.9407120	-5.4118230	-0.5175080
H	2.7299200	-3.8432470	-0.3592240
P	-1.9288460	0.7594320	0.2062410
P	1.1303520	-1.2375170	0.1746280
C	-1.9630010	1.0906820	2.0042530
C	-1.7217290	0.0543170	2.9088530
C	-2.0952140	2.3994340	2.4862010
C	-1.6428390	0.3148750	4.2729850
H	-1.5944900	-0.9639160	2.5456610
C	-2.0159630	2.6560250	3.8515550
H	-2.2691600	3.2277700	1.8026960
C	-1.7915690	1.6149410	4.7480920
H	-1.4609500	-0.5047650	4.9649130
H	-2.1338020	3.6748430	4.2133050
H	-1.7334870	1.8168940	5.8150490
C	-3.0684880	1.9483760	-0.5861640
C	-2.8671980	2.2187100	-1.9442670
C	-4.1941740	2.4753990	0.0565460
C	-3.7814680	2.9938110	-2.6500820
H	-1.9977670	1.8067250	-2.4557940
C	-5.1037560	3.2546220	-0.6517190
H	-4.3764900	2.2722620	1.1102070
C	-4.9013800	3.5113830	-2.0049810
H	-3.6161860	3.1938770	-3.7061540
H	-5.9773770	3.6565350	-0.1439460
H	-5.6167850	4.1162940	-2.5571340
C	1.0261680	-1.7156480	1.9313720
C	1.7137320	-0.9591170	2.8864800
C	0.1949960	-2.7572370	2.3494180
C	1.6104030	-1.2740820	4.2368560
H	2.3407950	-0.1236180	2.5738360
C	0.0865620	-3.0654800	3.7029540
H	-0.3797900	-3.3190770	1.6147570
C	0.8010850	-2.3319680	4.6459710
H	2.1587520	-0.6890580	4.9714180
H	-0.5568120	-3.8833470	4.0189280
H	0.7210830	-2.5783630	5.7022660
C	2.8979040	-1.3314700	-0.3149010
C	3.2211800	-1.0335420	-1.6443510
C	3.9234960	-1.6155750	0.5909630
C	4.5483180	-1.0158830	-2.0572410
H	2.4324070	-0.8048760	-2.3589340

C	5.2526840	-1.5909900	0.1725620
H	3.6954670	-1.8752540	1.6223320
C	5.5684530	-1.2891570	-1.1481450
H	4.7851510	-0.7886430	-3.0942630
H	6.0420480	-1.8157690	0.8861760
H	6.6069890	-1.2713010	-1.4702030
C	0.2320980	2.8377560	-0.1981210
H	-0.5116120	3.3875810	0.3778410
H	0.2051680	3.0013250	-1.2774490
C	2.4315900	1.8310830	-0.3603660
H	2.2783600	1.6890150	-1.4269760
H	3.1924100	1.2136410	0.1053570
C	1.6464520	2.6644910	1.9008250
H	1.8939310	3.7163730	2.0997200
H	0.7405660	2.4324190	2.4767440
H	2.4695050	2.0539030	2.2898340
C	1.4377200	2.4469600	0.4278870
Ni	0.2598800	0.8482820	-0.1151850
N	3.9714860	3.2992390	-0.7843860
H	4.5073250	2.8899770	-1.5521290
C	3.3032560	4.5187210	-1.2316950
H	2.5178320	4.7580640	-0.4963960
H	4.0127590	5.3629590	-1.2177640
C	4.8417010	3.5010250	0.3757250
H	4.2041210	3.7942440	1.2222660
H	5.5203020	4.3499360	0.1856180
C	5.6467770	2.2638680	0.7107040
H	6.2046240	1.9084650	-0.1656020
H	6.3733600	2.4881490	1.4982160
H	5.0195970	1.4373770	1.0689270
C	2.7119870	4.3602260	-2.6150100
H	2.2253270	5.2881760	-2.9317580
H	3.4919050	4.1253210	-3.3502520
H	1.9611440	3.5610870	-2.6520160

6 – Constrained P-Ni-P Angle Ground

Lowest Frequency Vibration = 31.0960 cm**-1
Electronic Energy = -3337.85225782
Electronic and Zero-Point Energy = -3337.125060
Enthalpy = -3337.077209
Free Energy = -3337.200552
E large = -5468.81674989

Ti	-0.0469740	-1.7158400	0.3872340
Cl	-0.3846600	-3.8374200	1.0600490
Cl	0.1425860	-2.4182840	-1.8428720
N	-1.5911040	-0.7888240	1.1401280

N	1.6956020	-1.1873100	0.9703060
C	-2.4686150	-1.0885190	2.3281850
C	-3.4187220	-2.2389230	2.0022580
H	-4.1378990	-1.9557380	1.2242910
H	-2.8761390	-3.1286370	1.6664380
H	-3.9874680	-2.5074460	2.9017680
C	-3.2887460	0.1262230	2.7475400
H	-3.8927260	-0.1524850	3.6198850
H	-2.6564350	0.9727370	3.0341340
H	-3.9867210	0.4537680	1.9688770
C	-1.5487180	-1.4612490	3.4845370
H	-0.9776230	-2.3716800	3.2756140
H	-0.8470960	-0.6434610	3.6982450
H	-2.1449730	-1.6428510	4.3869850
C	2.7184640	-1.8824900	1.8489400
C	2.0425790	-2.2424510	3.1678890
H	1.2156970	-2.9456520	3.0257600
H	2.7757260	-2.7218740	3.8277860
H	1.6636330	-1.3481610	3.6782720
C	3.1954630	-3.1455190	1.1372720
H	3.7396400	-2.8984490	0.2188680
H	3.8757880	-3.7026740	1.7936540
H	2.3592160	-3.8044190	0.8789820
C	3.9253920	-1.0005950	2.1541010
H	3.6518930	-0.0875050	2.6924790
H	4.6016030	-1.5730240	2.8003390
H	4.4900770	-0.7311730	1.2562580
P	-1.9378400	0.1695350	-0.1970050
P	1.9194580	0.1189170	-0.0894770
C	-2.1427340	1.9266830	0.2548290
C	-1.3866900	2.4312280	1.3174750
C	-2.9334060	2.7991860	-0.5009410
C	-1.4447630	3.7817280	1.6402200
H	-0.7546810	1.7622350	1.8997470
C	-2.9890870	4.1508240	-0.1721840
H	-3.5102320	2.4379030	-1.3499690
C	-2.2484260	4.6437330	0.8972860
H	-0.8602980	4.1591690	2.4763410
H	-3.6158600	4.8183360	-0.7587770
H	-2.2958150	5.6996170	1.1525370
C	-3.4739520	-0.4316560	-0.9720800
C	-3.3971530	-1.5861150	-1.7602920
C	-4.7252370	0.1291230	-0.6932650
C	-4.5551700	-2.1668210	-2.2644910
H	-2.4310160	-2.0425050	-1.9710660
C	-5.8801480	-0.4548390	-1.2045640

H	-4.8110140	1.0166880	-0.0702230
C	-5.7973860	-1.6015570	-1.9885510
H	-4.4853910	-3.0641280	-2.8743630
H	-6.8479290	-0.0114750	-0.9829530
H	-6.7025540	-2.0560880	-2.3841560
C	2.0716970	1.6596480	0.8789440
C	2.3532430	2.8752460	0.2435340
C	1.7960160	1.6551740	2.2496480
C	2.3947640	4.0567930	0.9757610
H	2.5504410	2.9109340	-0.8264800
C	1.8420440	2.8391630	2.9799510
H	1.5363810	0.7225450	2.7486560
C	2.1466180	4.0400930	2.3458050
H	2.6246280	4.9924530	0.4714920
H	1.6354500	2.8204720	4.0474950
H	2.1832220	4.9644770	2.9173800
C	3.4613420	-0.1376230	-1.0350960
C	3.5407510	-1.2411250	-1.8930530
C	4.5476150	0.7354510	-0.9295040
C	4.6973770	-1.4685050	-2.6298990
H	2.6999900	-1.9264500	-1.9815620
C	5.6998520	0.5047700	-1.6757810
H	4.5094770	1.5868740	-0.2534280
C	5.7757640	-0.5934100	-2.5262980
H	4.7520460	-2.3307920	-3.2899390
H	6.5412600	1.1875370	-1.5861490
H	6.6780350	-0.7717100	-3.1064450
C	-1.1420760	0.8556320	-2.8922350
H	-2.1501470	1.2626100	-2.8355410
H	-1.0446520	-0.1246270	-3.3609990
C	1.2114150	1.0673580	-2.7561150
H	1.3514870	0.1052630	-3.2513130
H	2.1150630	1.6504240	-2.5839030
C	-0.1640010	3.1788000	-2.5457330
H	0.3424230	3.7496750	-3.3328510
H	-1.2102520	3.4940880	-2.5119030
H	0.3084470	3.4458270	-1.5921810
C	-0.0339560	1.7153650	-2.8312480
Ni	0.0153490	0.3337880	-1.2407890

6 – Constrained P-NI-P Angle TS1

Lowest Frequency Vibration = -278.6261 cm**-1
Electronic Energy = -3551.49143389
Electronic and Zero-Point Energy = -3550.613563
Enthalpy = -3550.558363
Free Energy = -3550.698040

E large = -5682.52219805

Ti	-0.8837810	-1.2612800	-1.3406380
Cl	-1.8125180	-2.3916330	-3.0711070
Cl	0.0352180	0.3112660	-2.8684270
N	-2.4493620	-0.9774910	-0.1991550
N	0.5210870	-2.3800540	-0.6681570
C	-3.7441630	-1.7147910	-0.0205730
C	-4.6804640	-1.4124810	-1.1896230
H	-4.9843900	-0.3582120	-1.1943100
H	-4.2092340	-1.6410040	-2.1512260
H	-5.5887540	-2.0225430	-1.1009320
C	-4.4399710	-1.3283130	1.2803940
H	-5.3798940	-1.8894920	1.3515740
H	-3.8345410	-1.5727940	2.1597280
H	-4.6969310	-0.2631600	1.3161680
C	-3.4179750	-3.2023160	0.0358000
H	-3.0023770	-3.5626210	-0.9111690
H	-2.6979450	-3.4072930	0.8400060
H	-4.3307070	-3.7756790	0.2401870
C	0.9828130	-3.7791730	-1.0038960
C	-0.2034370	-4.7233700	-0.8481810
H	-1.0213880	-4.4658700	-1.5285200
H	0.1150560	-5.7468510	-1.0819970
H	-0.5830520	-4.7128370	0.1814050
C	1.4879360	-3.7909800	-2.4449720
H	2.3766170	-3.1568650	-2.5515700
H	1.7645370	-4.8138430	-2.7309630
H	0.7213570	-3.4363090	-3.1435160
C	2.1028560	-4.2627650	-0.0869890
H	1.8040000	-4.2842560	0.9658300
H	2.3594550	-5.2888410	-0.3771600
H	3.0132560	-3.6634090	-0.1853630
P	-2.0753050	0.6071630	0.2148190
P	1.3620430	-1.1375460	0.1265000
C	-2.1214810	0.8823520	2.0202440
C	-1.7540280	-0.1647280	2.8704020
C	-2.3612520	2.1507420	2.5618330
C	-1.6560660	0.0445820	4.2412750
H	-1.5451440	-1.1509240	2.4580070
C	-2.2602610	2.3562860	3.9350780
H	-2.6311540	2.9879680	1.9210140
C	-1.9096060	1.3052670	4.7769360
H	-1.3788410	-0.7823140	4.8915430
H	-2.4589010	3.3434920	4.3456970
H	-1.8344480	1.4677640	5.8494570
C	-3.2735720	1.7241690	-0.5833380

C	-3.0791100	1.9998720	-1.9417280
C	-4.4313520	2.1841920	0.0539310
C	-4.0325780	2.7192190	-2.6536680
H	-2.1851740	1.6351560	-2.4465260
C	-5.3804490	2.9064820	-0.6630270
H	-4.6085600	1.9729210	1.1067240
C	-5.1842930	3.1717780	-2.0154470
H	-3.8744120	2.9250160	-3.7096300
H	-6.2794620	3.2572060	-0.1618900
H	-5.9314270	3.7316230	-2.5730450
C	1.4208330	-1.5064990	1.9127320
C	2.1429650	-0.6664790	2.7666460
C	0.6590150	-2.5442380	2.4553690
C	2.1353880	-0.8860160	4.1397100
H	2.7298610	0.1547630	2.3567600
C	0.6566470	-2.7654020	3.8299110
H	0.0608500	-3.1764440	1.8000220
C	1.3986560	-1.9415260	4.6721120
H	2.7110980	-0.2347350	4.7932030
H	0.0709890	-3.5836130	4.2428600
H	1.3974880	-2.1176800	5.7452470
C	3.0910720	-1.0888000	-0.4808150
C	3.3219600	-0.7247020	-1.8136690
C	4.1792970	-1.3687510	0.3513920
C	4.6214620	-0.6373030	-2.2997680
H	2.4823690	-0.5014420	-2.4699360
C	5.4789690	-1.2761680	-0.1408220
H	4.0227330	-1.6761900	1.3829000
C	5.7026290	-0.9074950	-1.4634110
H	4.7887600	-0.3588690	-3.3376600
H	6.3172310	-1.5017200	0.5140330
H	6.7182220	-0.8353620	-1.8453620
C	-0.1371710	2.7243590	-0.1177440
H	-0.9117920	3.1902640	0.4907820
H	-0.2176310	2.8896790	-1.1933380
C	2.1438290	1.9640830	-0.3624300
H	1.9845170	1.8348580	-1.4290020
H	3.0005380	1.4632390	0.0734080
C	1.3439240	2.6656400	1.9357540
H	1.3615960	3.7387950	2.1677310
H	0.5421760	2.2172840	2.5361520
H	2.2990140	2.2404390	2.2633450
C	1.1183180	2.4578200	0.4640180
Ni	0.0984720	0.7136930	-0.1016040
N	3.5227510	3.6554370	-0.7954930
H	4.0532530	3.3834580	-1.6248360

C	2.6916420	4.8167250	-1.0919630
H	1.9217190	4.8914240	-0.3064870
H	3.2912610	5.7408220	-1.0300520
C	4.4315330	3.8455180	0.3350170
H	3.8202790	3.9220670	1.2467050
H	4.9632400	4.8073850	0.2327200
C	5.4327710	2.7159000	0.4492480
H	6.0094840	2.6097250	-0.4787300
H	6.1413920	2.9151270	1.2593930
H	4.9553310	1.7488090	0.6586910
C	2.0508230	4.7037140	-2.4575210
H	1.4122360	5.5698370	-2.6579950
H	2.8136890	4.6632450	-3.2451560
H	1.4315830	3.8018760	-2.5433490

8 – Fluorinated Bridge Ground

Lowest Frequency Vibration = 33.3158 cm**-1
Electronic Energy = -2834.62831896
Electronic and Zero-Point Energy = -2833.874781
Enthalpy = -2833.828651
Free Energy = -2833.946673
E large = -4174.34752804

C	-2.3962320	-1.0396790	2.3968700
C	-3.2434570	-2.3147390	2.3630080
H	-3.8606390	-2.3469410	1.4564310
H	-2.6658370	-3.2373450	2.4272900
H	-3.9212400	-2.2972400	3.2243560
C	-3.3812700	0.1228910	2.4760190
H	-4.0141200	-0.0708100	3.3493540
H	-2.8950260	1.0860210	2.6408800
H	-4.0496350	0.2017400	1.6165180
C	-1.5479230	-0.9282360	3.6654740
H	-0.8211170	-1.7310760	3.7914430
H	-1.0161120	0.0318130	3.6714970
H	-2.2145590	-0.9420480	4.5364830
C	2.8493050	-2.1319280	1.3590760
C	2.3259130	-3.0389670	2.4750300
H	1.7907470	-3.9193150	2.1180780
H	3.1928680	-3.3898800	3.0467590
H	1.6803370	-2.4804240	3.1621620
C	3.7132940	-2.9241850	0.3749070
H	4.3249210	-2.2621180	-0.2478280
H	4.3986200	-3.5600820	0.9490960
H	3.1261730	-3.5734200	-0.2788840
C	3.7479450	-1.1134070	2.0541370
H	3.2549220	-0.6242500	2.8980220

H	4.6053560	-1.6681310	2.4517610
H	4.1556710	-0.3519630	1.3867470
P	-1.7286820	0.0188440	-0.2772350
P	1.7911590	0.1464980	-0.0975170
C	-2.3193430	1.6684310	0.2279380
C	-1.5057540	2.4239060	1.0807330
C	-3.4450940	2.2624460	-0.3481620
C	-1.8354900	3.7380130	1.3861790
H	-0.6232970	1.9729840	1.5309650
C	-3.7648690	3.5848750	-0.0477420
H	-4.0826010	1.7008770	-1.0274350
C	-2.9681580	4.3225630	0.8221250
H	-1.2003200	4.3049920	2.0638420
H	-4.6481010	4.0356170	-0.4945300
H	-3.2266090	5.3522630	1.0576830
C	-3.0356130	-0.8171130	-1.2514090
C	-2.6015080	-1.5297450	-2.3759200
C	-4.3938570	-0.8551220	-0.9119660
C	-3.5013100	-2.2554360	-3.1483580
H	-1.5450670	-1.5296620	-2.6376730
C	-5.2937080	-1.5771540	-1.6893270
H	-4.7672860	-0.3153030	-0.0454840
C	-4.8498810	-2.2780490	-2.8069380
H	-3.1467820	-2.8063990	-4.0162110
H	-6.3464540	-1.5907120	-1.4176630
H	-5.5557740	-2.8443350	-3.4099200
C	1.9009910	1.3759930	1.2370470
C	2.2342240	2.6953110	0.9078520
C	1.4428990	1.0856510	2.5246890
C	2.1480420	3.6987800	1.8673620
H	2.5515900	2.9473050	-0.1036410
C	1.3554580	2.0927440	3.4810770
H	1.1300090	0.0716860	2.7706330
C	1.7127480	3.3988810	3.1564360
H	2.4179140	4.7189680	1.6046990
H	1.0007330	1.8536720	4.4814370
H	1.6435130	4.1846310	3.9050280
C	3.3614030	0.1228480	-1.0379620
C	3.3831680	-0.7128010	-2.1620830
C	4.4870190	0.8896480	-0.7322290
C	4.5208460	-0.7936960	-2.9542760
H	2.5089860	-1.3166860	-2.4072480
C	5.6246360	0.8101160	-1.5324360
H	4.4899090	1.5457930	0.1367320
C	5.6448530	-0.0322410	-2.6390670
H	4.5317130	-1.4533770	-3.8186760

H	6.4986730	1.4071210	-1.2830210
H	6.5359220	-0.0936690	-3.2592710
C	-1.0872340	1.3613140	-2.9159550
H	-2.1283440	1.6564510	-2.7918490
H	-0.9000640	0.5107720	-3.5746350
C	1.2382160	1.7409350	-2.6653800
H	1.4770970	0.9100720	-3.3321400
H	2.0837220	2.3443110	-2.3359410
C	-0.3387380	3.6619550	-2.1607680
H	-0.2865390	4.3808040	-2.9886130
H	-1.3424330	3.7305780	-1.7275280
H	0.3998180	3.9726900	-1.4128010
C	-0.0575490	2.2919540	-2.6860640
Ni	0.0680280	0.7089520	-1.3705390
N	-1.4458300	-0.9442150	1.1653620
N	1.6768390	-1.4220830	0.6373480
C	-0.7738380	-2.1690880	0.8606050
C	0.6137570	-2.2144420	0.1056500
F	-1.5688010	-3.0076490	0.1211600
F	-0.5099150	-2.8449130	1.9985240
F	0.3998920	-1.9578300	-1.2245620
F	0.9250910	-3.5253910	0.1241530

8 – Fluorinated Bridge TS1

Lowest Frequency Vibration = -381.3830 cm**-1
Electronic Energy = -3048.25412621
Electronic and Zero-Point Energy = -3047.348166
Enthalpy = -3047.295079
Free Energy = -3047.427842
E large = -4388.03795331

C	-3.8780630	-0.2730900	-1.7114350
C	-4.1194310	0.8554870	-2.7170220
H	-4.1256870	1.8323170	-2.2214060
H	-3.3778600	0.8772920	-3.5186930
H	-5.1056150	0.7132910	-3.1767320
C	-4.8676850	-0.0828220	-0.5628520
H	-5.8625950	0.0050550	-1.0145480
H	-4.8929950	-0.9376550	0.1173080
H	-4.7079740	0.8295850	0.0144110
C	-4.2294570	-1.6322650	-2.3212530
H	-3.7018180	-1.8570270	-3.2481260
H	-4.0495480	-2.4427780	-1.6063290
H	-5.3023330	-1.6248510	-2.5460430
C	0.2031290	-3.9005010	-0.5175170
C	-1.0877390	-4.4420170	0.0979790
H	-1.9664620	-4.2942050	-0.5326060

H	-0.9757080	-5.5200730	0.2692790
H	-1.2683440	-3.9674370	1.0714830
C	0.5401090	-4.5921870	-1.8438470
H	1.4792800	-4.2050080	-2.2565750
H	0.6798440	-5.6604750	-1.6418830
H	-0.2365280	-4.5052870	-2.6042140
C	1.3299960	-4.2862040	0.4361690
H	1.1585510	-3.9797530	1.4686440
H	1.3772490	-5.3808500	0.4358600
H	2.3079800	-3.9331080	0.1032110
P	-1.8700880	0.6520510	0.1943600
P	1.1651080	-1.1485450	-0.0504790
C	-2.5704380	-0.1654630	1.6650630
C	-2.9853450	-1.4992920	1.6210370
C	-2.4776680	0.4797990	2.9044700
C	-3.3419430	-2.1644730	2.7902670
H	-3.0151310	-2.0229280	0.6662100
C	-2.8475890	-0.1834360	4.0703010
H	-2.1087500	1.5028090	2.9654250
C	-3.2831270	-1.5053470	4.0156030
H	-3.6649080	-3.2022640	2.7412760
H	-2.7853200	0.3325460	5.0256580
H	-3.5660800	-2.0250820	4.9281110
C	-2.6443780	2.3070100	0.0077230
C	-2.1783530	3.0743610	-1.0689690
C	-3.5703730	2.8688650	0.8873640
C	-2.6479610	4.3649900	-1.2748690
H	-1.4469950	2.6497180	-1.7581010
C	-4.0349540	4.1675880	0.6845120
H	-3.9500410	2.2925000	1.7293580
C	-3.5793130	4.9154460	-0.3952680
H	-2.2854320	4.9439980	-2.1213400
H	-4.7614550	4.5898720	1.3750150
H	-3.9465300	5.9270600	-0.5516480
C	1.4918800	-1.5764910	1.6943730
C	2.7590910	-1.4421220	2.2696090
C	0.4010220	-1.8604210	2.5262430
C	2.9370040	-1.6339100	3.6380730
H	3.6202090	-1.1709020	1.6631390
C	0.5822750	-2.0530620	3.8901600
H	-0.5952570	-1.9566890	2.0990770
C	1.8538820	-1.9474670	4.4510200
H	3.9318510	-1.5345410	4.0665550
H	-0.2772200	-2.2907390	4.5138470
H	1.9963840	-2.1030790	5.5178040
C	2.7477920	-1.2993050	-0.9913720

C	2.8305320	-0.4936190	-2.1373040
C	3.8543840	-2.0918510	-0.6598150
C	3.9779480	-0.4760940	-2.9214640
H	1.9819040	0.1261960	-2.4213610
C	5.0069640	-2.0687580	-1.4405460
H	3.8426930	-2.7273680	0.2213570
C	5.0735220	-1.2597470	-2.5703070
H	4.0151740	0.1532450	-3.8077630
H	5.8563230	-2.6870730	-1.1594420
H	5.9758370	-1.2423810	-3.1771460
C	0.2946400	2.6788750	1.0957260
H	-0.2477890	2.8702830	2.0239570
H	-0.0045600	3.3092480	0.2571280
C	2.3530480	2.0254290	-0.0358640
H	1.8682520	2.2519420	-0.9849560
H	3.1583900	1.2994240	-0.0776990
C	2.2394130	1.8553150	2.4986810
H	2.6014060	2.7688260	2.9914140
H	1.5043570	1.3962480	3.1743160
H	3.0900890	1.1714280	2.4019040
C	1.6213050	2.1797610	1.1677720
N	3.7157550	3.5621300	-0.2815280
H	3.9542820	3.5499940	-1.2753000
C	3.0546840	4.8240290	0.0541310
H	2.5405570	4.6852270	1.0177470
H	3.8115340	5.6099990	0.2077550
C	4.9195430	3.2888160	0.5125340
H	4.5996970	3.1013060	1.5472230
H	5.5530530	4.1902220	0.5357630
C	5.7109980	2.1194630	-0.0349090
H	5.9660140	2.2796660	-1.0906660
H	6.6489150	2.0099040	0.5188910
H	5.1722160	1.1656470	0.0382280
C	2.0781910	5.2445390	-1.0221030
H	1.5823010	6.1792920	-0.7418920
H	2.5929800	5.4127760	-1.9763850
H	1.2981110	4.4902490	-1.1874800
N	-2.4210540	-0.2563380	-1.1892060
N	0.0539070	-2.3579060	-0.6743440
C	-1.3631670	-0.5872070	-2.0890510
C	-0.6129980	-1.9668200	-1.8711270
Ni	0.3061950	0.8410030	0.3886390
F	-1.8292780	-0.7150740	-3.3494830
F	-0.4350230	0.4173890	-2.1983980
F	0.2402140	-2.0258360	-2.9495660
F	-1.6007720	-2.8516250	-2.1453380