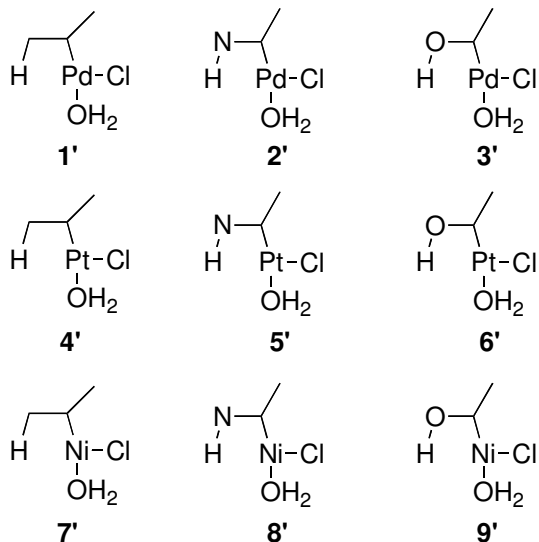


Supplemental Information



Supplemental Scheme 1. Reactant structures for the *cis*-chloride isomers. BHE from these reactant complexes occurs in an identical manner to the species in the manuscript.

Supplemental Table 1. Enthalpies (kcal/mol) for the species represented in supplemental scheme 1. As in table 1, the values in parenthesis are the enthalpies including solvation corrections for water.

Species	Reactant	Planar Reactant	TS	Product
1'	0	-	6.8 (7.7)	5.6 (6.3)
2'	0	18.8	33.9 (37.2)	27.5 (10.3)
3'	0	7.9	31.9 (35.1)	16.2 (9.1)
4'	0	-	0.7 (-0.7)	-8.5 (-11.9)
5'	0	23.9	31.2 (14.1)	16.9 (16.9)
6'	0	12.4	25.6 (28.2)	6.7 (1.3)
7'	0	-	9.8 (11.0)	8.5 (8.5)
8'	0	24.1	37.5 (40.5)	7.7 (8.5)
9'	0	16.7	34 (36.3)	3.8 (2.6)

Supplemental Table 2. Bond lengths (Å) and dihedral angles, θ (degrees), for complexes **1-8** in their reactant, TS, and product forms.

Species	Reactant					TS					Product				
	β -H	M-H	M- β	α - β	θ	β -H	M-H	M- β	α - β	θ	β -H	M-H	M- β	α - β	θ
1	1.21	1.78	2.32	1.48	0.7	1.21	1.78	2.32	1.48	1.3	2.62	1.50	2.21	1.38	35.4
2	1.01	2.70	2.10	1.42	107.9	1.51	1.57	2.24	1.34	21.1	2.55	1.51	2.07	1.28	39.6
3	0.97	2.71	2.29	1.41	96.8	1.35	1.61	2.26	1.30	21.6	2.72	1.50	2.17	1.25	32.8
4	1.02	2.65	2.03	1.46	109.9	1.36	1.65	2.18	1.38	28.6	2.65	1.52	2.15	1.35	35.9
5	0.97	2.61	2.14	1.45	101.2	1.31	1.67	2.13	1.36	42.4	2.64	1.52	2.11	1.28	35.9
6	1.18	1.67	2.15	1.49	0.9	1.91	1.42	2.05	1.38	17.5	2.47	1.41	2.06	1.38	35.5
7	1.02	2.51	1.88	1.44	109.1	1.58	1.44	2.05	1.34	16.0	2.41	1.42	1.87	1.28	15.3
8	0.97	2.42	1.93	1.45	101.3	1.39	1.48	2.00	1.31	24.8	2.44	1.43	1.89	1.23	6.0

Supplemental Table 3. Bond lengths (Å) and dihedral angles, θ (degrees) for complexes **1'-8'** in their reactant, TS, and product forms.

Species	Reactant					TS					Product				
	β -H	M-H	M- β	α - β	θ	β -H	M-H	M- β	α - β	θ	β -H	M-H	M- β	α - β	θ
1'	1.16	1.93	2.39	1.50	1.1	1.77	1.56	2.22	1.41	7.5	2.53	1.54	2.17	1.39	37.1
2'	1.01	2.78	2.16	1.43	109.0	1.50	1.56	2.23	1.35	17.9	2.63	1.55	2.10	1.35	37.2
3'	0.97	2.77	2.36	1.42	95.1	1.47	1.58	2.24	1.30	13.4	2.54	1.51	2.11	1.25	36.3
4'	1.21	1.80	2.30	1.50	0.7	1.51	1.62	2.20	1.45	2.4	2.55	1.56	2.12	1.41	37.9
5'	1.01	2.73	2.10	1.46	110.1	1.55	1.60	2.17	1.40	26.5	2.63	1.55	2.10	1.35	37.2
6'	0.97	2.67	2.25	1.46	97.1	1.44	1.61	2.12	1.38	41.7	2.51	1.55	2.07	1.29	37.3
7'	1.16	1.73	2.17	1.50	1.5	2.04	1.43	2.08	1.38	26.5	2.45	1.44	2.07	1.38	36.5
8'	1.02	2.57	1.92	1.45	110.5	1.60	1.45	2.06	1.34	16.8	2.42	1.45	2.42	1.28	9.0
9'	0.97	2.47	1.98	1.45	102.1	1.52	1.44	1.89	1.34	41.8	2.35	1.46	1.90	1.23	38.1

XYZ Structure Files

These are .xyz coordinates for the reactants, "pre", transition states, "TS", and products "post" of all the complexes in table 1. H2OH or HCl refers to the ligand "trans" to the vacant site in the reactant. CCH is an alkane, OCH is a methoxy, CNH is an amine, and COH is an alcohol, and in each of these cases the letters denote the $\alpha\beta\gamma$ atoms on the reactive portion of the molecule.

15

Ni.CCH.H2OH.TS.xyz

Ni1 0.109685 -0.432427 0.761096
H2 0.179487 -1.792717 1.132387
C3 1.934641 -0.133407 1.671817
Cl4 -2.058115 -0.686749 0.546210
O5 -0.212795 1.600154 0.229397
H6 -0.119043 1.705262 -0.728754
H7 -1.177109 1.499333 0.362009
C8 2.172502 -0.369042 0.333246
H9 2.223949 0.494445 -0.331129
H10 2.081218 -0.914293 2.411945
H11 1.816274 0.880608 2.044179
H12 2.144408 -1.940347 -1.150127
H13 2.596308 -2.482935 0.476371
Cl4 2.684387 -1.662350 -0.239351
H15 3.742462 -1.549622 -0.511377

15

Ni.CCH.H2OH.post.xyz

Ni1 0.109685 -0.432427 0.761096
H2 0.179487 -1.792717 1.132387
C3 1.934641 -0.133407 1.671817
Cl4 -2.058115 -0.686749 0.546210
O5 -0.212795 1.600154 0.229397
H6 -0.119043 1.705262 -0.728754
H7 -1.177109 1.499333 0.362009
C8 2.172502 -0.369042 0.333246
H9 2.223949 0.494445 -0.331129
H10 2.081218 -0.914293 2.411945
H11 1.816274 0.880608 2.044179
H12 2.144408 -1.940347 -1.150127
H13 2.596308 -2.482935 0.476371
Cl4 2.684387 -1.662350 -0.239351
H15 3.742462 -1.549622 -0.511377

15

Ni.CCH.H2OH.pre.xyz

Ni1 0.230259 -0.136345 0.840487
H2 0.471647 -0.636519 2.417328
C3 1.650325 -0.582118 2.385421
Cl4 -2.021227 -0.273993 1.011375
O5 -0.027972 0.487610 -0.996596
H6 0.215353 -0.199364 -1.634025
H7 -1.009740 0.468261 -0.934543
C8 2.124469 -0.156770 1.040248
H9 2.506394 0.865724 0.989736
H10 1.914133 -1.603421 2.671763
H11 1.846098 0.120563 3.197944
H12 2.916379 -0.801442 -0.867713
H13 2.433246 -2.137628 0.196037
Cl4 2.884650 -1.139172 0.174650
H15 3.929232 -1.246274 0.501757

15

Ni.CCH.HCl.TS.xyz

Ni1 0.057662 -0.395687 -0.138595

H2 -0.020708 -1.610340 0.638936
C3 1.732951 0.063884 0.980637
Cl4 -0.018319 1.466812 -1.512270
O5 -1.839163 -0.587470 -0.641320
H6 -1.852475 0.140190 -1.301521
H7 -2.045876 -1.415869 -1.094609
C8 2.177707 -0.524415 -0.185015
H9 2.367699 0.125373 -1.036881
H10 1.700007 -0.493822 1.911620
H11 1.619864 1.142762 1.039151
Cl2 2.663729 -1.940492 -0.301253
H13 2.268914 -2.424253 -1.200410
H14 3.757974 -1.936688 -0.396258
H15 2.389842 -2.540757 0.569411

15

Ni.CCH.HCl.post.xyz

Ni1 0.057662 -0.395687 -0.138595
H2 -0.020708 -1.610340 0.638936
C3 1.732951 0.063884 0.980637
Cl4 -0.018319 1.466812 -1.512270
O5 -1.839163 -0.587470 -0.641320
H6 -1.852475 0.140190 -1.301521
H7 -2.045876 -1.415869 -1.094609
C8 2.177707 -0.524415 -0.185015
H9 2.367699 0.125373 -1.036881
H10 1.700007 -0.493822 1.911620
H11 1.619864 1.142762 1.039151
Cl2 2.663729 -1.940492 -0.301253
H13 2.268914 -2.424253 -1.200410
H14 3.757974 -1.936688 -0.396258
H15 2.389842 -2.540757 0.569411

15

Ni.CCH.HCl.pre.xyz

Ni1 0.134688 -0.053042 -0.123293
H2 0.302939 -0.026798 1.600745
C3 1.466514 -0.042201 1.595536
Cl4 0.028658 -0.049411 -2.306139
O5 -1.934044 0.092491 -0.085847
H6 -1.965299 0.254295 -1.051125
H7 -2.336781 -0.780307 0.030077
C8 1.987630 -0.112305 0.190271
H9 2.437973 0.813100 -0.174416
H10 1.685583 -0.921951 2.206446
H11 1.706262 0.876761 2.135093
Cl2 2.712950 -1.360820 -0.261098
H13 2.781959 -1.386082 -1.351478
H14 3.735927 -1.395665 0.142623
H15 2.199504 -2.272115 0.065560

14

Ni.CNH.H2OH.post.xyz

Ni1 -0.199938 -0.043634 -0.058593
H2 -0.389212 0.020401 1.350752
N3 1.562022 -0.657120 0.104993
Cl4 -2.190478 0.776969 -0.393134
C5 2.248874 -1.303133 0.971762
H6 3.303705 -1.494998 0.761471
C7 1.712181 -1.819709 2.256869
H8 0.658431 -1.570951 2.369036
H9 1.846472 -2.906206 2.301257
H10 2.283585 -1.398468 3.091268
O11 0.001373 -0.068329 -2.187096
H12 -0.259895 -0.934722 -2.523893
H13 -0.794565 0.487379 -2.291676
H14 2.108769 -0.393175 -0.715307

14

Ni.CNH.H2OH.pre.xyz

Ni1 0.026710 0.014220 -0.000336
H2 -0.074652 0.025390 2.504361
N3 0.638921 -0.014716 1.781694
Cl4 -0.932526 1.982129 -0.618271
C5 0.875072 -1.270982 1.116165
H6 1.936162 -1.448649 0.932714
C7 0.108755 -2.471542 1.621802
H8 -0.948192 -2.235149 1.787074
H9 0.145509 -3.270418 0.875453
H10 0.520942 -2.874557 2.558482
O11 -0.416750 -0.629168 -1.821788
H12 -0.862263 0.215572 -2.061557
H13 0.384630 -0.669188 -2.362487
H14 1.428917 0.587202 1.992298

14

Ni.CNH.HCl.post.xyz

Ni1 -0.205738 -0.089105 -0.073970
H2 -0.467035 -0.321278 1.335853
N3 1.529464 -0.781347 0.040746
Cl4 0.113116 0.461208 -2.313924
C5 2.254042 -1.401522 0.895128
H6 3.267937 -1.686955 0.597385
C7 1.829881 -1.772986 2.272000
H8 0.816343 -1.425857 2.473888
H9 1.880958 -2.862518 2.389329
H10 2.528130 -1.343913 3.000868
O11 -1.995629 0.615599 -0.328748
H12 -2.148961 1.391214 0.228439
H13 -1.868459 0.929321 -1.250559
H14 1.981154 -0.617744 -0.860963

14

Ni.CNH.HCl.pre.xyz

Ni1 0.112046 0.006774 -0.150321
H2 0.779046 -0.440611 2.288553
N3 1.078685 0.138467 1.508724
Cl4 -0.216838 -0.577801 -2.255371
C5 1.797759 -0.515260 0.436150
H6 2.616177 0.095570 0.050965
C7 2.116685 -1.981352 0.600672
H8 1.262594 -2.539245 0.999905
H9 2.349776 -2.406949 -0.378896
H10 2.980359 -2.152365 1.260155
O11 -1.841205 0.722639 -0.160626
H12 -1.831301 1.679438 -0.306344
H13 -1.983054 0.337960 -1.051580
H14 1.415400 1.043037 1.823164

13

Ni.CO.H2OH.pre.xyz

Ni1 0.103976 -0.128812 0.099162
H2 0.039354 -0.115998 2.518400
O3 0.789965 -0.165979 1.903403
C4 0.829508 -1.441791 1.224099
H5 1.878566 -1.696964 1.063405
C6 -0.022478 -2.535133 1.813041
H7 -1.062407 -2.215187 1.947546
H8 -0.034918 -3.385400 1.123761
H9 0.361094 -2.896772 2.777660
Cl10 -0.800071 1.828999 -0.604984
O11 -0.387573 -0.847656 -1.656739
H12 -0.809495 -0.005169 -1.946844
H13 0.402491 -0.955243 -2.206375

13

Ni.CO.HCl.pre.xyz

Ni1 0.015088 -0.006543 -0.035875
H2 1.051615 -0.178551 2.201819
O3 1.436600 0.031480 1.336192

C14 -1.101276 -0.869579 -1.710179
C5 1.373389 -1.137585 0.472945
H6 2.243881 -1.111605 -0.184745
C7 1.113507 -2.450683 1.158412
H8 0.236666 -2.402571 1.814634
H9 0.900457 -3.203789 0.394444
H10 1.976304 -2.796093 1.745299
O11 -1.289325 1.593992 -0.052284
H12 -0.880471 2.356246 -0.487144
H13 -1.856955 1.182191 -0.734898

15

Pd.CCH.H2OH.TS.xyz

Pd1 0.106819 -0.147685 0.873182
H2 0.574352 -0.594533 2.512796
C3 1.781219 -0.504106 2.427289
C14 -2.332271 -0.217794 0.846260
O5 -0.236140 0.494857 -1.243141
H6 -0.803357 -0.254439 -1.494747
H7 -0.903367 1.167698 -1.018250
C8 2.163176 -0.132768 1.053655
H10 2.487820 0.900698 0.916691
H11 2.071918 -1.507227 2.745704
H12 1.974737 0.246040 3.194924
H13 2.736135 -0.833655 -0.901003
H15 2.437755 -2.136616 0.269453
C15 2.845396 -1.127689 0.147585
H16 3.923257 -1.175746 0.361036

15

Pd.CCH.H2OH.post.xyz

Pd1 0.050138 -0.408387 0.787661
H2 0.080319 -1.854309 1.191824
C3 2.037131 -0.192208 1.721139
C14 -2.283171 -0.548085 0.491555
O5 -0.305749 1.817009 0.151328
H6 -0.205062 1.871943 -0.809882
H7 -1.265146 1.679865 0.277443
C8 2.261426 -0.412551 0.373525
H10 2.356626 0.461137 -0.271725
H11 2.167742 -0.991461 2.444603
H12 1.986437 0.817887 2.117773
H13 2.225181 -1.936632 -1.158808
H15 2.585628 -2.548881 0.466605
C15 2.737914 -1.711788 -0.218895
H16 3.810526 -1.637780 -0.442865

15

Pd.CCH.H2OH.pre.xyz

Pd1 0.154337 -0.155127 0.886018
H2 0.528570 -0.681706 2.543205
C3 1.732204 -0.628316 2.517617
C14 -2.297471 -0.175090 0.668824
O5 -0.121334 0.554432 -1.196086
H6 -0.002114 -0.205316 -1.784316
H7 -1.096004 0.583293 -1.027413
C8 2.191980 -0.196657 1.182690
H10 2.543705 0.834974 1.116707
H11 1.987895 -1.653190 2.794201
H12 1.915651 0.075523 3.330664
H13 2.899495 -0.817591 -0.758951
H15 2.492474 -2.167306 0.323985
C15 2.922559 -1.161285 0.280274
H16 3.981229 -1.239465 0.567631

15

Pd.CCH.HCl.TS.xyz

Pd1 0.013700 -0.055756 -0.034124
H2 -0.106977 -0.151707 1.516023
C3 1.661528 -0.030161 1.458984

C14 0.049923 0.079478 -2.472343
O5 -2.174882 0.019751 -0.467473
H6 -1.995962 0.133424 -1.427610
H7 -2.533257 -0.875143 -0.380660
C8 2.138185 -0.153378 0.136485
H10 2.452024 0.756834 -0.371848
H11 1.695879 -0.891057 2.121240
H12 1.666663 0.938052 1.950191
C13 2.693520 -1.438074 -0.423440
H14 2.459925 -1.526679 -1.486688
H15 3.786991 -1.439455 -0.316732
H16 2.299812 -2.314766 0.098940

15

Pd.CCH.HCl.post.xyz

Pd1 0.015335 -0.363004 -0.129289
H2 -0.033590 -1.594206 0.786320
C3 1.817921 0.123572 0.970613
C14 -0.124398 1.544605 -1.708569
O5 -2.081029 -0.502209 -0.773379
H6 -1.983125 0.279207 -1.365980
H7 -2.219813 -1.266621 -1.349839
C8 2.224903 -0.477980 -0.216108
H10 2.406738 0.170933 -1.071166
H11 1.848215 -0.424892 1.907341
H12 1.740382 1.205074 1.036073
C13 2.754881 -1.880351 -0.322252
H14 2.392478 -2.376203 -1.227313
H15 3.850295 -1.840976 -0.394566
H16 2.484933 -2.488017 0.544716

15

Pd.CCH.HCl.pre.xyz

Pd1 0.056621 -0.033416 -0.114035
H2 0.497699 -0.001138 1.765891
C3 1.652274 -0.038273 1.661533
C14 -0.050147 -0.067833 -2.476268
O5 -2.252430 0.082827 -0.325465
H6 -2.139343 0.210918 -1.288200
H7 -2.594977 -0.818314 -0.243364
C8 2.044057 -0.112308 0.213375
H10 2.470935 0.807789 -0.191209
H11 1.918683 -0.925575 2.241372
H12 1.965230 0.875876 2.170445
C13 2.720468 -1.362828 -0.298328
H14 2.704214 -1.385699 -1.390248
H15 3.771239 -1.389158 0.027142
H16 2.234719 -2.271112 0.073382

14

Pd.CNH.H2OH.post.xyz

Pd1 0.107820 0.235152 -0.039349
H2 0.447170 0.692134 1.357973
N3 1.945622 -0.716932 -0.143893
C14 -1.966532 1.314636 0.107394
C5 2.324518 -1.829446 0.366801
H6 3.342967 -2.183149 0.182388
C7 1.443137 -2.680183 1.208105
H8 0.470736 -2.209415 1.338477
H9 1.323958 -3.666427 0.744116
H10 1.914446 -2.843932 2.181282
O11 -0.701428 -0.338650 -2.177178
H12 -1.573568 -0.007889 -1.888013
H13 -0.382924 0.346997 -2.783444
H14 2.671059 -0.247134 -0.683756

14

Pd.CNH.H2OH.pre.xyz

Pd1 0.037728 -0.087454 -0.000334
H2 -0.197946 0.155353 2.674504

N3 0.574093 0.084368 2.019491
C4 0.896086 -1.187866 1.478584
C5 0.150629 -2.395043 1.989997
O6 -0.216771 -0.153937 -1.942294
C17 -1.031850 1.629453 -1.439551
H8 1.967323 -1.324053 1.325095
H9 -0.916318 -2.186684 2.119027
H10 0.238637 -3.208923 1.265088
H11 0.555334 -2.754001 2.946918
H12 -0.717321 -0.365005 -2.270146
H13 0.631816 -1.108351 -2.405283
H14 1.319365 0.745333 2.208585

14

Pd.CNH.HCl.post.xyz

Pd1 -0.151515 -0.165168 0.058481
H2 -0.565024 -1.012301 1.292570
N3 1.824422 -0.045301 0.766249
C14 0.288721 1.287392 -1.920476
C5 1.804952 -1.191785 0.058493
H6 2.164687 -1.198081 -0.976103
C7 1.761327 -2.525137 0.745698
H8 1.390365 -2.429375 1.766887
H9 1.145095 -3.236962 0.190016
H10 2.784017 -2.926113 0.773689
O11 -2.154803 0.099029 -0.663436
H12 -2.694618 0.601798 -0.035035
H13 -1.932185 0.697913 -1.413121
H14 2.165415 0.719320 0.175285

14

Pd.CNH.HCl.pre.xyz

Pd1 0.072860 0.023022 -0.050099
H2 1.070290 -0.499494 2.494097
N3 1.322899 0.094590 1.711620
C14 -0.293979 -0.612603 -2.321804
C5 1.890257 -0.525027 0.559172
H6 2.660687 0.085827 0.086206
C7 2.191155 -2.002071 0.623628
H8 1.384896 -2.558499 1.112346
H9 2.292396 -2.392513 -0.391622
H10 3.128895 -2.198825 1.162929
O11 -2.119099 0.795237 -0.334610
H12 -2.038255 1.730645 -0.567255
H13 -2.110357 0.334550 -1.199430
H14 1.677949 0.998921 1.998686

13

Pd.COH.H2OH.post.xyz

Pd1 -0.176619 -0.148588 0.004756
H2 -0.521746 -1.571081 0.326030
O3 1.276049 0.017594 1.605302
C14 -1.795743 -0.285778 -1.649197
C5 2.041028 -0.657114 0.885703
H6 2.668572 -0.143575 0.132711
C7 2.338959 -2.108663 1.116522
H8 1.607047 -2.552470 1.792977
H9 2.368823 -2.655865 0.169463
H10 3.340623 -2.181071 1.563709
O11 0.030675 2.064656 -0.690285
H12 0.790925 2.197412 -1.273287
H13 -0.732977 1.984116 -1.290232

13

Pd.COH.H2OH.pre.xyz

Pd1 0.071893 -0.084156 -0.021689
H2 0.957090 -0.263406 2.538166
O3 1.494890 -0.023283 1.765918
C14 -1.800824 1.286150 -0.891023
C5 1.545302 -1.097059 0.855005

H6 2.468001 -1.013078 0.275139
C7 1.220122 -2.465851 1.389476
H8 0.270560 -2.469411 1.937730
H9 1.119709 -3.165814 0.555669
H10 2.010608 -2.840323 2.054224
O11 -0.599402 -1.249361 -1.779173
H12 -1.361256 -0.615782 -1.846606
H13 -0.022305 -1.003293 -2.517046

13

Pt.COH.HCl.post.xyz

Pd1 -0.387789 -0.076689 0.131401
H2 -1.173119 -1.269827 0.633036
O3 1.057907 -0.542140 1.595616
Cl4 0.671922 1.888921 -0.956823
C5 2.055152 -0.829174 0.903926
H6 2.398886 -0.117087 0.113967
C7 2.834858 -2.073470 1.130455
H8 2.334505 -2.716063 1.882079
H9 2.948731 -2.609368 0.166187
H10 3.849409 -1.796596 1.468050
O11 -1.860572 0.311006 -1.338006
H12 -1.397142 1.109337 -1.688290
H13 -1.827939 -0.324655 -2.050561

13

Pd.COH.HCl.pre.xyz

Pd1 0.022866 0.046820 -0.047584
H2 1.255079 -0.722643 2.308716
O3 1.478897 0.079913 1.810931
Cl4 0.022853 -0.555148 -2.333894
C5 1.882328 -0.286960 0.504723
H6 2.514675 0.510984 0.108100
C7 2.424261 -1.682138 0.337165
H8 1.737223 -2.433409 0.744124
H9 2.545558 -1.892255 -0.727876
H10 3.399055 -1.790174 0.832309
O11 -2.236416 0.471277 -0.454926
H12 -2.326688 1.417119 -0.636751
H13 -2.132571 0.064138 -1.336686

14

Pt.CNH.H2OH.post.xyz

Pt1 0.012346 0.052078 0.025359
H2 -0.075526 0.110996 1.539755
N3 2.151646 -0.147391 0.127287
Cl4 -2.239185 0.626492 -0.204793
C5 1.674972 -1.405277 0.147773
H6 1.665868 -2.005482 -0.769494
C7 1.625838 -2.188910 1.429868
H8 1.642722 -1.524639 2.295258
H9 0.738028 -2.825896 1.470603
H10 2.506915 -2.843846 1.471714
O11 -0.009443 0.051246 -2.342434
H12 -0.973876 -0.073893 -2.396664
H13 0.117375 0.981665 -2.581873
H14 2.421011 0.104964 -0.827243

14

Pt.CNH.H2OH.pre.xyz

Pt1 0.035374 -0.087407 -0.017464
H2 -0.246543 0.230412 2.599027
N3 0.526126 0.141878 1.943269
C4 0.878269 -1.190226 1.473051
C5 0.142234 -2.354976 2.095454
O6 -0.248469 -0.972106 -1.988466
Cl7 -1.068122 1.715615 -1.332873
H8 1.959872 -1.323418 1.416431
H9 -0.930007 -2.155244 2.185957
H10 0.252741 -3.231110 1.449957

H11 0.539745 -2.615732 3.085932
H12 -0.726955 -0.182921 -2.349592
H13 0.618113 -0.971530 -2.422660
H14 1.275496 0.798944 2.142643

14

Pt.CNH.HCl.post.xyz

Pt1 -0.151515 -0.165168 0.058481
H2 -0.565024 -1.012301 1.292570
N3 1.824422 -0.045301 0.766249
Cl4 0.288721 1.287392 -1.920476
C5 1.804952 -1.191785 0.058493
H6 2.164687 -1.198081 -0.976103
C7 1.761327 -2.525137 0.745698
H8 1.390365 -2.429375 1.766887
H9 1.145095 -3.236962 0.190016
H10 2.784017 -2.926113 0.773689
O11 -2.154803 0.099029 -0.663436
H12 -2.694618 0.601798 -0.035035
H13 -1.932185 0.697913 -1.413121
H14 2.165415 0.719320 0.175285

14

Pt.CNH.HCl.pre.xyz

Pt1 0.041297 -0.002844 -0.090016
H2 1.072842 -0.422798 2.399817
N3 1.345759 0.075915 1.558277
Cl4 -0.785175 -0.611750 -2.217458
C5 1.831569 -0.713387 0.435227
H6 2.671959 -0.227813 -0.065518
C7 2.029966 -2.194450 0.666651
H8 1.192061 -2.636005 1.214550
H9 2.087056 -2.698106 -0.301976
H10 2.960937 -2.399011 1.212623
O11 -2.049199 1.083620 -0.119967
H12 -1.824644 1.980704 -0.406818
H13 -2.307216 0.626175 -0.945927
H14 1.810646 0.954893 1.760294

13

Pt.COH.H2OH.post.xyz

Pt1 -0.173415 -0.189984 0.053707
H2 -0.573042 -1.584567 0.504581
O3 1.126059 0.042910 1.701467
Cl4 -1.784154 -0.247766 -1.609335
C5 1.877417 -0.529749 0.832839
H6 2.522532 0.106057 0.201694
C7 2.298023 -1.968999 0.951670
H8 1.574670 -2.540256 1.535294
H9 2.425903 -2.421550 -0.035610
H10 3.271554 -2.000827 1.460298
O11 0.254486 1.977044 -0.757408
H12 0.942015 1.919123 -1.436455
H13 -0.574897 2.059980 -1.260176

13

Pt.COH.H2OH.pre.xyz

Pt1 0.052988 -0.076488 -0.020119
H2 0.841543 -0.064017 2.467276
O3 1.350962 0.133796 1.662456
Cl4 -1.795055 1.472674 -0.653775
C5 1.550895 -1.074603 0.877269
H6 2.530473 -0.986261 0.405991
C7 1.312871 -2.362278 1.621902
H8 0.333479 -2.361854 2.122442
H9 1.308888 -3.189632 0.900247
H10 2.102659 -2.567818 2.365522
O11 -0.704902 -0.930215 -1.841445
H12 -1.461494 -0.291436 -1.897455
H13 -0.052413 -0.567249 -2.461519

13

Pt.COH.HCl.post.xyz

Pt1 -0.207262 -0.165672 0.190474
H2 -0.692945 -1.410840 0.981562
O3 1.206854 0.065767 1.679564
Cl4 0.360356 1.739815 -1.353772
C5 1.917357 -0.464007 0.744999
H6 2.429739 0.209249 0.042608
C7 2.410514 -1.877225 0.826949
H8 1.757742 -2.488427 1.451524
H9 2.505509 -2.313003 -0.171461
H10 3.415859 -1.856380 1.271215
O11 -1.774709 -0.222426 -1.215340
H12 -1.439670 0.522228 -1.781269
H13 -1.754090 -1.035252 -1.742169

13

Pt.COH.HCl.pre.xyz

Pt1 -0.026687 0.032506 0.015030
H2 1.005065 -0.297455 2.459632
O3 1.496875 -0.022402 1.668498
Cl4 -1.093428 -0.884033 -1.837373
C5 1.443342 -1.099508 0.686910
H6 2.354128 -1.022941 0.088080
C7 1.201673 -2.477027 1.253035
H8 0.303687 -2.512576 1.878922
H9 1.046531 -3.172334 0.423150
H10 2.063053 -2.827814 1.836299
O11 -1.616700 1.702248 -0.397358
H12 -1.127506 2.373504 -0.895283
H13 -2.083874 1.182739 -1.079552