Supporting Information

The optimized geometries (in Cartesian and internal coordinates, in Å), absolute energies (in hartrees) and symmetry point groups of all the structures reported in the paper. The structure labels correspond to those of Figures 1, 3, 5, 7, and 9.

R1-Cr

Coordinates (Angstroms)

ATOM		X	Y	Z
1	Cr	0.000000	0.000000	0.148813
2	Cl	2.302956	0.000000	0.353783
3	Cl	0.000000	-1.886461	-0.814677
4	Cl	0.000000	1.886461	-0.814677
5	Cl	-2.302956	0.000000	0.353783
6	C	0.000000	0.000000	1.904818
7	H	0.000000	-0.935480	2.469384
8	H	0.000000	0.935480	2.469384

Point Group: C_{2v} Number of degrees of freedom: 7

Energy is -1966.378887383

Distance Matrix (Angstroms)

	Cr(1)	Cl(2)	Cl(3)	Cl(4)	Cl(5)	C (6)
Cl(2)	2.312059					
Cl(3)	2.118266	3.198068				
Cl(4)	2.118266	3.198068	3.772922			
Cl(5)	2.312059	4.605912	3.198068	3.198068		
C (6)	1.756005	2.776565	3.309742	3.309742	2.776565	
H (7)	2.502033	3.264122	3.418980	4.329944	3.264122	1.092638
H (8)	2.502033	3.264122	4.329944	3.418980	3.264122	1.092638

	H (7)
H (8)	1.870961

R2-Cr

Coordinates (Angstroms)

ATOM		X	Y	Z
1	Cr	-0.402782	-0.019828	0.000000
2	Cl	2.707349	-0.203836	0.000000
3	Cl	-1.289703	-0.613850	-1.821759
4	Cl	-0.132923	2.088829	0.000000
5	Cl	-1.289703	-0.613850	1.821759
6	C	1.227891	-1.183983	0.000000
7	H	1.192046	-1.797115	0.901233
8	H	1.192046	-1.797115	-0.901233

Point Group: C_s Number of degrees of freedom: 11

Energy is -1966.434393933

Distance Matrix (Angstroms)

	Cr(1)	Cl(2)	Cl(3)	Cl(4)	Cl(5)	C (6)
Cl(2)	3.115570					
Cl(3)	2.111468	4.411728				
Cl(4)	2.125855	3.650131	3.458529			
Cl(5)	2.111468	4.411728	3.643518	3.458529		
C (6)	2.003585	1.774679	3.159452	3.544448	3.159452	
H (7)	2.552342	2.376321	3.869610	4.203371	2.899408	1.090613
H (8)	2.552342	2.376321	2.899408	4.203371	3.869610	1.090613

	H (7)
H (8)	1.802465

R3-Cr

Coordinates (Angstroms)

ATOM	X	Y	Z
1 Cr	0.000000	0.000000	0.566060
2 Cl	1.893166	0.000000	1.695274
3 Cl	-1.893166	0.000000	1.695274
4 Cl	0.000000	1.464207	-1.462672
5 Cl	0.000000	-1.464207	-1.462672
6 C	0.000000	0.000000	-2.537648
7 H	-0.910101	0.000000	-3.134009
8 H	0.910101	0.000000	-3.134009

Point Group: C_{2v} Number of degrees of freedom: 7

Energy is -1966.404774410

Distance Matrix (Angstroms)

	Cr(1)	Cl(2)	Cl(3)	Cl(4)	Cl(5)	C (6)
Cl(2)	2.204359					
Cl(3)	2.204359	3.786332				
Cl(4)	2.501931	3.962399	3.962399			
Cl(5)	2.501931	3.962399	3.962399	2.928414		
C (6)	3.103708	4.636993	4.636993	1.816446	1.816446	
H (7)	3.810354	5.583930	4.928325	2.401157	2.401157	1.088086
H (8)	3.810354	4.928325	5.583930	2.401157	2.401157	1.088086

	H (7)
H (8)	1.820202

Ethylene

Coordinates (Angstroms)

ATOM	X	Y	Z
1 H	1.240641	-0.922990	0.000000
2 C	0.665417	0.000000	0.000000
3 C	-0.665417	0.000000	0.000000
4 H	1.240641	0.922990	0.000000
5 H	-1.240641	-0.922990	0.000000
6 H	-1.240641	0.922990	0.000000

Point Group: D_{2h} Number of degrees of freedom: 3

Energy is -78.587447729

Distance Matrix (Angstroms)

	H (1)	C (2)	C (3)	H (4)	H (5)
C (2)	1.087562				
C (3)	2.117774	1.330835			
H (4)	1.845980	1.087562	2.117774		
H (5)	2.481281	2.117774	1.087562	3.092636	
H (6)	3.092636	2.117774	1.087562	2.481281	1.845980

p1-Cr

Coordinates (Angstroms)

ATOM	X	Y	Z
1 Cr	-0.295118	0.000336	-0.077082
2 C	1.365239	0.000524	-1.324347
3 H	1.421109	0.922501	-1.891751
4 H	1.421670	-0.921266	-1.892034
5 Cl	2.510679	0.000356	0.018981
6 Cl	-2.345301	0.000176	-0.623082
7 Cl	-0.053191	2.266403	-0.310740
8 Cl	-0.052787	-2.266198	-0.312265
9 C	-0.308282	-0.683017	2.134758
10 H	0.606025	-1.255280	2.244785
11 H	-1.234092	-1.248992	2.164541
12 C	-0.308847	0.679973	2.135165
13 H	0.605123	1.252885	2.245826
14 H	-1.235473	1.244656	2.165950

Point Group: C_1 Number of degrees of freedom: 36

Energy is -2045.018131456

Distance Matrix (Angstroms)

	Cr(1)	C (2)	H (3)	H (4)	Cl(5)	Cl(6)
C (2)	2.076645					
H (3)	2.662489	1.084024				
H (4)	2.662848	1.084043	1.843766			
Cl(5)	2.807441	1.765379	2.385038	2.384807		
Cl(6)	2.121642	3.776225	4.079957	4.080363	4.898243	
Cl(7)	2.290891	2.858942	2.545433	3.851874	3.437603	3.238381
Cl(8)	2.291552	2.858870	3.851616	2.545297	3.437783	3.238622
C (9)	2.315033	3.902987	4.667039	4.389140	3.590272	3.495980
H (10)	2.789211	3.859036	4.745316	4.229671	3.187246	4.302459
H (11)	2.732649	4.526605	5.312154	4.859658	4.493063	3.250546
C (12)	2.314331	3.902875	4.389489	4.666581	3.590242	3.495310
H (13)	2.788407	3.859057	4.230192	4.745057	3.187289	4.301733
H (14)	2.731994	4.527001	4.860673	5.312142	4.493485	3.249483

	Cl(7)	Cl(8)	C (9)	H (10)	H (11)	C (12)
Cl(8)	4.532601					
C (9)	3.839871	2.925689				
H (10)	4.400855	2.827453	1.084227			
H (11)	4.458649	2.926560	1.085513	1.841876		
C (12)	2.926528	3.838671	1.362990	2.143411	2.139591	
H (13)	2.827830	4.400070	2.143447	2.508166	3.106237	1.084350
H (14)	2.928438	4.457172	2.139294	3.105963	2.493648	1.085564

	H (13)
H (14)	1.842347

TS1-Cr

Coordinates (Angstroms)

ATOM	X	Y	Z
1 Cr	0.148630	0.046957	0.184932
2 Cl	2.086776	-0.955537	-0.229401
3 Cl	1.029415	1.939211	0.718756
4 Cl	-2.169727	0.485889	0.535502
5 Cl	-0.426995	0.865871	-1.895889
6 C	-0.185691	-0.706972	1.807046
7 H	0.768495	-0.895714	2.315671
8 H	-1.081106	-0.869375	2.396735
9 C	-0.714614	-1.934135	-0.965707
10 H	0.105301	-2.081482	-1.656783
11 H	-1.652055	-1.575011	-1.371542
12 C	-0.646044	-2.377675	0.339615
13 H	-1.567484	-2.456056	0.908551
14 H	0.224217	-2.929402	0.683392

Point Group: C_1 Number of degrees of freedom: 36

Energy is -2044.954388231

Distance Matrix (Angstroms)

	Cr(1)	Cl(2)	Cl(3)	Cl(4)	Cl(5)	C (6)
Cl(2)	2.221053					
Cl(3)	2.154385	3.224373				
Cl(4)	2.385444	4.558575	3.518556			
Cl(5)	2.309065	3.523316	3.179553	3.015488		
C (6)	1.819735	3.061537	3.108560	2.641238	4.030359	
H (7)	2.410998	2.866851	3.264202	3.702834	4.719070	1.097632
H (8)	2.691466	4.115761	3.893337	2.546767	4.676063	1.084378
C (9)	2.448242	3.057382	4.569668	3.198046	2.964456	3.077962
H (10)	2.814968	2.689129	4.760583	4.071027	3.004564	3.737923
H (11)	2.880253	3.958168	4.889722	2.855190	2.780939	3.606540
C (12)	2.556223	3.132820	4.646118	3.249612	3.945384	2.270799
H (13)	3.119895	4.110974	5.108647	3.026037	4.494530	2.403318
H (14)	3.018756	2.863295	4.934874	4.173374	4.634746	2.523849

	H (7)	H (8)	C (9)	H (10)	H (11)	C (12)
H (8)	1.851565					
C (9)	3.747716	3.545990				
H (10)	4.198365	4.394061	1.082385			
H (11)	4.462740	3.876056	1.082805	1.850993		
C (12)	2.846389	2.587661	1.380324	2.153567	2.141117	
H (13)	3.141887	2.229083	2.124295	3.085361	2.445856	1.085764
H (14)	2.663918	2.980456	2.142776	2.491893	3.094758	1.086250

	H (13)
H (14)	1.866801

pdt1-Cr

Coordinates (Angstroms)

ATOM	X	Y	Z
1 Cr	0.282480	0.073847	0.000000
2 Cl	0.433170	-2.139825	0.000000
3 Cl	1.105910	0.221197	2.039102
4 Cl	-0.384484	2.182519	0.000000
5 Cl	1.105910	0.221197	-2.039102
6 C	-1.559153	-0.282310	1.194356
7 H	-1.326461	-1.154965	1.794201
8 H	-1.682019	0.623525	1.777880
9 C	-1.559153	-0.282310	-1.194356
10 H	-1.326461	-1.154965	-1.794201
11 H	-1.682019	0.623525	-1.777880
12 C	-2.464029	-0.475182	0.000000
13 H	-3.270255	0.267405	0.000000
14 H	-2.893732	-1.483042	0.000000

Point Group: C_s Number of degrees of freedom: 21

Energy is -2044.984558072

Distance Matrix (Angstroms)

	Cr(1)	Cl(2)	Cl(3)	Cl(4)	Cl(5)	C (6)
Cl(2)	2.218796					
Cl(3)	2.204016	3.191386				
Cl(4)	2.211637	4.399002	3.197811			
Cl(5)	2.204016	3.191386	4.078205	3.197811		
C (6)	2.223724	2.974257	2.840718	2.980220	4.220348	
H (7)	2.705148	2.699150	2.805392	3.904519	4.743887	1.084199
H (8)	2.705967	3.907811	2.828896	2.697205	4.743814	1.084497
C (9)	2.223724	2.974257	4.220348	2.980220	2.840718	2.388711
H (10)	2.705148	2.699150	4.743887	3.904519	2.805392	3.122041
H (11)	2.705967	3.907811	4.743814	2.697205	2.828896	3.109633
C (12)	2.800848	3.341378	4.169814	3.374593	4.169814	1.510790
H (13)	3.558005	4.417027	4.828136	3.463428	4.828136	2.157902
H (14)	3.537263	3.391113	4.802032	4.442146	4.802032	2.156234

	H (7)	H (8)	C (9)	H (10)	H (11)	C (12)
H (8)	1.813757					
C (9)	3.122041	3.109633				
H (10)	3.588402	4.006146	1.084199			
H (11)	4.006146	3.555759	1.084497	1.813757		
C (12)	2.230543	2.231491	1.510790	2.230543	2.231491	
H (13)	3.003437	2.410430	2.157902	3.003437	2.410430	1.096101
H (14)	2.404814	3.011101	2.156234	2.404814	3.011101	1.095640

	H (13)
H (14)	1.790485

TS2-Cr

Coordinates (Angstroms)

ATOM	X	Y	Z
1 Cl	-1.374037	-1.598068	-0.135754
2 C	-3.222890	0.550796	0.176061
3 H	-3.392639	0.042790	1.119607
4 H	-3.490505	0.006794	-0.721529
5 C	-2.738502	1.823805	0.122863
6 H	-2.747743	2.362202	-0.820278
7 H	-2.702912	2.430471	1.022593
8 C	-0.603836	1.458369	0.192642
9 H	-0.525317	2.184243	-0.611901
10 H	-0.563057	1.868842	1.199270
11 Cr	0.350939	-0.150478	-0.025261
12 Cl	0.926971	-0.534302	-2.034352
13 Cl	1.033826	-1.042484	1.791646
14 Cl	2.024475	1.511226	0.170760

Point Group: C_1 Number of degrees of freedom: 36

Energy is -2044.971282245

Distance Matrix (Angstroms)

	Cl(1)	C (2)	H (3)	H (4)	C (5)	H (6)
C (2)	2.851859					
H (3)	2.888442	1.084972				
H (4)	2.719954	1.083154	1.844086			
C (5)	3.692947	1.363090	2.143223	2.140101		
H (6)	4.247279	2.121238	3.091718	2.471719	1.086036	
H (7)	4.397363	2.126070	2.487198	3.088118	1.085737	1.844680
C (8)	3.169047	2.771897	3.261986	3.357921	2.166844	2.537570
H (9)	3.905498	3.250528	3.975610	3.680440	2.359657	2.239256
H (10)	3.802557	3.139891	3.368582	3.965683	2.427600	3.015764
Cr(11)	2.254610	3.647543	3.919497	3.907201	3.669384	4.067855
Cl(12)	3.167162	4.825424	5.379547	4.640085	4.863121	4.833967
Cl(13)	3.133903	4.823722	4.606848	5.280777	5.023038	5.719642
Cl(14)	4.616443	5.334538	5.692252	5.785715	4.773463	4.947765

	H (7)	C (8)	H (9)	H (10)	Cr(11)	Cl(12)
C (8)	2.457625					
H (9)	2.733883	1.086437				
H (10)	2.219374	1.087865	1.838815			
Cr(11)	4.133437	1.883472	2.561814	2.532295		
Cl(12)	5.595609	3.357619	3.394554	4.295532	2.124989	
Cl(13)	5.159076	3.390135	4.315058	3.372946	2.136155	3.861078
Cl(14)	4.890687	2.628933	2.750809	2.807320	2.366518	3.201752

	Cl(13)
Cl(14)	3.182780

pdt2-Cr

Coordinates (Angstroms)

ATOM	X	Y	Z
1 Cl	-2.743254	-0.445581	0.639108
2 C	-2.672509	0.150576	-1.075170
3 H	-3.682551	0.486159	-1.315604
4 H	-2.429556	-0.715390	-1.695730
5 C	-1.672911	1.287154	-1.261681
6 H	-1.923944	1.767042	-2.222763
7 H	-1.829612	2.050576	-0.491156
8 C	-0.199285	0.920061	-1.331432
9 H	0.013726	0.107672	-2.056132
10 H	0.422414	1.785875	-1.586048
11 Cr	0.808887	-0.028756	0.042193
12 Cl	0.432209	-2.120878	0.117239
13 Cl	2.830651	0.174555	-0.651698
14 Cl	0.477463	1.283908	1.658286

Point Group: C_1 Number of degrees of freedom: 36

Energy is -2045.069618158

Distance Matrix (Angstroms)

	Cl(1)	C (2)	H (3)	H (4)	C (5)	H (6)
C (2)	1.816359					
H (3)	2.360364	1.091151				
H (4)	2.371218	1.092711	1.777136			
C (5)	2.785858	1.525055	2.164060	2.184283		
H (6)	3.709080	2.119029	2.357180	2.587639	1.103172	
H (7)	2.888432	2.159063	2.561347	3.075956	1.095937	1.757200
C (8)	3.495681	2.602809	3.510223	2.789538	1.520262	2.118088
H (9)	3.895042	2.860068	3.788681	2.603257	2.206144	2.556529
H (10)	4.466786	3.537478	4.314295	3.795009	2.178147	2.431287
Cr(11)	3.625984	3.660708	4.720357	3.738898	3.096938	3.977849
Cl(12)	3.628021	4.027482	5.077492	3.667690	4.236464	5.113021
Cl(13)	5.754926	5.519482	6.554363	5.436155	4.678892	5.254564
Cl(14)	3.795111	4.321869	5.175533	4.867995	3.626338	4.589413

	H (7)	C (8)	H (9)	H (10)	Cr(11)	Cl(12)
C (8)	2.154552					
H (9)	3.101923	1.109297				
H (10)	2.518031	1.095889	1.790075			
Cr(11)	3.401435	1.950259	2.248080	2.468484		
Cl(12)	4.784037	3.427060	3.140876	4.261925	2.127086	
Cl(13)	5.026260	3.193483	3.148329	3.044498	2.147172	3.407756
Cl(14)	3.245069	3.086873	3.923708	3.283399	2.108242	3.737572

	Cl(13)
Cl(14)	3.479107

TS3-Cr

Coordinates (Angstroms)

ATOM	X	Y	Z
1 Cr	0.585199	0.003313	-0.222090
2 Cl	1.487610	1.834062	0.368931
3 Cl	1.491166	-1.835187	0.338659
4 Cl	-0.868477	0.014201	-1.899458
5 Cl	-1.515113	-0.009670	1.333890
6 C	-2.919336	-0.005837	0.450555
7 H	-3.305814	-0.956225	0.109900
8 H	-3.308727	0.947810	0.122669

Point Group: C_1 Number of degrees of freedom: 18

Energy is -1966.362913047

Distance Matrix (Angstroms)

	Cr(1)	Cl(2)	Cl(3)	Cl(4)	Cl(5)	C (6)
Cl(2)	2.124922					
Cl(3)	2.124922	3.669375				
Cl(4)	2.219652	3.742810	3.741299			
Cl(5)	2.613915	3.653332	3.655230	3.297460		
C (6)	3.568515	4.776302	4.776146	3.119132	1.658957	
H (7)	4.021307	5.552451	4.882204	3.304521	2.366585	1.081040
H (8)	4.021640	4.883742	5.552539	3.303852	2.366616	1.081007

	H (7)
H (8)	1.904080

R1-Mo

Coordinates (Angstroms)

ATOM	X	Y	Z
1 Mo	0.000000	0.000000	0.169456
2 Cl	2.380303	0.000000	-0.054973
3 Cl	0.000000	-2.112168	-0.664127
4 Cl	0.000000	2.112168	-0.664127
5 Cl	-2.380303	0.000000	-0.054973
6 C	0.000000	0.000000	2.025767
7 H	0.000000	-0.937257	2.588838
8 H	0.000000	0.937257	2.588838

Point Group: C_{2v} Number of degrees of freedom: 7

Energy is -1947.702885268

Distance Matrix (Angstroms)

	Mo(1)	Cl(2)	Cl(3)	Cl(4)	Cl(5)	C (6)
Cl(2)	2.390860					
Cl(3)	2.270708	3.240088				
Cl(4)	2.270708	3.240088	4.224337			
Cl(5)	2.390860	4.760607	3.240088	3.240088		
C (6)	1.856312	3.161539	3.420057	3.420057	3.161539	
H (7)	2.594583	3.678863	3.458642	4.458787	3.678863	1.093389
H (8)	2.594583	3.678863	4.458787	3.458642	3.678863	1.093389

	H (7)
H (8)	1.874515

R4-Mo

Coordinates (Angstroms)

ATOM	X	Y	Z
1 Mo	0.052746	0.205328	0.000000
2 Cl	-2.234299	-0.010639	0.000000
3 Cl	0.926900	0.314083	-2.094351
4 Cl	0.271240	-2.209161	0.000000
5 Cl	0.926900	0.314083	2.094351
6 C	-0.022762	2.152716	0.000000
7 H	-0.055669	2.758734	0.909874
8 H	-0.055669	2.758734	-0.909874

Point Group: C_s Number of degrees of freedom: 11

Energy is -1947.682401258

Distance Matrix (Angstroms)

	Mo(1)	Cl(2)	Cl(3)	Cl(4)	Cl(5)	C (6)
Cl(2)	2.297219					
Cl(3)	2.272065	3.805907				
Cl(4)	2.424354	3.333350	3.344093			
Cl(5)	2.272065	3.805907	4.188702	3.344093		
C (6)	1.948852	3.093703	2.944271	4.371774	2.944271	
H (7)	2.712842	3.639193	3.995889	5.061099	2.888727	1.093715
H (8)	2.712842	3.639193	2.888727	5.061099	3.995889	1.093715

	H (7)
H (8)	1.819749

R2-Mo

Coordinates (Angstroms)

ATOM		X	Y	Z
1	Mo	-0.466268	-0.053487	0.000000
2	Cl	2.887555	-0.354043	0.000000
3	Cl	-1.286302	-0.496932	-2.047443
4	Cl	0.234652	2.117551	0.000000
5	Cl	-1.286302	-0.496932	2.047443
6	C	1.286220	-1.194079	0.000000
7	H	1.261350	-1.836521	0.888122
8	H	1.261350	-1.836521	-0.888122

Point Group: C_s Number of degrees of freedom: 11

Energy is -1947.690641634

Distance Matrix (Angstroms)

	Mo(1)	Cl(2)	Cl(3)	Cl(4)	Cl(5)	C (6)
Cl(2)	3.367264					
Cl(3)	2.249693	4.651185				
Cl(4)	2.281380	3.625834	3.652512			
Cl(5)	2.249693	4.651185	4.094885	3.652512		
C (6)	2.090972	1.808296	3.360939	3.474577	3.360939	
H (7)	2.636785	2.372982	4.111274	4.180616	3.103072	1.096408
H (8)	2.636785	2.372982	3.103072	4.180616	4.111274	1.096408

	H (7)
H (8)	1.776244

p1-Mo

Coordinates (Angstroms)

ATOM		X	Y	Z
1	Mo	-0.258101	-0.000148	-0.025783
2	C	1.446856	0.000328	-1.365347
3	H	1.569013	0.917503	-1.934464
4	H	1.569911	-0.917030	-1.933956
5	Cl	2.564460	0.001210	0.040996
6	Cl	-2.455698	-0.001297	-0.505533
7	Cl	-0.010113	2.369053	-0.372149
8	Cl	-0.007559	-2.369133	-0.371608
9	C	-0.156724	-0.706211	2.059441
10	H	0.754399	-1.270401	2.233634
11	H	-1.072666	-1.261517	2.252400
12	C	-0.157880	0.707020	2.059299
13	H	0.752254	1.272835	2.233498
14	H	-1.074684	1.260862	2.252429

Point Group: C_1 Number of degrees of freedom: 36

Energy is -2026.314240052

Distance Matrix (Angstroms)

	Mo(1)	C (2)	H (3)	H (4)	Cl(5)	Cl(6)
C (2)	2.168250					
H (3)	2.797050	1.086290				
H (4)	2.797038	1.086280	1.834533			
Cl(5)	2.823352	1.796341	2.394358	2.394312		
Cl(6)	2.249354	3.996150	4.368562	4.368580	5.049821	
Cl(7)	2.407193	2.952974	2.653575	3.966618	3.522187	3.408407
Cl(8)	2.407168	2.952488	3.966116	2.652913	3.521939	3.408515
C (9)	2.203852	3.847056	4.643909	4.355793	3.461128	3.515861
H (10)	2.782745	3.879035	4.777401	4.261307	3.114639	4.406630
H (11)	2.728495	4.585666	5.408920	4.962606	4.439985	3.332736
C (12)	2.204019	3.847439	4.356214	4.644231	3.461625	3.515686
H (13)	2.783102	3.879875	4.262072	4.778257	3.115796	4.406434
H (14)	2.728957	4.586438	4.963577	5.409520	4.440780	3.332657

	Cl(7)	Cl(8)	C (9)	H (10)	H (11)	C (12)
Cl(8)	4.738187					
C (9)	3.923184	2.949163				
H (10)	4.540948	2.928323	1.085726			
H (11)	4.604162	3.040836	1.088369	1.827183		
C (12)	2.948920	3.923598	1.413231	2.184683	2.179279	
H (13)	2.927848	4.541786	2.184756	2.543237	3.123080	1.085742
H (14)	3.041350	4.604475	2.179282	3.123010	2.522380	1.088379

	H (13)
H (14)	1.827075

TS1-Mo

Coordinates (Angstroms)

ATOM	X	Y	Z
1 Mo	0.087131	0.015259	0.116380
2 Cl	2.276674	-0.645336	-0.472636
3 Cl	0.984888	1.971515	0.947232
4 Cl	-2.277279	-0.086245	0.719370
5 Cl	-0.899634	1.334141	-1.631789
6 C	0.035254	-1.237652	1.635824
7 H	1.032541	-1.516508	1.991886
8 H	-0.789774	-1.577219	2.252394
9 C	-0.382071	-1.710564	-1.316903
10 H	0.413033	-1.755226	-2.050360
11 H	-1.377118	-1.504931	-1.695118
12 C	-0.254681	-2.431078	-0.095865
13 H	-1.165892	-2.800635	0.364345
14 H	0.658743	-2.992002	0.077366

Point Group: C_1 Number of degrees of freedom:36

Energy is -2026.281920802

Distance Matrix (Angstroms)

	Mo(1)	Cl(2)	Cl(3)	Cl(4)	Cl(5)	C (6)
Cl(2)	2.361657					
Cl(3)	2.307211	3.245404				
Cl(4)	2.442198	4.740458	3.863681			
Cl(5)	2.401926	3.918022	3.257149	3.073003		
C (6)	1.970072	3.133753	3.416828	2.741064	4.262091	
H (7)	2.599544	2.894940	3.641412	3.823592	4.999052	1.095045
H (8)	2.804907	4.206816	4.176887	2.604963	4.855405	1.084498
C (9)	2.291924	2.986038	4.533497	3.221278	3.104392	3.019337
H (10)	2.817018	2.682206	4.816761	4.206504	3.382674	3.741463
H (11)	2.781462	3.947603	4.964551	2.941549	2.879641	3.627865
C (12)	2.479203	3.120672	4.691206	3.202147	4.117268	2.122987
H (13)	3.092056	4.146940	5.266785	2.954511	4.599110	2.345703
H (14)	3.061352	2.902937	5.049707	4.180408	4.905635	2.428018

	H (7)	H (8)	C (9)	H (10)	H (11)	C (12)
H (8)	1.841843					
C (9)	3.603729	3.594980				
H (10)	4.096404	4.471255	1.082656			
H (11)	4.404610	3.991622	1.084182	1.842141		
C (12)	2.617648	2.555331	1.423482	2.173170	2.162226	
H (13)	3.021751	2.280995	2.151563	3.068661	2.442305	1.085666
H (14)	2.445852	2.971625	2.160870	2.473298	3.081852	1.085813

	H (13)
H (14)	1.856952

pdt1-Mo

Coordinates (Angstroms)

ATOM	X	Y	Z
1 Mo	0.178978	0.092463	0.000000
2 Cl	0.886199	-2.099659	0.000000
3 Cl	0.925873	0.312974	2.222527
4 Cl	-0.420076	2.318505	0.000000
5 Cl	0.925873	0.312974	-2.222527
6 C	-1.659595	-0.533557	1.144978
7 H	-1.356254	-1.153536	1.987068
8 H	-2.076580	0.413707	1.490654
9 C	-1.659595	-0.533557	-1.144978
10 H	-1.356254	-1.153536	-1.987068
11 H	-2.076580	0.413707	-1.490654
12 C	-2.401338	-1.184799	0.000000
13 H	-3.482094	-0.985144	0.000000
14 H	-2.249928	-2.268658	0.000000

Point Group: C_s Number of degrees of freedom: 21

Energy is -2026.309727837

Distance Matrix (Angstroms)

	Mo(1)	Cl(2)	Cl(3)	Cl(4)	Cl(5)	C (6)
Cl(2)	2.303381					
Cl(3)	2.355017	3.280549				
Cl(4)	2.305239	4.607226	3.282280			
Cl(5)	2.355017	3.280549	4.445054	3.282280		
C (6)	2.254601	3.200737	2.926153	3.313855	4.329128	
H (7)	2.803193	3.142004	2.722903	4.108520	5.007939	1.088809
H (8)	2.722643	4.161384	3.092008	2.931605	4.776252	1.091181
C (9)	2.254601	3.200737	4.329128	3.313855	2.926153	2.289956
H (10)	2.803193	3.142004	5.007939	4.108520	2.722903	3.207196
H (11)	2.722643	4.161384	4.776252	2.931605	3.092008	2.831562
C (12)	2.879137	3.412458	4.272386	4.024741	4.272386	1.511712
H (13)	3.816371	4.508230	5.104402	4.504448	5.104402	2.199184
H (14)	3.387399	3.140677	4.657270	4.938665	4.657270	2.161028

	H (7)	H (8)	C (9)	H (10)	H (11)	C (12)
H (8)	1.794867					
C (9)	3.207196	2.831562				
H (10)	3.974137	3.881967	1.088809			
H (11)	3.881967	2.981308	1.091181	1.794867		
C (12)	2.245355	2.209692	1.511712	2.245355	2.209692	
H (13)	2.914789	2.480787	2.199184	2.914789	2.480787	1.099044
H (14)	2.447568	3.073626	2.161028	2.447568	3.073626	1.094383

	H (13)
H (14)	1.779225

TS2-Mo

Coordinates (Angstroms)

ATOM	X	Y	Z
1 Cl	-1.601945	1.408828	0.000000
2 C	-3.445015	-0.556521	0.000000
3 H	-3.759533	-0.079446	-0.921432
4 H	-3.759533	-0.079446	0.921432
5 C	-2.805006	-1.771850	0.000000
6 H	-2.796596	-2.349804	0.919568
7 H	-2.796596	-2.349804	-0.919568
8 C	-0.673541	-1.592274	0.000000
9 H	-0.565165	-2.176876	0.916110
10 H	-0.565165	-2.176876	-0.916110
11 Mo	0.348012	0.054657	0.000000
12 Cl	0.799235	0.766345	2.113420
13 Cl	0.799235	0.766345	-2.113420
14 Cl	2.421821	-1.150256	0.000000

Point Group: C_s Number of degrees of freedom: 21

Energy is -2026.279298220

Distance Matrix (Angstroms)

	Cl(1)	C (2)	H (3)	H (4)	C (5)	H (6)
C (2)	2.694347					
H (3)	2.778342	1.084232				
H (4)	2.778342	1.084232	1.842864			
C (5)	3.400599	1.373549	2.150439	2.150439		
H (6)	4.049705	2.117054	3.077507	2.466126	1.086143	
H (7)	4.049705	2.117054	2.466126	3.077507	1.086143	1.839135
C (8)	3.141424	2.958691	3.558235	3.558235	2.139017	2.434506
H (9)	3.843364	3.429044	4.240255	3.821417	2.453608	2.238124
H (10)	3.843364	3.429044	3.821417	4.240255	2.453608	2.894633
Mo(11)	2.374049	3.841952	4.211763	4.211763	3.643852	4.063939
Cl(12)	3.262667	4.922416	5.541485	4.787334	4.888715	4.905678
Cl(13)	3.262667	4.922416	4.787334	5.541485	4.888715	5.642641
Cl(14)	4.768606	5.896803	6.340726	6.340726	5.263659	5.432899

	H (7)	C (8)	H (9)	H (10)	Mo(11)	Cl(12)
C (8)	2.434506					
H (9)	2.894633	1.092136				
H (10)	2.238124	1.092136	1.832219			
Mo(11)	4.063939	1.938028	2.579320	2.579320		
Cl(12)	5.642641	3.492663	3.457990	4.438715	2.275224	
Cl(13)	4.905678	3.492663	4.438715	3.457990	2.275224	4.226840
Cl(14)	5.432899	3.126762	3.288660	3.288660	2.398437	3.282177

	Cl(13)
Cl(14)	3.282177

pdt2-Mo

Coordinates (Angstroms)

ATOM		X	Y	Z
1	Cl	-2.146163	0.315611	0.908031
2	C	-2.860920	0.187431	-0.786846
3	H	-2.827875	1.202358	-1.188065
4	H	-3.895760	-0.124059	-0.640772
5	C	-2.044261	-0.797324	-1.602448
6	H	-2.171601	-1.806384	-1.191953
7	H	-2.476352	-0.811962	-2.615613
8	C	-0.553862	-0.449959	-1.670622
9	H	0.006041	-1.183138	-2.262952
10	H	-0.388334	0.542974	-2.139760
11	Mo	0.474500	0.031454	0.084164
12	Cl	0.397483	-1.923519	1.247300
13	Cl	2.589998	-0.240744	-0.822625
14	Cl	0.615512	2.277892	0.478261

Point Group: C_1 Number of degrees of freedom: 36

Energy is -2026.332828092

Distance Matrix (Angstroms)

	Cl(1)	C (2)	H (3)	H (4)	C (5)	H (6)
C (2)	1.843887					
H (3)	2.375852	1.091854				
H (4)	2.377644	1.090531	1.788656			
C (5)	2.748002	1.517195	2.187348	2.192294		
H (6)	2.985539	2.148156	3.079488	2.471183	1.096779	
H (7)	3.714366	2.119214	2.493782	2.527435	1.101553	1.763110
C (8)	3.125855	2.551439	2.852043	3.512134	1.531861	2.164738
H (9)	4.115017	3.503829	3.857079	4.356279	2.188346	2.505514
H (10)	3.525718	2.840857	2.700347	3.872200	2.197088	3.098042
Mo(11)	2.761770	3.450799	3.727635	4.432706	3.142561	3.465252
Cl(12)	3.405722	4.383041	5.109310	5.023426	3.918098	3.544554
Cl(13)	5.073058	5.467826	5.618669	6.489356	4.732257	5.025978
Cl(14)	3.414981	4.249247	3.973705	5.231938	4.567351	5.219092

	H (7)	C (8)	H (9)	H (10)	Mo(11)	Cl(12)
C (8)	2.172561					
H (9)	2.534643	1.096311				
H (10)	2.534187	1.110588	1.774872			
Mo(11)	4.087502	2.090110	2.683960	2.439667		
Cl(12)	4.941313	3.404512	3.608775	4.263011	2.276122	
Cl(13)	5.404534	3.262932	3.104751	3.349555	2.317691	3.453033
Cl(14)	5.355266	3.664192	4.456954	3.297223	2.285100	4.276776

	Cl(13)
Cl(14)	3.454625

R1-W

Coordinates (Angstroms)

ATOM		X	Y	Z
1	W	0.000000	0.000000	0.127888
2	Cl	2.349686	0.000000	-0.221974
3	Cl	0.000000	-2.171449	-0.558750
4	Cl	0.000000	2.171449	-0.558750
5	Cl	-2.349686	0.000000	-0.221974
6	C	0.000000	0.000000	1.991042
7	H	0.000000	-0.929034	2.567355
8	H	0.000000	0.929034	2.567355

Point Group: C_{2v} Number of degrees of freedom: 7

Energy is -1948.028406028

Distance Matrix (Angstroms)

	W (1)	Cl(2)	Cl(3)	Cl(4)	Cl(5)	C (6)
Cl(2)	2.375589					
Cl(3)	2.277425	3.217084				
Cl(4)	2.277425	3.217084	4.342898			
Cl(5)	2.375589	4.699371	3.217084	3.217084		
C (6)	1.863154	3.227764	3.349124	3.349124	3.227764	
H (7)	2.610384	3.763574	3.363946	4.402900	3.763574	1.093271
H (8)	2.610384	3.763574	4.402900	3.363946	3.763574	1.093271

	H (7)
H (8)	1.858069

R4-W

Coordinates (Angstroms)

ATOM		X	Y	Z
1	W	0.056565	0.169389	0.000000
2	Cl	-2.232867	0.181143	0.000000
3	Cl	0.896406	0.138882	-2.112134
4	Cl	0.067442	-2.256282	0.000000
5	Cl	0.896406	0.138882	2.112134
6	C	0.247104	2.095078	0.000000
7	H	0.308793	2.708199	0.904011
8	H	0.308793	2.708199	-0.904011

Point Group: C_s Number of degrees of freedom: 11

Energy is -1948.007162653

Distance Matrix (Angstroms)

	W (1)	Cl(2)	Cl(3)	Cl(4)	Cl(5)	C (6)
Cl(2)	2.289462					
Cl(3)	2.273185	3.775612				
Cl(4)	2.425696	3.351487	3.299258			
Cl(5)	2.273185	3.775612	4.224267	3.299258		
C (6)	1.935092	3.132635	2.951170	4.355068	2.951170	
H (7)	2.706734	3.696387	4.005472	5.051887	2.899352	1.094056
H (8)	2.706734	3.696387	2.899352	5.051887	4.005472	1.094056

	H (7)
H (8)	1.808021

R2-W

Coordinates (Angstroms)

ATOM		X	Y	Z
1	W	-0.378347	-0.048741	0.000000
2	Cl	3.001797	-0.325780	0.000000
3	Cl	-1.154040	-0.480690	-2.065579
4	Cl	0.306796	2.128348	0.000000
5	Cl	-1.154040	-0.480690	2.065579
6	C	1.370367	-1.173811	0.000000
7	H	1.383374	-1.825275	0.882129
8	H	1.383374	-1.825275	-0.882129

Point Group: C_s Number of degrees of freedom: 11

Energy is -1947.978633867

Distance Matrix (Angstroms)

	W (1)	Cl(2)	Cl(3)	Cl(4)	Cl(5)	C (6)
Cl(2)	3.391478					
Cl(3)	2.248310	4.643446				
Cl(4)	2.282354	3.644965	3.634245			
Cl(5)	2.248310	4.643446	4.131158	3.634245		
C (6)	2.079371	1.838674	3.334616	3.469213	3.334616	
H (7)	2.652902	2.376116	4.115260	4.191457	3.105951	1.096689
H (8)	2.652902	2.376116	3.105951	4.191457	4.115260	1.096689

	H (7)
H (8)	1.764259

p1-W

Coordinates (Angstroms)

ATOM	X	Y	Z
1 W	-0.191379	-0.000011	-0.005935
2 C	1.477261	0.000112	-1.379308
3 H	1.637567	0.911070	-1.950042
4 H	1.637466	-0.910776	-1.950149
5 Cl	2.604520	-0.000081	0.047324
6 Cl	-2.408464	0.000130	-0.405544
7 Cl	-0.031543	2.354995	-0.431000
8 Cl	-0.031754	-2.355025	-0.431063
9 C	-0.015450	-0.717378	2.027673
10 H	0.896747	-1.277269	2.215159
11 H	-0.919849	-1.262359	2.298464
12 C	-0.015652	0.717327	2.027759
13 H	0.896441	1.277406	2.215202
14 H	-0.920179	1.262031	2.298658

Point Group: C_1 Number of degrees of freedom: 36

Energy is -2026.621537896

Distance Matrix (Angstroms)

	W (1)	C (2)	H (3)	H (4)	Cl(5)	Cl(6)
C (2)	2.161137					
H (3)	2.820401	1.086867				
H (4)	2.820307	1.086849	1.821846			
Cl(5)	2.796406	1.818238	2.398888	2.398845		
Cl(6)	2.252810	4.005880	4.425568	4.425505	5.033398	
Cl(7)	2.398391	2.953177	2.679242	3.969718	3.567072	3.346010
Cl(8)	2.398397	2.953467	3.970052	2.679510	3.567150	3.346066
C (9)	2.163592	3.788205	4.605054	4.311913	3.361627	3.487389
H (10)	2.783643	3.858612	4.763039	4.246500	3.040922	4.407296
H (11)	2.726619	4.567930	5.414238	4.971336	4.368313	3.334894
C (12)	2.163647	3.788310	4.312026	4.605135	3.361859	3.487246
H (13)	2.783630	3.858670	4.246495	4.763129	3.041249	4.407056
H (14)	2.726728	4.568106	4.971588	5.414332	4.368630	3.334681

	Cl(7)	Cl(8)	C (9)	H (10)	H (11)	C (12)
Cl(8)	4.710020					
C (9)	3.935074	2.954241				
H (10)	4.588814	3.004357	1.086615			
H (11)	4.617825	3.071311	1.090078	1.818567		
C (12)	2.954268	3.935151	1.434705	2.201364	2.193174	
H (13)	3.004120	4.588989	2.201335	2.554675	3.123500	1.086617
H (14)	3.071689	4.617767	2.193177	3.123497	2.524389	1.090072

	H (13)
H (14)	1.818601

TS1-W

Coordinates (Angstroms)

ATOM	X	Y	Z
1 W	0.047743	-0.018181	0.099651
2 Cl	2.191519	-0.757147	-0.456354
3 Cl	0.985120	1.905695	1.009482
4 Cl	-2.257535	0.070857	0.676609
5 Cl	-0.660022	1.422927	-1.716980
6 C	0.015859	-1.247470	1.652497
7 H	0.964771	-1.680871	1.983029
8 H	-0.826563	-1.535570	2.276064
9 C	-0.534479	-1.656536	-1.376314
10 H	0.242890	-1.731953	-2.127937
11 H	-1.520345	-1.394696	-1.745162
12 C	-0.440767	-2.440542	-0.198316
13 H	-1.353464	-2.747797	0.301292
14 H	0.441330	-3.049962	-0.032467

Point Group: C_1 Number of degrees of freedom: 36

Energy is -2026.611182571

Distance Matrix (Angstroms)

	W (1)	Cl(2)	Cl(3)	Cl(4)	Cl(5)	C (6)
Cl(2)	2.334735					
Cl(3)	2.325461	3.270291				
Cl(4)	2.378049	4.665113	3.740621			
Cl(5)	2.424432	3.804364	3.220738	3.179530		
C (6)	1.980783	3.069392	3.360861	2.803331	4.352151	
H (7)	2.674433	2.882493	3.716405	3.893397	5.095448	1.094314
H (8)	2.793502	4.144981	4.090077	2.680772	4.972408	1.086974
C (9)	2.280715	3.014348	4.548702	3.188620	3.100791	3.105463
H (10)	2.817311	2.746196	4.860739	4.167460	3.307174	3.818108
H (11)	2.785145	3.980632	4.975742	2.925110	2.946176	3.731714
C (12)	2.489028	3.135176	4.730931	3.220756	4.157019	2.248875
H (13)	3.074874	4.135653	5.255997	2.983793	4.685000	2.439628
H (14)	3.060075	2.915449	5.093123	4.186427	4.904824	2.503819

	H (7)	H (8)	C (9)	H (10)	H (11)	C (12)
H (8)	1.820951					
C (9)	3.678795	3.666034				
H (10)	4.174178	4.536245	1.083941			
H (11)	4.489667	4.083067	1.084685	1.835553		
C (12)	2.703868	2.662775	1.418142	2.166315	2.156854	
H (13)	3.056270	2.376308	2.162394	3.079194	2.459005	1.084911
H (14)	2.492113	3.038133	2.167894	2.483449	3.085677	1.084893

	H (13)
H (14)	1.850402

pdt1-W

Coordinates (Angstroms)

ATOM		X	Y	Z
1	W	0.113559	0.068559	0.000000
2	Cl	0.980042	-2.054939	0.000000
3	Cl	0.901967	0.348811	2.198532
4	Cl	-0.509913	2.282504	0.000000
5	Cl	0.901967	0.348811	-2.198532
6	C	-1.664427	-0.624302	1.139482
7	H	-1.368183	-1.229257	1.998082
8	H	-2.146407	0.291536	1.494548
9	C	-1.664427	-0.624302	-1.139482
10	H	-1.368183	-1.229257	-1.998082
11	H	-2.146407	0.291536	-1.494548
12	C	-2.398574	-1.308252	0.000000
13	H	-3.485867	-1.156136	0.000000
14	H	-2.205831	-2.386187	0.000000

Point Group: C_s Number of degrees of freedom: 21

Energy is -2026.636744262

Distance Matrix (Angstroms)

	W (1)	Cl(2)	Cl(3)	Cl(4)	Cl(5)	C (6)
Cl(2)	2.293477					
Cl(3)	2.352376	3.258474				
Cl(4)	2.300058	4.586216	3.250557			
Cl(5)	2.352376	3.258474	4.397065	3.250557		
C (6)	2.222546	3.215332	2.941924	3.328790	4.321535	
H (7)	2.805748	3.191903	2.772014	4.130548	5.025481	1.091295
H (8)	2.718609	4.185009	3.129131	2.979218	4.789019	1.094136
C (9)	2.222546	3.215332	4.321535	3.328790	2.941924	2.278964
H (10)	2.805748	3.191903	5.025481	4.130548	2.772014	3.209056
H (11)	2.718609	4.185009	4.789019	2.979218	3.129131	2.830049
C (12)	2.864685	3.460142	4.298020	4.057163	4.298020	1.518282
H (13)	3.802071	4.555458	5.133372	4.547587	5.133372	2.213349
H (14)	3.377180	3.203047	4.687448	4.967173	4.687448	2.166974

	H (7)	H (8)	C (9)	H (10)	H (11)	C (12)
H (8)	1.781008					
C (9)	3.209056	2.830049				
H (10)	3.996165	3.888047	1.091295			
H (11)	3.888047	2.989095	1.094136	1.781008		
C (12)	2.249506	2.203766	1.518282	2.249506	2.203766	
H (13)	2.912433	2.474587	2.213349	2.912433	2.474587	1.097883
H (14)	2.456109	3.067149	2.166974	2.456109	3.067149	1.095031

	H (13)
H (14)	1.775252

TS2-W

Coordinates (Angstroms)

ATOM		X	Y	Z
1	Cl	-1.672662	1.348864	0.000000
2	C	-3.469879	-0.539792	0.000000
3	H	-3.822436	-0.089869	-0.921212
4	H	-3.822436	-0.089869	0.921212
5	C	-2.773949	-1.740434	0.000000
6	H	-2.815639	-2.328079	0.913645
7	H	-2.815639	-2.328079	-0.913645
8	C	-0.760703	-1.598413	0.000000
9	H	-0.595976	-2.193006	0.903669
10	H	-0.595976	-2.193006	-0.903669
11	W	0.289096	0.049200	0.000000
12	Cl	0.664159	0.688969	2.158283
13	Cl	0.664159	0.688969	-2.158283
14	Cl	2.409176	-1.029570	0.000000

Point Group: C_s Number of degrees of freedom: 21

Energy is -2026.593764066

Distance Matrix (Angstroms)

	Cl(1)	C (2)	H (3)	H (4)	C (5)	H (6)
C (2)	2.607109					
H (3)	2.745927	1.084139				
H (4)	2.745927	1.084139	1.842424			
C (5)	3.279725	1.387753	2.161555	2.161555		
H (6)	3.957405	2.112048	3.064298	2.454237	1.087112	
H (7)	3.957405	2.112048	2.454237	3.064298	1.087112	1.827290
C (8)	3.085144	2.908662	3.535328	3.535328	2.018250	2.364301
H (9)	3.810606	3.436430	4.261856	3.851432	2.401043	2.223791
H (10)	3.810606	3.436430	3.851432	4.261856	2.401043	2.871894
W (11)	2.353215	3.804840	4.215764	4.215764	3.547540	4.015667
Cl(12)	3.248750	4.822687	5.497219	4.718736	4.730832	4.770817
Cl(13)	3.248750	4.822687	4.718736	5.497219	4.730832	5.536092
Cl(14)	4.724230	5.899421	6.369038	6.369038	5.231646	5.460729

	H (7)	C (8)	H (9)	H (10)	W (11)	Cl(12)
C (8)	2.364301					
H (9)	2.871894	1.094209				
H (10)	2.223791	1.094209	1.807339			
W (11)	4.015667	1.953639	2.574385	2.574385		
Cl(12)	5.536092	3.452612	3.386410	4.389678	2.282140	
Cl(13)	4.770817	3.452612	4.389678	3.386410	2.282140	4.316565
Cl(14)	5.460729	3.220514	3.346811	3.346811	2.378756	3.264451

	Cl(13)
Cl(14)	3.264451

pdt2-W

Coordinates (Angstroms)

ATOM	X	Y	Z
1 Cl	-2.073109	0.244772	0.970731
2 C	-2.991642	0.211673	-0.655264
3 H	-3.030324	1.256366	-0.969984
4 H	-3.988653	-0.151549	-0.405634
5 C	-2.220879	-0.676586	-1.608476
6 H	-2.338778	-1.724799	-1.307913
7 H	-2.689956	-0.574755	-2.598623
8 C	-0.721832	-0.324105	-1.686536
9 H	-0.197051	-1.014615	-2.359448
10 H	-0.582987	0.688297	-2.121460
11 W	0.353740	0.020365	0.073910
12 Cl	0.376663	-2.043964	1.037444
13 Cl	2.489064	-0.181409	-0.832574
14 Cl	0.532270	2.270107	0.466830

Point Group: C_1 Number of degrees of freedom: 36

Energy is -2026.624358131

Distance Matrix (Angstroms)

	Cl(1)	C (2)	H (3)	H (4)	C (5)	H (6)
C (2)	1.867795					
H (3)	2.388714	1.091755				
H (4)	2.391811	1.090080	1.794188			
C (5)	2.742817	1.513834	2.190702	2.201708		
H (6)	3.023576	2.145252	3.078924	2.451797	1.096808	
H (7)	3.713813	2.118047	2.474129	2.583586	1.100360	1.764046
C (8)	3.034903	2.550023	2.887987	3.513204	1.541907	2.172512
H (9)	4.024393	3.495392	3.887853	4.351841	2.184972	2.489394
H (10)	3.461043	2.859811	2.763703	3.904863	2.192886	3.093168
W (11)	2.596968	3.429268	3.750907	4.372172	3.153543	3.493520
Cl(12)	3.353230	4.393022	5.150680	4.971890	3.951942	3.602247
Cl(13)	4.924120	5.497644	5.705236	6.491840	4.799041	5.090781
Cl(14)	3.338247	4.232517	3.972931	5.202341	4.535386	5.229904

	H (7)	C (8)	H (9)	H (10)	W (11)	Cl(12)
C (8)	2.183630					
H (9)	2.542687	1.097729				
H (10)	2.502459	1.110583	1.762240			
W (11)	4.093982	2.091575	2.701071	2.478556		
Cl(12)	4.978324	3.403626	3.595495	4.285423	2.278240	
Cl(13)	5.485973	3.325578	3.200123	3.443126	2.328526	3.380579
Cl(14)	5.279486	3.597178	4.394217	3.231898	2.290763	4.354425

	Cl(13)
Cl(14)	3.395206

R1-Ru

Coordinates (Angstroms)

ATOM		X	Y	Z
1	Ru	0.000000	0.000000	-0.001091
2	Cl	0.000000	-2.270669	0.461498
3	Cl	2.339333	0.000000	0.003936
4	Cl	-2.339333	0.000000	0.003936
5	Cl	0.000000	2.270669	0.461498
6	C	0.000000	0.000000	-1.834501
7	H	0.942864	0.000000	-2.384882
8	H	-0.942864	0.000000	-2.384882

Point Group: C_{2v} Number of degrees of freedom: 7

Energy is -1973.972019323

Distance Matrix (Angstroms)

	Ru(1)	Cl(2)	Cl(3)	Cl(4)	Cl(5)	C (6)
Cl(2)	2.317310					
Cl(3)	2.339338	3.292078				
Cl(4)	2.339338	3.292078	4.678666			
Cl(5)	2.317310	4.541337	3.292078	3.292078		
C (6)	1.833410	3.229172	2.975287	2.975287	3.229172	
H (7)	2.563484	3.761225	2.767052	4.059467	3.761225	1.091747
H (8)	2.563484	3.761225	4.059467	2.767052	3.761225	1.091747

	H (7)
H (8)	1.885728

R2-Ru

Coordinates (Angstroms)

ATOM		X	Y	Z
1	Ru	-0.338012	0.032841	0.000000
2	Cl	2.840218	-0.492841	0.000000
3	Cl	-1.432883	-0.539656	-1.855176
4	Cl	0.324570	2.161206	0.000000
5	Cl	-1.432883	-0.539656	1.855176
6	C	1.248672	-1.281915	0.000000
7	H	1.148558	-1.883713	0.905983
8	H	1.148558	-1.883713	-0.905983

Point Group: C_s Number of degrees of freedom: 11

Energy is -1974.025450210

Distance Matrix (Angstroms)

	Ru(1)	Cl(2)	Cl(3)	Cl(4)	Cl(5)	C (6)
Cl(2)	3.221411					
Cl(3)	2.228940	4.658676				
Cl(4)	2.229115	3.656836	3.718196			
Cl(5)	2.228940	4.658676	3.710351	3.718196		
C (6)	2.060618	1.776417	3.344153	3.564975	3.344153	
H (7)	2.589184	2.370030	4.011773	4.226243	3.061257	1.092240
H (8)	2.589184	2.370030	3.061257	4.226243	4.011773	1.092240

	H (7)
H (8)	1.811966

p1-Ru

Coordinates (Angstroms)

ATOM		X	Y	Z
1	Ru	-0.168064	-0.000317	-0.027422
2	C	1.399323	0.003809	-1.378341
3	H	1.439139	0.937200	-1.933442
4	H	1.444251	-0.929306	-1.933525
5	Cl	2.519059	0.006790	-0.017350
6	Cl	-2.360384	-0.006674	-0.474303
7	Cl	-0.157431	2.399657	-0.336425
8	Cl	-0.143319	-2.400338	-0.336521
9	C	-0.089005	-0.706550	2.033127
10	H	0.826431	-1.269604	2.180119
11	H	-1.007409	-1.263794	2.191039
12	C	-0.093094	0.705666	2.033351
13	H	0.819067	1.273974	2.180445
14	H	-1.014742	1.257512	2.191309

Point Group: C_1 Number of degrees of freedom: 36

Energy is -2052.623463781

Distance Matrix (Angstroms)

	Ru(1)	C (2)	H (3)	H (4)	Cl(5)	Cl(6)
C (2)	2.069227					
H (3)	2.663634	1.086711				
H (4)	2.663796	1.086716	1.866513			
Cl(5)	2.687150	1.762417	2.388157	2.388140		
Cl(6)	2.237412	3.866884	4.178081	4.178018	4.900811	
Cl(7)	2.419808	3.041243	2.690405	4.024688	3.604333	3.265340
Cl(8)	2.419970	3.040569	4.024114	2.689747	3.603386	3.265577
C (9)	2.179651	3.789175	4.557500	4.258500	3.393421	3.454880
H (10)	2.733742	3.822620	4.708161	4.173676	3.053366	4.335521
H (11)	2.687460	4.487722	5.276487	4.809839	4.350557	3.242675
C (12)	2.179637	3.789400	4.258731	4.557704	3.393692	3.454904
H (13)	2.733665	3.822954	4.173964	4.708509	3.053855	4.335512
H (14)	2.687334	4.487970	4.810166	5.276654	4.350888	3.242592

	Cl(7)	Cl(8)	C (9)	H (10)	H (11)	C (12)
Cl(8)	4.800016					
C (9)	3.907426	2.913263				
H (10)	4.556803	2.924457	1.084739			
H (11)	4.531160	2.902920	1.085782	1.833882		
C (12)	2.913689	3.907182	1.412221	2.183748	2.177064	
H (13)	2.924952	4.556521	2.183752	2.543589	3.126723	1.084735
H (14)	2.903259	4.530913	2.177051	3.126717	2.521317	1.085781

	H (13)
H (14)	1.833915

TS1-Ru

Coordinates (Angstroms)

ATOM	X	Y	Z
1 Ru	-0.145433	0.035712	0.061115
2 Cl	-2.387140	0.490328	-0.296734
3 Cl	-0.719011	-2.220780	0.483057
4 Cl	2.271135	0.017843	0.865835
5 Cl	1.084767	-0.829306	-1.730454
6 C	-0.256726	0.500850	1.879811
7 H	-1.264826	0.631023	2.280166
8 H	0.579091	0.592350	2.568484
9 C	0.381060	2.087716	-1.075251
10 H	-0.409113	2.090069	-1.819972
11 H	1.393579	1.899090	-1.412318
12 C	0.147841	2.551757	0.191990
13 H	0.976040	2.716591	0.874923
14 H	-0.837795	2.899260	0.485690

Point Group: C_1 Number of degrees of freedom: 36

Energy is -2052.558692808

Distance Matrix (Angstroms)

	Ru(1)	Cl(2)	Cl(3)	Cl(4)	Cl(5)	C (6)
Cl(2)	2.315164					
Cl(3)	2.366175	3.277321				
Cl(4)	2.547094	4.824348	3.754853			
Cl(5)	2.339096	3.981347	3.176389	2.977558		
C (6)	1.880530	3.045672	3.093847	2.766139	4.074670	
H (7)	2.555705	2.814214	3.414717	3.857375	4.872189	1.092472
H (8)	2.668648	4.125338	3.734672	2.468215	4.556061	1.086846
C (9)	2.404005	3.289478	4.711859	3.409482	3.071403	3.414279
H (10)	2.797927	2.965133	4.897285	4.323356	3.280616	4.029545
H (11)	2.830501	4.186044	5.002880	3.082073	2.764185	3.939123
C (12)	2.536458	3.303705	4.859348	3.373894	4.000651	2.686752
H (13)	3.017797	4.200000	5.234920	2.993425	4.401500	2.727457
H (14)	2.976497	2.969109	5.121418	4.255880	4.744444	2.834358

	H (7)	H (8)	C (9)	H (10)	H (11)	C (12)
H (8)	1.866723					
C (9)	4.011199	3.943620				
H (10)	4.435335	4.741124	1.085812			
H (11)	4.723299	4.268225	1.083692	1.858050		
C (12)	3.169437	3.110141	1.369534	2.138070	2.133458	
H (13)	3.368350	2.745563	2.133697	3.094130	2.464573	1.086040
H (14)	2.923594	3.415762	2.140268	2.480854	3.095449	1.085586

	H (13)
H (14)	1.864099

pdt1-Ru

Coordinates (Angstroms)

ATOM	X	Y	Z
1 Ru	-0.252247	0.136795	0.000000
2 Cl	-2.490603	-0.348827	0.000000
3 Cl	-0.036824	1.107679	-2.031749
4 Cl	2.236006	0.599234	0.000000
5 Cl	-0.036824	1.107679	2.031749
6 C	0.534867	-1.653881	-1.099696
7 H	-0.430185	-1.944543	-1.515992
8 H	1.236348	-1.226549	-1.807055
9 C	0.534867	-1.653881	1.099696
10 H	-0.430185	-1.944543	1.515992
11 H	1.236348	-1.226549	1.807055
12 C	1.076578	-2.518710	0.000000
13 H	2.166446	-2.548701	0.000000
14 H	0.662756	-3.533025	0.000000

Point Group: C_s Number of degrees of freedom: 21

Energy is -2052.586035507

Distance Matrix (Angstroms)

	Ru(1)	Cl(2)	Cl(3)	Cl(4)	Cl(5)	C (6)
Cl(2)	2.290429					
Cl(3)	2.262085	3.502919				
Cl(4)	2.530860	4.820751	3.090675			
Cl(5)	2.262085	3.502919	4.063498	3.090675		
C (6)	2.243970	3.473610	2.970146	3.029806	4.214142	
H (7)	2.581058	3.014939	3.120384	3.984671	4.696515	1.090465
H (8)	2.709256	4.233911	2.668346	2.756491	4.669689	1.083995
C (9)	2.243970	3.473610	4.214142	3.029806	2.970146	2.199391
H (10)	2.581058	3.014939	4.696515	3.984671	3.120384	2.803147
H (11)	2.709256	4.233911	4.669689	2.756491	2.668346	3.020577
C (12)	2.969424	4.175305	4.303297	3.326536	4.303297	1.500236
H (13)	3.614134	5.150490	4.727739	3.148703	4.727739	2.161500
H (14)	3.782170	4.481382	5.114054	4.421615	5.114054	2.181025

	H (7)	H (8)	C (9)	H (10)	H (11)	C (12)
H (8)	1.837816					
C (9)	2.803147	3.020577				
H (10)	3.031983	3.786223	1.090465			
H (11)	3.786223	3.614109	1.083995	1.837816		
C (12)	2.213196	2.227252	1.500236	2.213196	2.227252	
H (13)	3.066877	2.424586	2.161500	3.066877	2.424586	1.090280
H (14)	2.452759	2.985681	2.181025	2.452759	2.985681	1.095484

	H (13)
H (14)	1.797214

TS2-Ru

Coordinates (Angstroms)

ATOM	X	Y	Z
1 Cl	1.668141	-1.544022	0.100509
2 C	3.275931	0.748322	-0.148169
3 H	3.524394	0.326190	-1.116667
4 H	3.634576	0.209208	0.720262
5 C	2.605591	1.940879	-0.030078
6 H	2.583768	2.423968	0.942725
7 H	2.565634	2.600619	-0.892523
8 C	0.530260	1.610962	-0.181146
9 H	0.375015	2.309235	0.635411
10 H	0.469104	2.003648	-1.193199
11 Ru	-0.219215	-0.178418	0.021341
12 Cl	-1.022593	-0.611813	2.062938
13 Cl	-1.060889	-1.003170	-1.884502
14 Cl	-2.058947	1.520339	-0.137806

Point Group: C_1 Number of degrees of freedom: 36

Energy is -2052.565871521

Distance Matrix (Angstroms)

	Cl(1)	C (2)	H (3)	H (4)	C (5)	H (6)
C (2)	2.810991					
H (3)	2.902565	1.085319				
H (4)	2.706433	1.083255	1.843945			
C (5)	3.611150	1.373133	2.152230	2.149536		
H (6)	4.158442	2.115875	3.086510	2.461473	1.086369	
H (7)	4.355417	2.118865	2.478404	3.076127	1.086584	1.843820
C (8)	3.365713	2.878184	3.389790	3.523383	2.106813	2.478095
H (9)	4.099498	3.386112	4.113494	3.878408	2.356699	2.232979
H (10)	3.961986	3.247493	3.486333	4.111151	2.433385	3.034904
Ru(11)	2.330934	3.619893	3.945161	3.935791	3.531797	3.934218
Cl(12)	3.458351	5.021581	5.627152	4.915901	4.905169	4.845274
Cl(13)	3.417658	4.989046	4.835451	5.504730	5.054640	5.746477
Cl(14)	4.830971	5.390458	5.792914	5.905214	4.684695	4.851689

	H (7)	C (8)	H (9)	H (10)	Ru(11)	Cl(12)
C (8)	2.372388					
H (9)	2.686689	1.085564				
H (10)	2.200504	1.087288	1.856354			
Ru(11)	4.039007	1.950537	2.630325	2.590425		
Cl(12)	5.650651	3.519659	3.538880	4.434888	2.236374	
Cl(13)	5.207973	3.502408	4.402704	3.443796	2.240729	3.966978
Cl(14)	4.808675	2.591155	2.672899	2.781813	2.509126	3.234714

	Cl(13)
Cl(14)	3.227253

pdt2-Ru

Coordinates (Angstroms)

ATOM		X	Y	Z
1	Cl	-2.125068	0.110859	0.947689
2	C	-2.872866	0.164224	-0.719993
3	H	-2.853667	1.212551	-1.024957
4	H	-3.904084	-0.170139	-0.599413
5	C	-2.060879	-0.735052	-1.632793
6	H	-2.140892	-1.772257	-1.289323
7	H	-2.513801	-0.695842	-2.636838
8	C	-0.597425	-0.332011	-1.742230
9	H	0.002644	-1.077082	-2.276974
10	H	-0.449850	0.645427	-2.229517
11	Ru	0.443780	0.002817	-0.009497
12	Cl	0.641522	-1.735495	1.410065
13	Cl	2.509666	-0.111368	-0.959930
14	Cl	0.481374	2.158650	0.662150

Point Group: C_1 Number of degrees of freedom: 36

Energy is -2052.663958050

Distance Matrix (Angstroms)

	Cl(1)	C (2)	H (3)	H (4)	C (5)	H (6)
C (2)	1.828445					
H (3)	2.374008	1.091953				
H (4)	2.374316	1.090756	1.787819			
C (5)	2.716353	1.516978	2.188866	2.187328		
H (6)	2.924140	2.147063	3.080100	2.480242	1.095522	
H (7)	3.694687	2.131416	2.521039	2.521974	1.102172	1.764519
C (8)	3.124978	2.543393	2.826796	3.502317	1.521879	2.159103
H (9)	4.041883	3.497655	3.868912	4.347330	2.188626	2.460381
H (10)	3.631357	2.895034	2.747896	3.905652	2.203909	3.096576
Ru(11)	2.743512	3.395732	3.656196	4.391108	3.074550	3.386646
Cl(12)	3.358100	4.527361	5.180411	5.210650	4.190805	3.876838
Cl(13)	5.016888	5.394921	5.524702	6.424143	4.661718	4.949217
Cl(14)	3.326939	4.139925	3.855377	5.123187	4.483673	5.112392

	H (7)	C (8)	H (9)	H (10)	Ru(11)	Cl(12)
C (8)	2.145972					
H (9)	2.570475	1.095977				
H (10)	2.494957	1.102094	1.781583			
Ru(11)	4.017255	2.049044	2.549949	2.477904		
Cl(12)	5.235873	3.666295	3.799465	4.484020	2.252995	
Cl(13)	5.328120	3.211650	2.992051	3.308069	2.276894	3.427044
Cl(14)	5.291741	3.626050	4.397453	3.393930	2.258348	3.968550

	Cl(13)
Cl(14)	3.449361

R1-Re/d

Coordinates (Angstroms)

ATOM		X	Y	Z
1	Re	0.000000	0.000000	-0.061182
2	Cl	0.000000	-2.258026	0.496843
3	Cl	2.310442	0.000000	0.051352
4	Cl	-2.310442	0.000000	0.051352
5	Cl	0.000000	2.258026	0.496843
6	C	0.000000	0.000000	-1.923290
7	H	0.930316	0.000000	-2.493857
8	H	-0.930316	0.000000	-2.493857

Point Group: C_{2v} Number of degrees of freedom: 7

Energy is -1959.257911679

Distance Matrix (Angstroms)

	Re(1)	Cl(2)	Cl(3)	Cl(4)	Cl(5)	C (6)
Cl(2)	2.325956					
Cl(3)	2.313181	3.261179				
Cl(4)	2.313181	3.261179	4.620884			
Cl(5)	2.325956	4.516052	3.261179	3.261179		
C (6)	1.862108	3.309943	3.039301	3.039301	3.309943	
H (7)	2.604495	3.861146	2.895313	4.120752	3.861146	1.091345
H (8)	2.604495	3.861146	4.120752	2.895313	3.861146	1.091345

	H (7)
H (8)	1.860631

R2-Re/d

Coordinates (Angstroms)

ATOM		X	Y	Z
1	Re	0.216207	-0.001244	-0.007826
2	Cl	-0.034607	1.900636	1.199406
3	Cl	2.236638	0.002424	-0.997137
4	Cl	-2.588511	0.001225	-0.555757
5	Cl	-0.033453	-1.910521	1.188533
6	C	-1.091038	0.005040	-1.580740
7	H	-1.088018	-0.895709	-2.203211
8	H	-1.088047	0.910771	-2.195790

Point Group: C_1 Number of degrees of freedom: 18

Energy is -1959.249696116

Distance Matrix (Angstroms)

	Re(1)	Cl(2)	Cl(3)	Cl(4)	Cl(5)	C (6)
Cl(2)	2.266598					
Cl(3)	2.249643	3.685996				
Cl(4)	2.857739	3.634664	4.845295			
Cl(5)	2.266924	3.811173	3.686438	3.636707		
C (6)	2.045235	3.526832	3.378466	1.814670	3.529410	
H (7)	2.705695	4.528468	3.648917	2.402098	3.694033	1.094910
H (8)	2.705556	3.690112	3.649027	2.401743	4.530508	1.094826

	H (7)
H (8)	1.806495

p1-Re/d

Coordinates (Angstroms)

ATOM		X	Y	Z
1	Re	-0.161368	0.000789	0.057225
2	C	1.369564	-0.013087	-1.385089
3	H	1.470605	0.905288	-1.957842
4	H	1.455759	-0.934737	-1.955192
5	Cl	2.563667	-0.020691	-0.035368
6	Cl	-2.383825	0.025874	-0.283750
7	Cl	-0.099269	2.380902	-0.344958
8	Cl	-0.149898	-2.379518	-0.347025
9	C	0.074938	-0.717765	2.071777
10	H	0.989026	-1.289374	2.200472
11	H	-0.827410	-1.256680	2.355075
12	C	0.089432	0.712460	2.071253
13	H	1.014931	1.265315	2.199557
14	H	-0.801749	1.269878	2.352982

Point Group: C_1 Number of degrees of freedom: 36

Energy is -2037.871496373

Distance Matrix (Angstroms)

	Re(1)	C (2)	H (3)	H (4)	Cl(5)	Cl(6)
C (2)	2.103382					
H (3)	2.746260	1.087045				
H (4)	2.745930	1.087146	1.840087			
Cl(5)	2.726692	1.802134	2.397525	2.397637		
Cl(6)	2.248602	3.911828	4.293318	4.296383	4.953943	
Cl(7)	2.414652	2.995083	2.691344	4.000554	3.599267	3.281631
Cl(8)	2.414417	2.997722	4.001338	2.692903	3.608965	3.283344
C (9)	2.151878	3.757999	4.562895	4.262655	3.334629	3.485257
H (10)	2.753441	3.824914	4.726524	4.196803	3.014636	4.390599
H (11)	2.702769	4.512433	5.343803	4.888243	4.329122	3.321260
C (12)	2.150741	3.756522	4.263617	4.559865	3.331247	3.483452
H (13)	2.751780	3.822272	4.197764	4.721917	3.007870	4.388003
H (14)	2.700218	4.509299	4.886688	5.340135	4.323866	3.317057

	Cl(7)	Cl(8)	C (9)	H (10)	H (11)	C (12)
Cl(8)	4.760689					
C (9)	3.933534	2.943225				
H (10)	4.597229	2.995881	1.085752			
H (11)	4.588286	3.003520	1.088540	1.823297		
C (12)	2.942343	3.932642	1.430298	2.198478	2.190585	
H (13)	2.993414	4.596380	2.198300	2.554820	3.127118	1.085661
H (14)	3.001122	4.586179	2.190521	3.127284	2.526689	1.088251

	H (13)
H (14)	1.823153

TS1-Re/d

Coordinates (Angstroms)

ATOM	X	Y	Z
1 Re	-0.053195	-0.021147	0.063425
2 Cl	1.318299	0.460896	-1.845238
3 Cl	2.078903	-0.861159	0.900286
4 Cl	0.272924	2.230510	0.583297
5 Cl	-2.271865	0.449873	-0.439153
6 C	-0.556697	-0.834743	1.750379
7 H	0.068392	-1.385067	2.445562
8 H	-1.581389	-0.658862	2.089330
9 C	-0.346429	-1.922083	-1.120859
10 H	0.638401	-2.216385	-1.466218
11 H	-1.080870	-1.694533	-1.886607
12 C	-0.782828	-2.372789	0.141545
13 H	-1.846472	-2.435503	0.350065
14 H	-0.111665	-2.984692	0.735757

Point Group: C_1 Number of degrees of freedom: 36

Energy is -2037.841240801

Distance Matrix (Angstroms)

	Re(1)	Cl(2)	Cl(3)	Cl(4)	Cl(5)	C (6)
Cl(2)	2.399240					
Cl(3)	2.439631	3.140740				
Cl(4)	2.333791	3.181528	3.594504			
Cl(5)	2.323132	3.855707	4.737308	3.269866		
C (6)	1.939398	4.257082	2.769430	3.383212	3.063672	
H (7)	2.747661	4.835371	2.589307	4.072133	4.143114	1.084838
H (8)	2.616553	5.014267	3.853893	3.749011	2.845922	1.093534
C (9)	2.258776	2.995770	3.330590	4.531200	3.130208	3.077422
H (10)	2.763545	2.788145	3.084157	4.910087	4.078412	3.699147
H (11)	2.767482	3.225461	4.294817	4.831060	2.848170	3.773812
C (12)	2.463470	4.048681	3.324187	4.743429	3.243742	2.237201
H (13)	3.021112	4.819155	4.264959	5.130099	3.021460	2.487335
H (14)	3.039416	4.536344	3.055332	5.231585	4.224111	2.418635

	H (7)	H (8)	C (9)	H (10)	H (11)	C (12)
H (8)	1.837404					
C (9)	3.630402	3.664174				
H (10)	4.039557	4.471607	1.084333			
H (11)	4.492689	4.138986	1.085150	1.845250		
C (12)	2.647388	2.714611	1.409697	2.151571	2.159227	
H (13)	3.026752	2.500354	2.162717	3.085691	2.477475	1.085704
H (14)	2.348330	3.066225	2.152040	2.449814	3.079068	1.085345

	H (13)
H (14)	1.860087

pdt1-Re/d

Coordinates (Angstroms)

ATOM	X	Y	Z
1 Re	-0.165975	-0.118197	0.000000
2 Cl	-0.508249	-0.818881	-2.189850
3 Cl	-2.259478	0.863206	0.000000
4 Cl	-0.508249	-0.818881	2.189850
5 Cl	1.910840	-1.140394	0.000000
6 C	0.715023	1.576127	1.142566
7 H	-0.141732	2.095373	1.573533
8 H	1.350802	1.163428	1.924515
9 C	0.715023	1.576127	-1.142566
10 H	-0.141732	2.095373	-1.573533
11 H	1.350802	1.163428	-1.924515
12 C	1.402604	2.292627	0.000000
13 H	2.479929	2.103829	0.000000
14 H	1.239261	3.377564	0.000000

Point Group: C_s Number of degrees of freedom: 21

Energy is -2037.867250341

Distance Matrix (Angstroms)

	Re(1)	Cl(2)	Cl(3)	Cl(4)	Cl(5)	C (6)
Cl(2)	2.324555					
Cl(3)	2.312122	3.269811				
Cl(4)	2.324555	4.379700	3.269811			
Cl(5)	2.314746	3.278842	4.626658	3.278842		
C (6)	2.225387	4.282226	3.265175	2.886047	3.180397	
H (7)	2.715968	4.773915	2.911888	3.001176	4.142371	1.090585
H (8)	2.765308	4.930884	4.102196	2.730572	3.053685	1.089027
C (9)	2.225387	2.886047	3.265175	4.282226	3.180397	2.285132
H (10)	2.715968	3.001176	2.911888	4.773915	4.142371	2.894968
H (11)	2.765308	2.730572	4.102196	4.930884	3.053685	3.159354
C (12)	2.876197	4.257733	3.931169	4.257733	3.470437	1.513802
H (13)	3.455171	4.718781	4.899095	4.718781	3.293758	2.167677
H (14)	3.767629	5.045729	4.308500	5.045729	4.567598	2.196692

	H (7)	H (8)	C (9)	H (10)	H (11)	C (12)
H (8)	1.794259					
C (9)	2.894968	3.159354				
H (10)	3.147066	3.915675	1.090585			
H (11)	3.915675	3.849029	1.089027	1.794259		
C (12)	2.213569	2.231934	1.513802	2.213569	2.231934	
H (13)	3.057643	2.421372	2.167677	3.057643	2.421372	1.093743
H (14)	2.455027	2.935744	2.196692	2.455027	2.935744	1.097164

	H (13)
H (14)	1.778105

TS2-Re/d

Coordinates (Angstroms)

ATOM	X	Y	Z
1 Cl	-1.528037	-1.408847	0.344724
2 C	-3.514158	0.309474	-0.189116
3 H	-3.834278	0.149631	0.834989
4 H	-3.758579	-0.472052	-0.899031
5 C	-2.966762	1.501584	-0.594364
6 H	-2.917053	1.713359	-1.658858
7 H	-3.057375	2.366776	0.056489
8 C	-0.818551	1.551490	-0.359018
9 H	-0.699641	2.073152	-1.310221
10 H	-0.856962	2.210555	0.513935
11 Re	0.311201	0.044647	-0.065766
12 Cl	2.331586	1.248880	-0.418409
13 Cl	0.707903	-1.121084	-1.964190
14 Cl	0.868441	-0.228731	2.115804

Point Group: C_1 Number of degrees of freedom: 36

Energy is -2037.834780161

Distance Matrix (Angstroms)

	Cl(1)	C (2)	H (3)	H (4)	C (5)	H (6)
C (2)	2.679979					
H (3)	2.826299	1.084812				
H (4)	2.720263	1.083745	1.843650			
C (5)	3.379708	1.372952	2.150213	2.148263		
H (6)	3.961298	2.118389	3.083151	2.462016	1.086493	
H (7)	4.083783	2.121666	2.474949	3.076304	1.086451	1.840939
C (8)	3.124454	2.972838	3.533479	3.609722	2.161640	2.473761
H (9)	3.943272	3.505559	4.257677	4.000530	2.445195	2.273305
H (10)	3.684975	3.342017	3.635230	4.196693	2.486408	3.035162
Re(11)	2.379903	3.836498	4.243511	4.186217	3.625896	3.967892
Cl(12)	4.747902	5.925182	6.387272	6.346866	5.307288	5.413193
Cl(13)	3.226968	4.798248	5.484664	4.637377	4.717836	4.611681
Cl(14)	3.205075	4.980913	4.888683	5.527906	5.004776	5.687684

	H (7)	C (8)	H (9)	H (10)	Re(11)	Cl(12)
C (8)	2.418609					
H (9)	2.740989	1.091356				
H (10)	2.252883	1.094481	1.836076			
Re(11)	4.093231	1.906020	2.585595	2.528204		
Cl(12)	5.524140	3.165196	3.265438	3.458456	2.378338	
Cl(13)	5.515943	3.471209	3.551337	4.437311	2.262811	3.262287
Cl(14)	5.137068	3.484232	4.415336	3.390150	2.268149	3.278165

	Cl(13)
Cl(14)	4.179524

pdt2-Re/d

Coordinates (Angstroms)

ATOM		X	Y	Z
1	Cl	-1.891273	0.225139	0.848566
2	C	-2.615466	0.252653	-0.852927
3	H	-2.611815	1.304398	-1.145027
4	H	-3.638399	-0.104921	-0.731273
5	C	-1.760918	-0.622786	-1.746415
6	H	-1.855968	-1.667523	-1.430443
7	H	-2.173940	-0.553668	-2.764396
8	C	-0.282703	-0.210340	-1.756875
9	H	0.314764	-0.930293	-2.329940
10	H	-0.143964	0.771087	-2.238968
11	Re	0.644585	0.021838	0.094531
12	Cl	2.813258	-0.144153	-0.648516
13	Cl	0.543800	-2.103777	0.951041
14	Cl	0.729785	2.265953	0.562791

Point Group: C_1 Number of degrees of freedom: 36

Energy is -2037.889616910

Distance Matrix (Angstroms)

	Cl(1)	C (2)	H (3)	H (4)	C (5)	H (6)
C (2)	1.849402					
H (3)	2.378737	1.091560				
H (4)	2.378504	1.090437	1.791995			
C (5)	2.733111	1.514914	2.190829	2.196277		
H (6)	2.962651	2.144163	3.079786	2.471361	1.095604	
H (7)	3.706742	2.121040	2.503298	2.545506	1.100749	1.766694
C (8)	3.092809	2.544261	2.844917	3.510508	1.534712	2.169124
H (9)	4.037886	3.488147	3.868168	4.343325	2.177961	2.462656
H (10)	3.589431	2.880660	2.751621	3.905331	2.190897	3.087310
Re(11)	2.653390	3.402776	3.712897	4.363712	3.096945	3.381162
Cl(12)	4.950782	5.447043	5.637041	6.452307	4.728378	4.973302
Cl(13)	3.371043	4.334515	5.095788	4.931166	3.844649	3.408911
Cl(14)	3.334147	4.153112	3.873954	5.135823	4.458794	5.111882

	H (7)	C (8)	H (9)	H (10)	Re(11)	Cl(12)
C (8)	2.170196					
H (9)	2.554260	1.097134				
H (10)	2.480293	1.102207	1.764483			
Re(11)	4.055707	2.083621	2.625528	2.574569		
Cl(12)	5.432936	3.289045	3.112503	3.480282	2.298437	
Cl(13)	4.857306	3.406027	3.492042	4.349025	2.293906	3.398404
Cl(14)	5.239471	3.540905	4.330834	3.293618	2.294031	3.408333

	Cl(13)
Cl(14)	4.390885