

## Supplementary Material

### Aminomethylpyridinequinones as new ligands for PEPPSI-type complexes

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#### Table of Contents

<b>Computational details</b> .....	S2
<b>Table S1.</b> Structural and electronic data from DFT calculations .....	S2
<b>Table S2.</b> Effect of the PEPPSI type ligands on the metal centre (%V <sub>Bur</sub> ).....	S2
<b>Table S3.</b> Effect of the PEPPSI type ligands on the NHC ligand (%V <sub>Bur</sub> ).....	S3
<b>Steric maps</b> .....	S4
<b>NCI plots</b> .....	S28
<b>xyz coordinates of all computed species</b> .....	S33
<b>Table S4.</b> Basic details about X-ray experiments for PEPPSI-BQ complexes.....	S317
<b>Table S5.</b> Basic details about X-ray experiments for PEPPSI-NQ complexes. ....	S318

**Computational details**

All DFT calculations were performed at the GGA level with Gaussian16 set of programs,<sup>1</sup> using the BP86 functional of Becke and Perdew,<sup>2,3</sup> adding the Grimme D3 dispersion term.<sup>4</sup> The electronic configuration of the molecular systems was described with the split valence basis set def2SVP for the main group atoms,<sup>5,6</sup> while for palladium we adopted the quasi-relativistic Stuttgart/Dresden effective core potential with an associated valence contracted basis set (standard SDD keywords in Gaussian 16).<sup>7-9</sup> The geometry optimizations were performed without symmetry constraints. All studied ligand-metal complexes were considered in singlet spin state, as ground state. All the geometry optimizations used the polarizable solvation model (PCM) with DMF as the solvent.<sup>10</sup> The reported energies are Gibbs free energies.

**Table S1.** Structural and electronic data from DFT calculations

	Pd-N	MBO	HOMA	LUMO	Chemical Potential	Chemical Hardness	Electro-philicity	Charge Pd	Charge N
<b>PEPPSI-Py</b>	2.132	0.409	-0.231	-0.067	-0.149	0.164	0.068	0.185	-0.487
<b>PEPPSI</b>	2.135	0.378	-0.232	-0.070	-0.151	0.162	0.070	0.186	-0.477
<b>7a</b>	2.132	0.387	-0.228	-0.118	-0.173	0.110	0.137	0.163	-0.490
<b>7b</b>	2.131	0.401	-0.230	-0.119	-0.175	0.111	0.137	0.191	-0.479
<b>7c</b>	2.131	0.410	-0.231	-0.118	-0.174	0.113	0.135	0.186	-0.491
<b>7d</b>	2.133	0.387	-0.225	-0.121	-0.173	0.104	0.145	0.163	-0.490
<b>7e</b>	2.120	0.400	-0.229	-0.122	-0.176	0.107	0.144	0.188	-0.477
<b>7f</b>	2.129	0.410	-0.228	-0.119	-0.174	0.109	0.139	0.184	-0.491

**Table S2.** Effect of the PEPPSI type ligands on the metal centre (%V<sub>Bur</sub>)

Catalyst	%V <sub>Bur</sub> (total)	%V <sub>Bur</sub> (SW)	%V <sub>Bur</sub> (NW)	%V <sub>Bur</sub> (NE)	%V <sub>Bur</sub> (SE)
<b>PEPPSI-Py</b>	19.5	19.5	19.5	19.5	19.5
<b>PEPPSI</b>	19.5	19.4	19.8	19.4	19.4
<b>7a</b>	28.0	27.7	44.2	20.8	19.4
<b>7b</b>	19.9	19.0	22.1	19.3	19.3
<b>7c</b>	19.4	19.5	19.3	19.4	19.4
<b>7d</b>	27.9	27.6	43.8	20.7	19.4
<b>7e</b>	19.8	19.1	21.1	19.6	19.6
<b>7f</b>	22.3	18.7	27.1	23.7	19.5

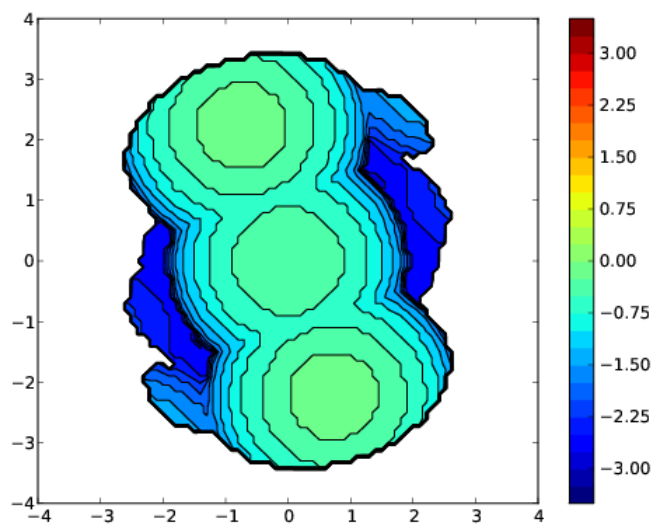
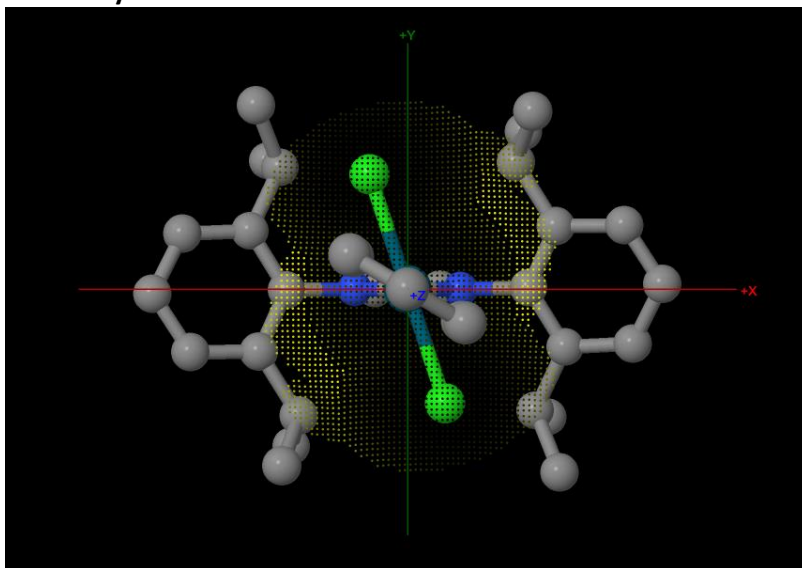
**Table S3.** Effect of the PEPPSI type ligands on the NHC ligand (%V<sub>Bur</sub>)

Catalyst	%V <sub>Bur</sub> (total)	%V <sub>Bur</sub> (SW)	%V <sub>Bur</sub> (NW)	%V <sub>Bur</sub> (NE)	%V <sub>Bur</sub> (SE)
<b>PEPPSI-Py</b>	37.0	30.2	43.8	30.2	43.7
<b>PEPPSI</b>	38.1	32.5	49.0	28.2	42.5
<b>7a</b>	37.1	29.8	42.9	32.1	43.4
<b>7b</b>	38.9	32.5	52.3	27.8	42.9
<b>7c</b>	36.6	30.4	42.4	30.8	43.0
<b>7d</b>	37.1	29.9	43.0	31.9	43.6
<b>7e</b>	39.1	33.5	51.5	27.9	43.4
<b>7f</b>	38.0	28.3	40.5	33.2	49.8

### Steric maps

Steric maps (xy plane). The linking N atom of the pyridine is at the centre, whereas the metal on the z axis, and 2 Å below the xy plane described by the metal and both halide atoms. The isocontour curves of the steric maps are given in Å.

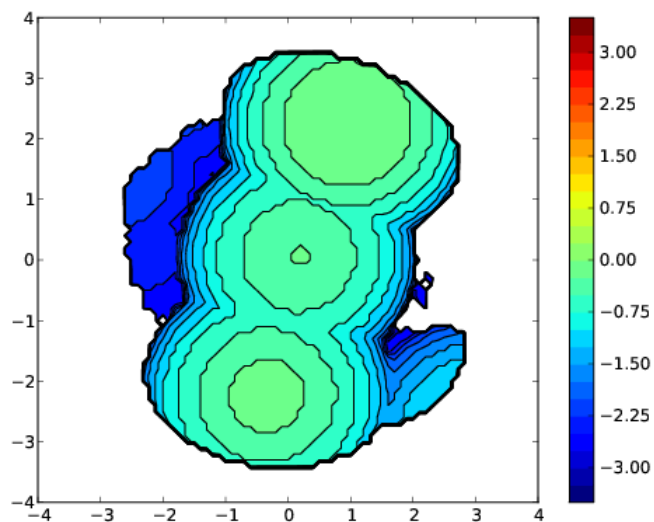
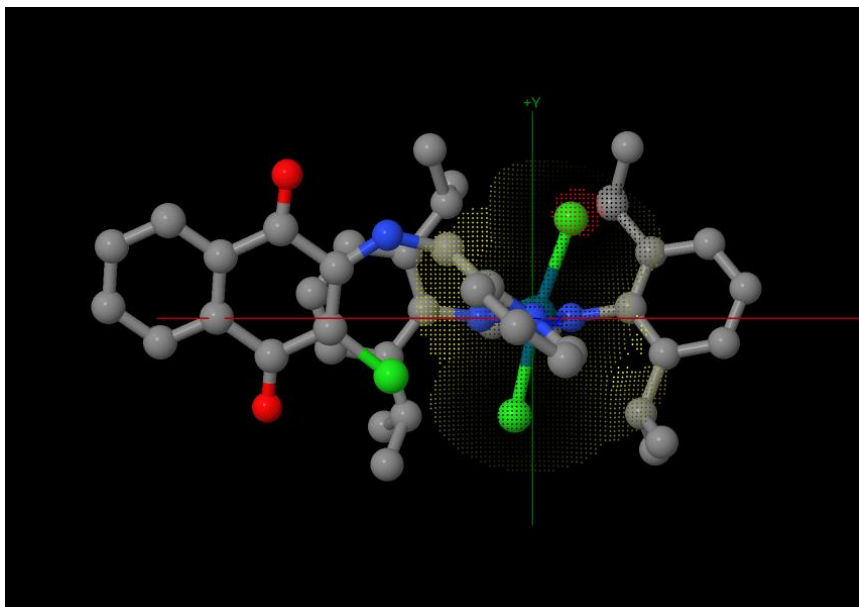
- **PEPPSI-Py:**



%V Free	%V Buried	% V Tot/V Ex
71.5	28.5	99.9

Quadrant	V f	V b	V t	%V f	%V b
SW	34.5	10.4	44.9	76.9	23.1
NW	29.6	15.2	44.9	66.0	34.0
NE	34.5	10.3	44.9	77.0	23.0
SE	29.7	15.2	44.9	66.1	33.9

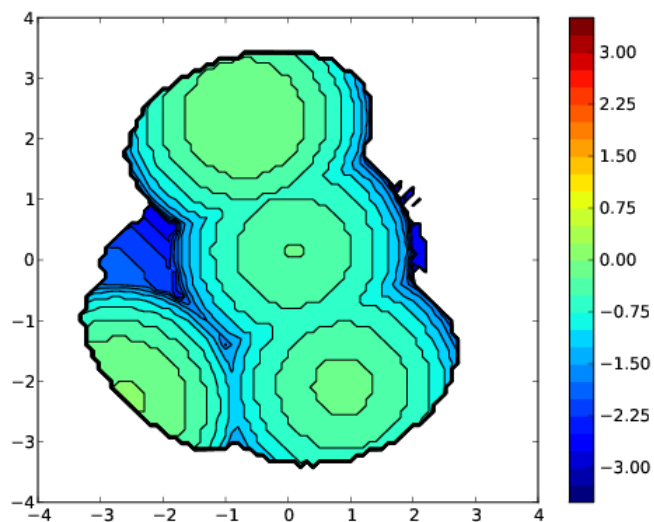
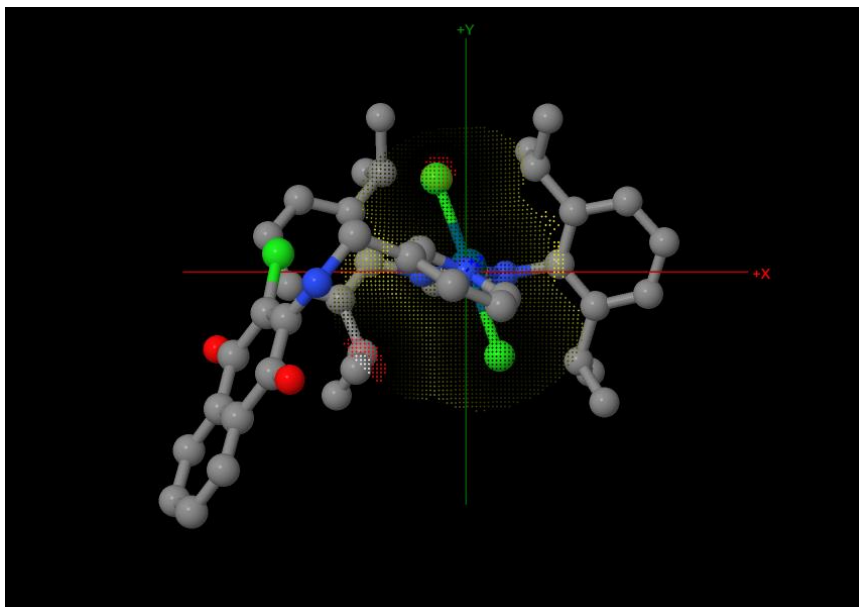
## ▪ 7a



%V Free	%V Buried	% V Tot/V Ex
70.9	29.1	99.9

Quadrant	V f	V b	V t	%V f	%V b
SW	31.3	13.5	44.9	69.9	30.1
NW	35.2	9.6	44.9	78.5	21.5
NE	28.0	16.9	44.9	62.4	37.6
SE	32.6	12.3	44.9	72.6	27.4

- 7b

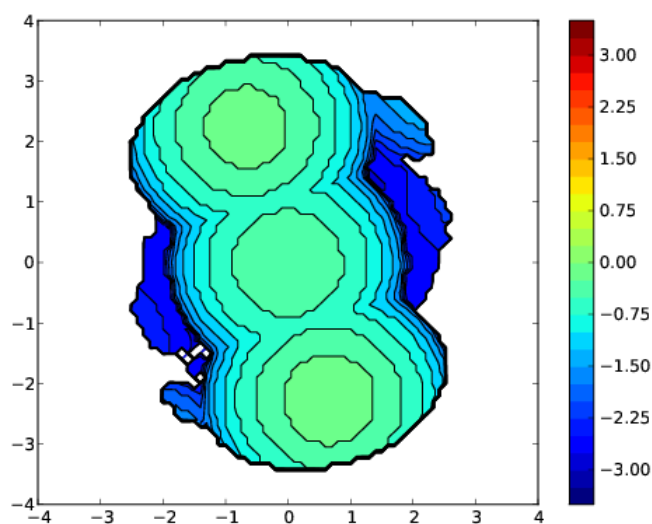
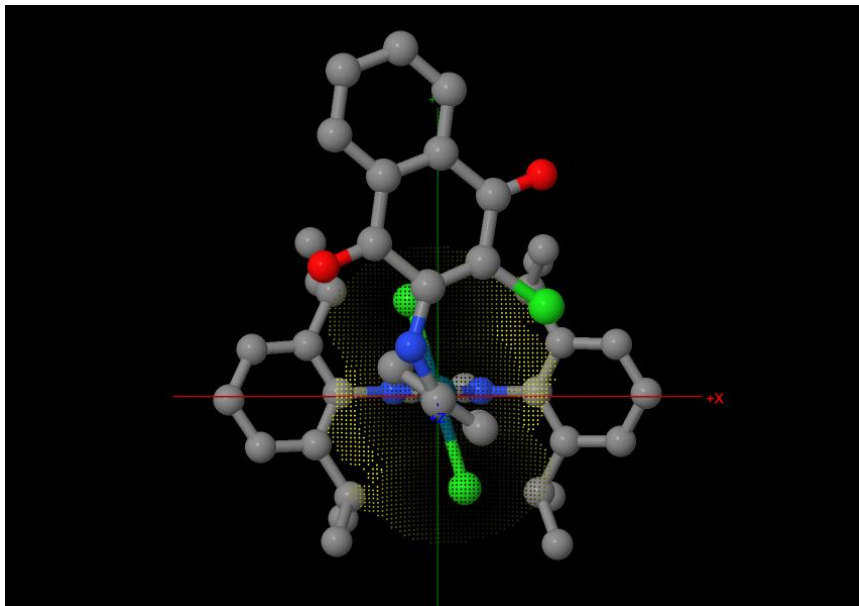


%V Free	%V Buried	% V Tot/V Ex
67.9	32.1	99.9

Quadrant	V f	V b	V t	%V f	%V b
SW	29.2	15.6	44.9	65.1	34.9
NW	29.2	15.7	44.9	65.0	35.0
NE	34.0	10.8	44.9	75.9	24.1
SE	29.4	15.4	44.9	65.6	34.4

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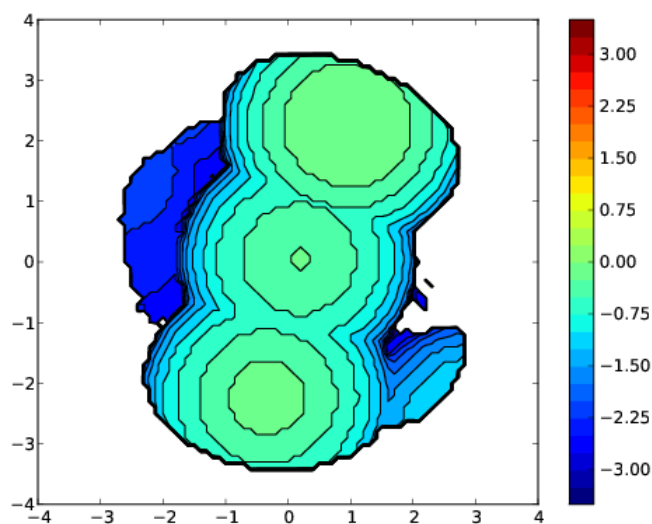
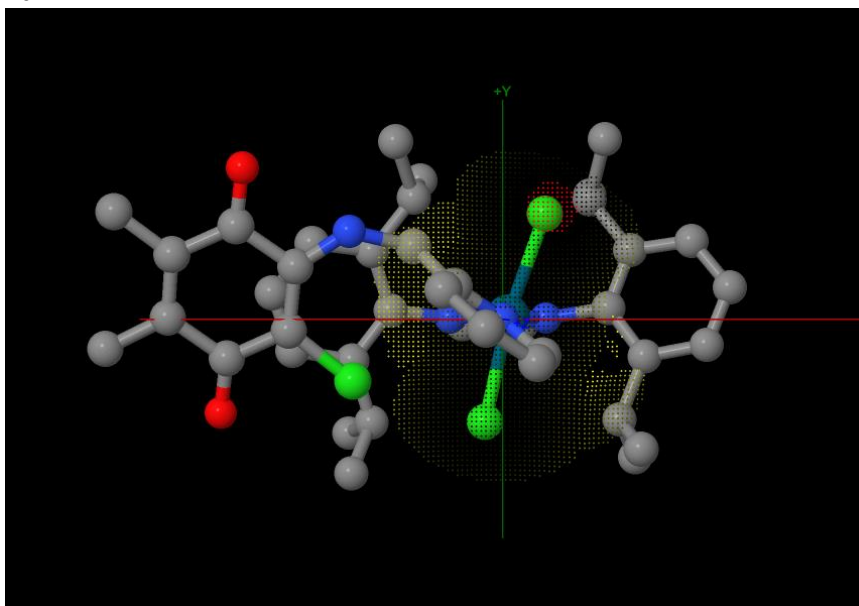
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- 7c



%V Free	%V Buried	% V Tot/V Ex
71.7	28.3	99.9

Quadrant	V f	V b	V t	%V f	%V b
SW	34.5	10.4	44.9	76.9	23.1
NW	30.0	14.9	44.9	66.9	33.1
NE	34.4	10.5	44.9	76.6	23.4
SE	29.9	15.0	44.9	66.6	33.4

▪ 7d

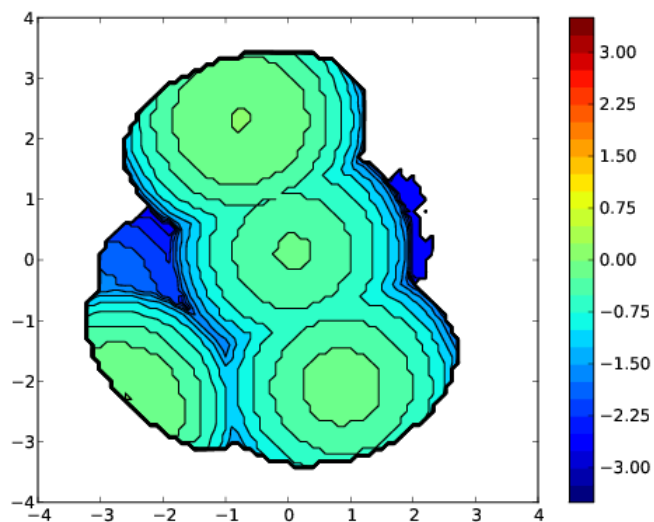
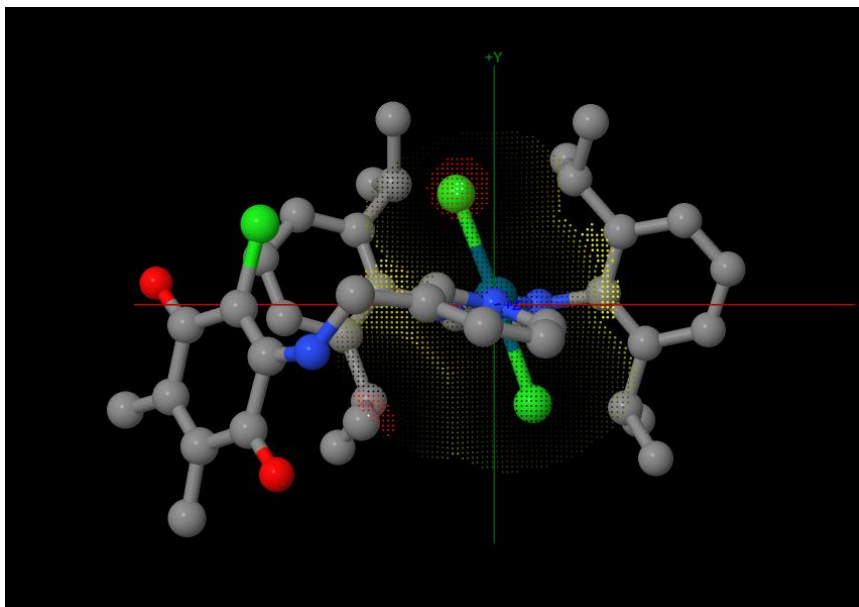


%V Free	%V Buried	% V Tot/V Ex
70.8	29.2	99.9

Quadrant	V f	V b	V t	%V f	%V b
SW	31.3	13.5	44.9	69.9	30.1
NW	35.2	9.7	44.9	78.5	21.5
NE	28.0	16.9	44.9	62.4	37.6
SE	32.5	12.4	44.9	72.4	27.6



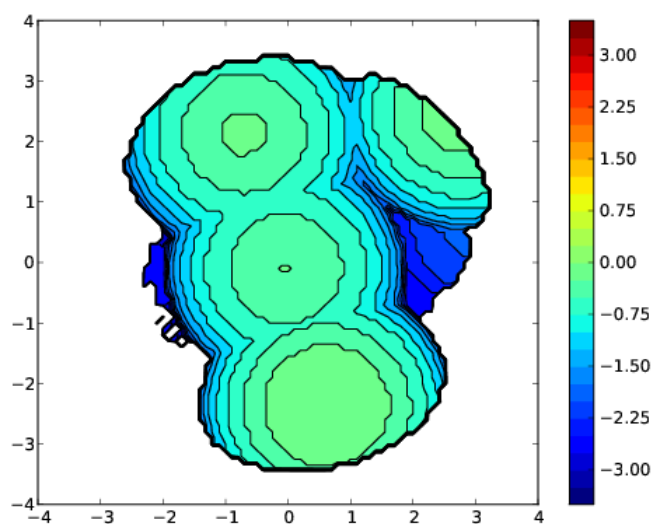
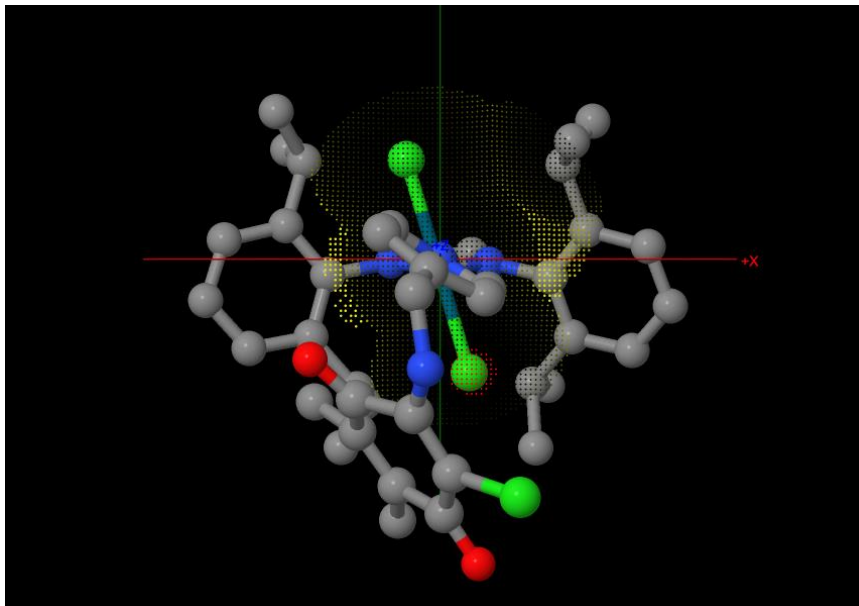
- 7e



%V Free	%V Buried	% V Tot/V Ex
67.5	32.5	99.9

Quadrant	V f	V b	V t	%V f	%V b
SW	29.4	15.4	44.9	65.6	34.4
NW	28.5	16.4	44.9	63.6	36.4
NE	34.1	10.8	44.9	75.9	24.1
SE	29.2	15.7	44.9	65.1	34.9

## ▪ 7f



%V Free

%V Buried

% V Tot/V Ex

69.1

30.9

99.9

Quadrant

V f

V b

V t

%V f

%V b

SW

33.9

10.9

44.9

75.6

24.4

NW

30.2

14.7

44.9

67.2

32.8

NE

30.5

14.4

44.9

68.0

32.0

SE

29.4

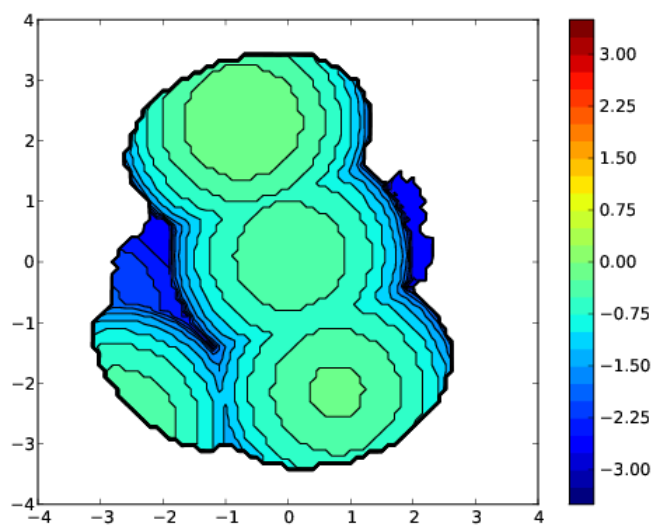
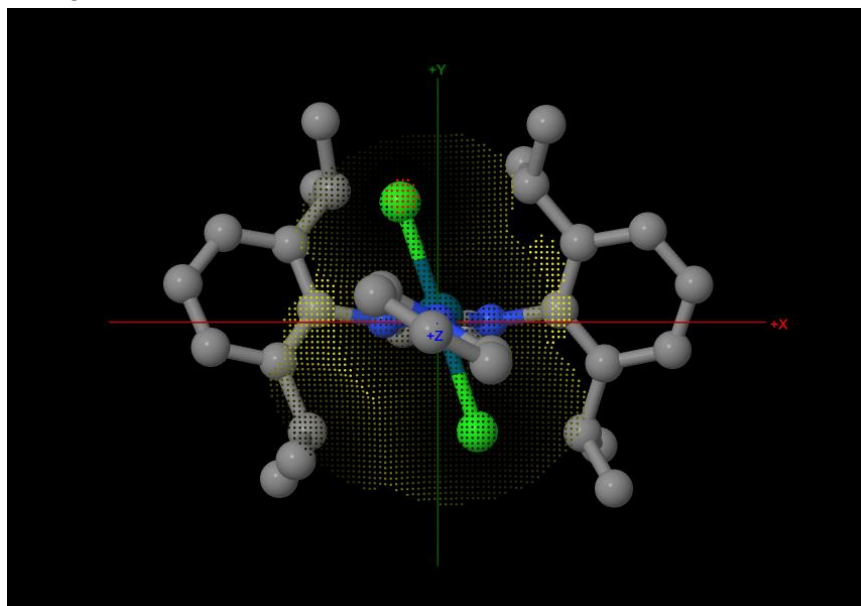
15.5

44.9

65.5

34.5

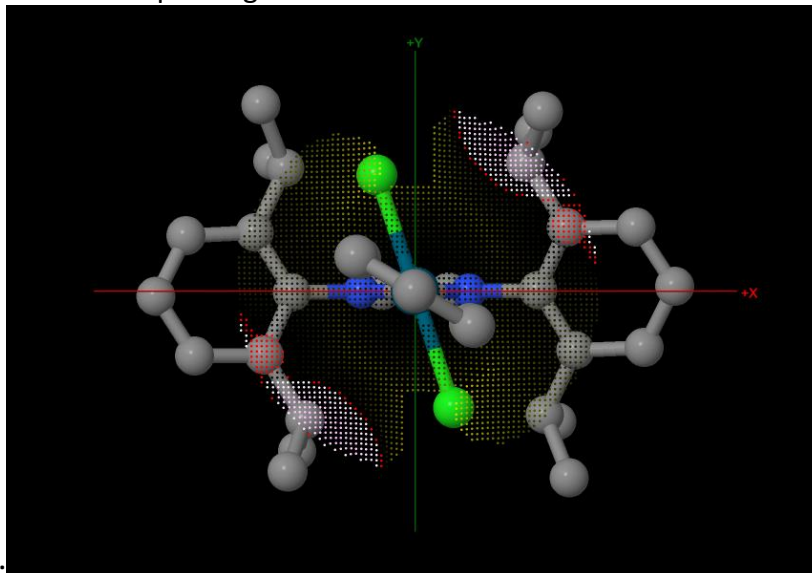
▪ PEPPSI



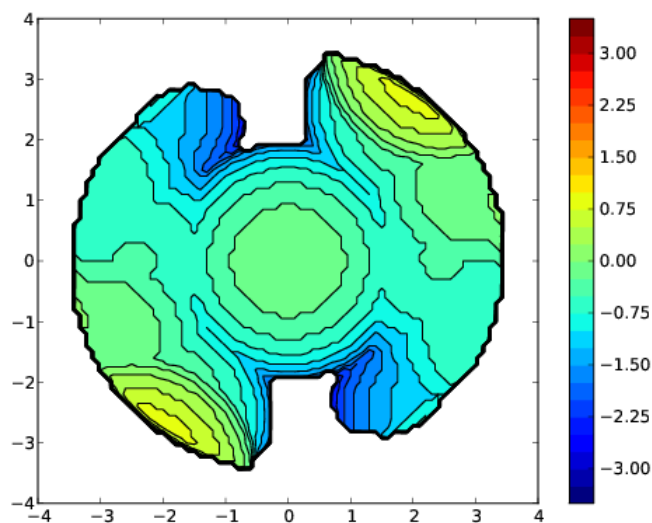
%V Free	%V Buried	% V Tot/V Ex
69.6	30.4	99.9

Quadrant	V f	V b	V t	%V f	%V b
SW	31.5	13.4	44.9	70.2	29.8
NW	29.2	15.6	44.9	65.1	34.9
NE	34.4	10.5	44.9	76.6	23.4
SE	29.9	15.0	44.9	66.6	33.4

Steric maps (xy plane). The metal is at the centre, whereas linking C atom of the NHC ligand on the z axis. The isocontour curves of the steric maps are given in Å.



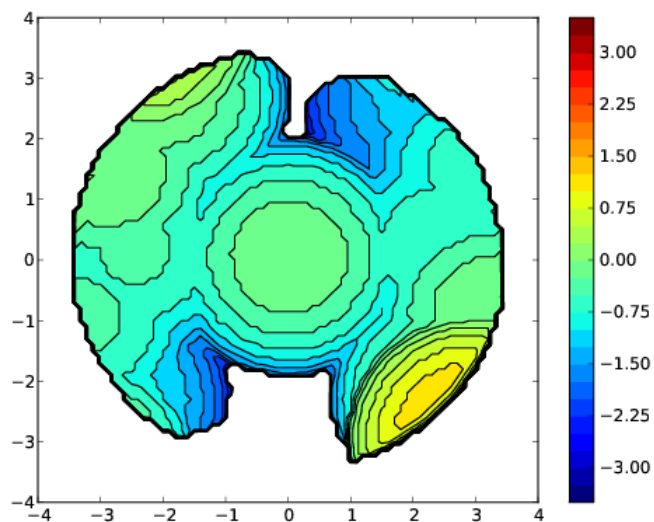
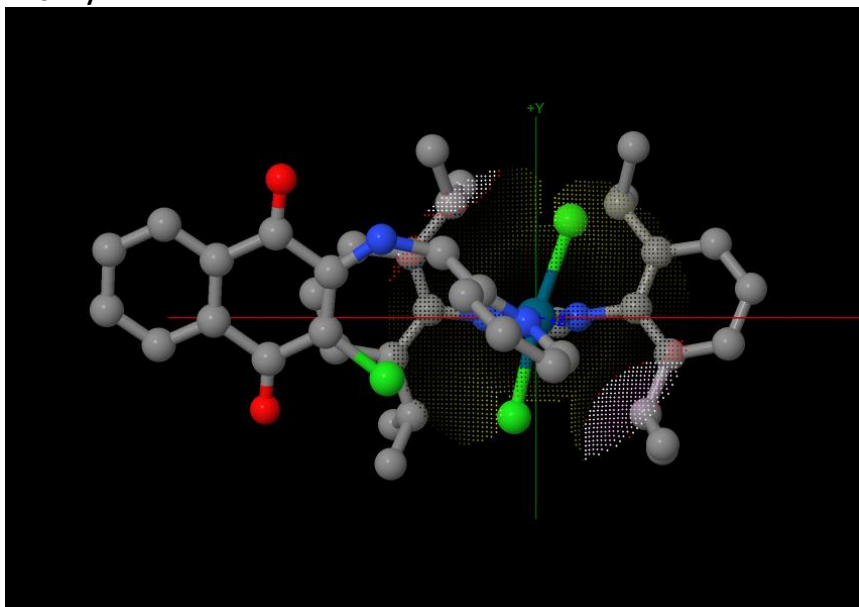
▪ IPrCl<sub>2</sub>Py:



%V Free	%V Buried	% V Tot/V Ex
63.0	37.0	99.9

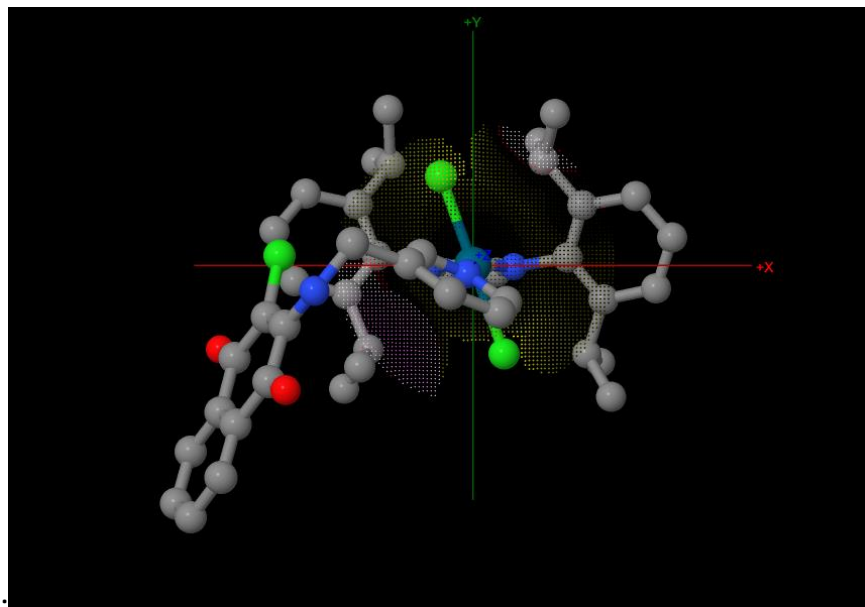
Quadrant	V f	V b	V t	%V f	%V b
SW	25.2	19.6	44.9	56.2	43.8
NW	31.3	13.6	44.9	69.8	30.2
NE	25.3	19.6	44.9	56.3	43.7
SE	31.3	13.5	44.9	69.8	30.2

- IPrCl<sub>2</sub>Py<sub>1</sub>:

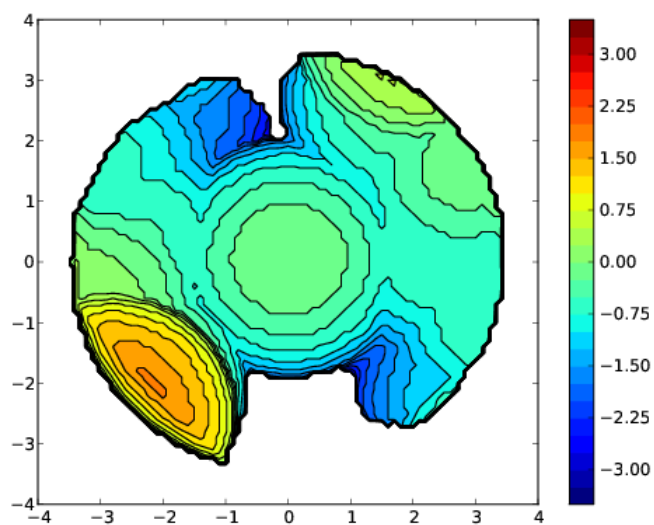


%V Free	%V Buried	% V Tot/V Ex
62.9	37.1	99.9

Quadrant	V f	V b	V t	%V f	%V b
SW	31.5	13.4	44.9	70.2	29.8
NW	25.6	19.3	44.9	57.1	42.9
NE	30.5	14.4	44.9	67.9	32.1
SE	25.4	19.5	44.9	56.6	43.4



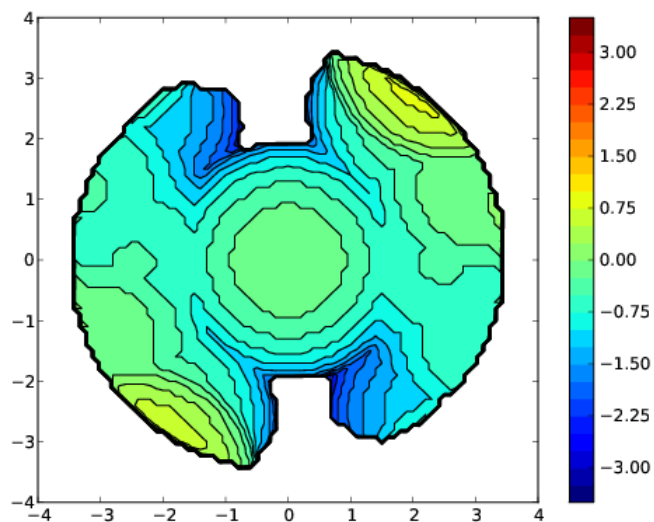
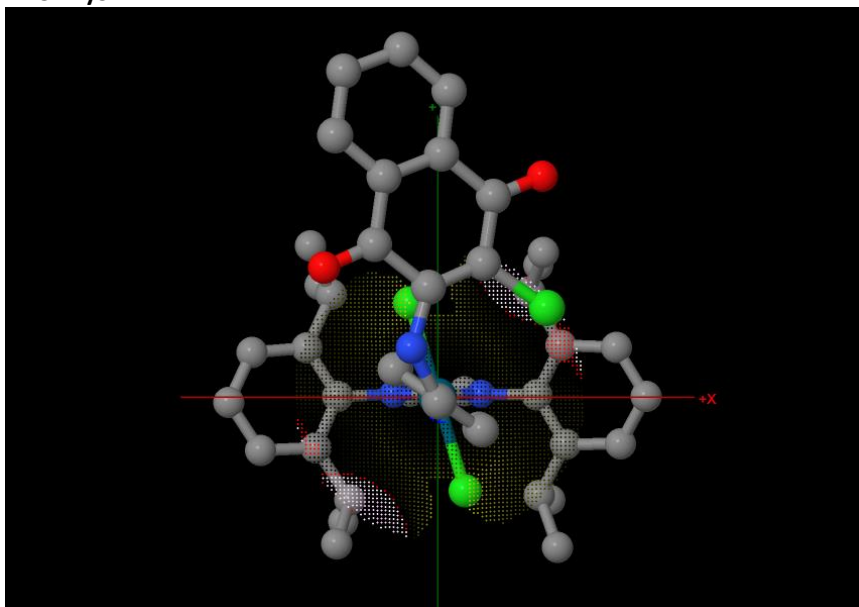
▪ IPrCl<sub>2</sub>Py<sub>2</sub>:



%V Free	%V Buried	% V Tot/V Ex
61.1	38.9	99.9

Quadrant	V f	V b	V t	%V f	%V b
SW	21.4	23.4	44.9	47.7	52.3
NW	30.3	14.6	44.9	67.5	32.5
NE	25.6	19.2	44.9	57.1	42.9
SE	32.4	12.5	44.9	72.2	27.8

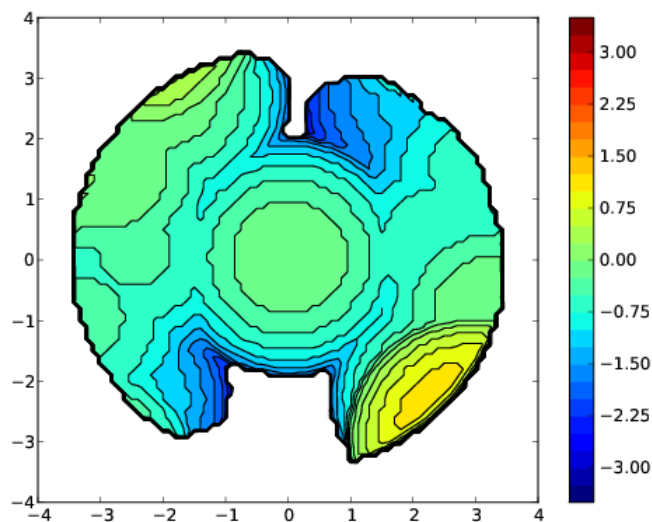
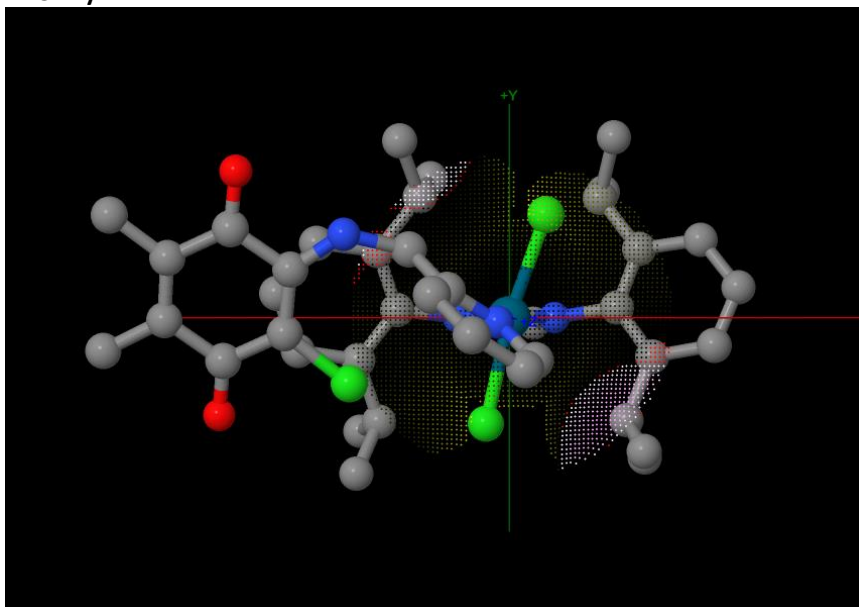
- IPrCl<sub>2</sub>Py<sub>3</sub>:



%V Free	%V Buried	% V Tot/V Ex
63.4	36.6	99.9

Quadrant	V f	V b	V t	%V f	%V b
SW	25.8	19.0	44.9	57.6	42.4
NW	31.2	13.6	44.9	69.6	30.4
NE	25.6	19.3	44.9	57.0	43.0
SE	31.0	13.8	44.9	69.2	30.8

- IPrCl<sub>2</sub>Py<sub>4</sub>:

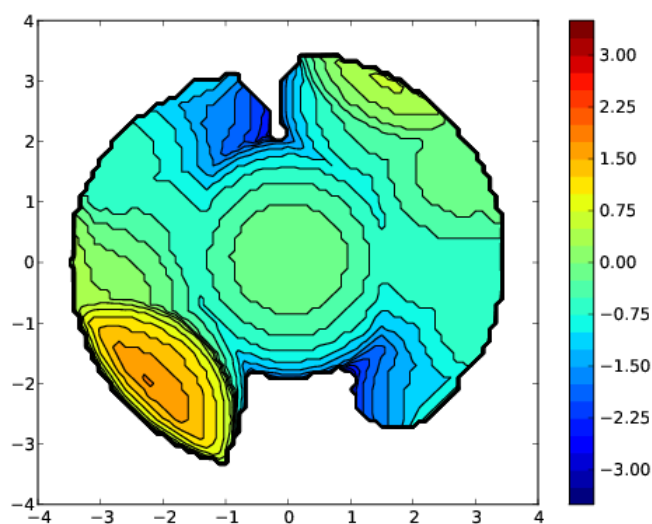
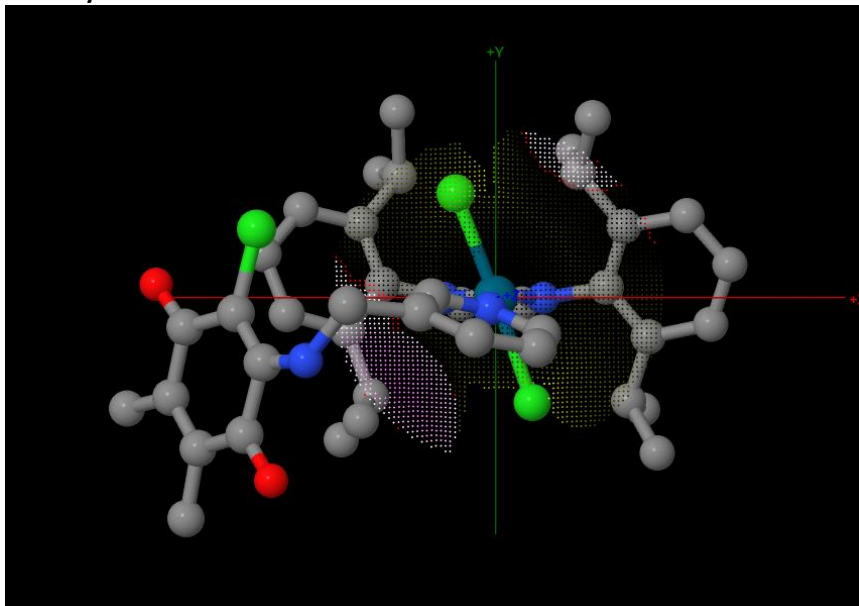


%V Free	%V Buried	% V Tot/V Ex
62.9	37.1	99.9

Quadrant	V f	V b	V t	%V f	%V b
SW	31.4	13.4	44.9	70.1	29.9
NW	25.6	19.3	44.9	57.0	43.0
NE	30.5	14.3	44.9	68.1	31.9
SE	25.3	19.6	44.9	56.4	43.6



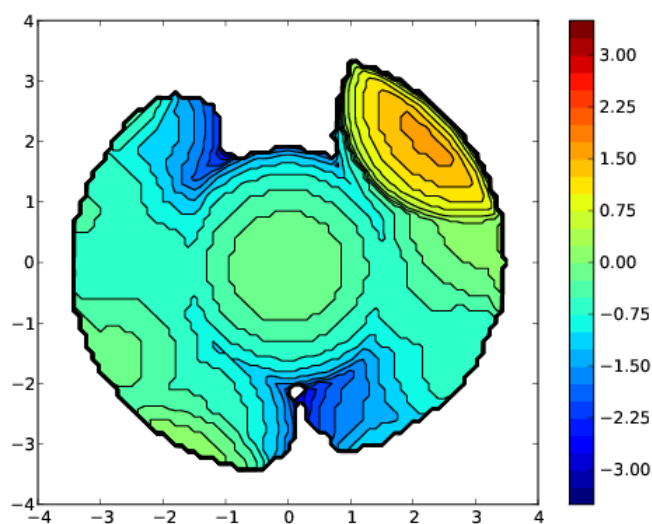
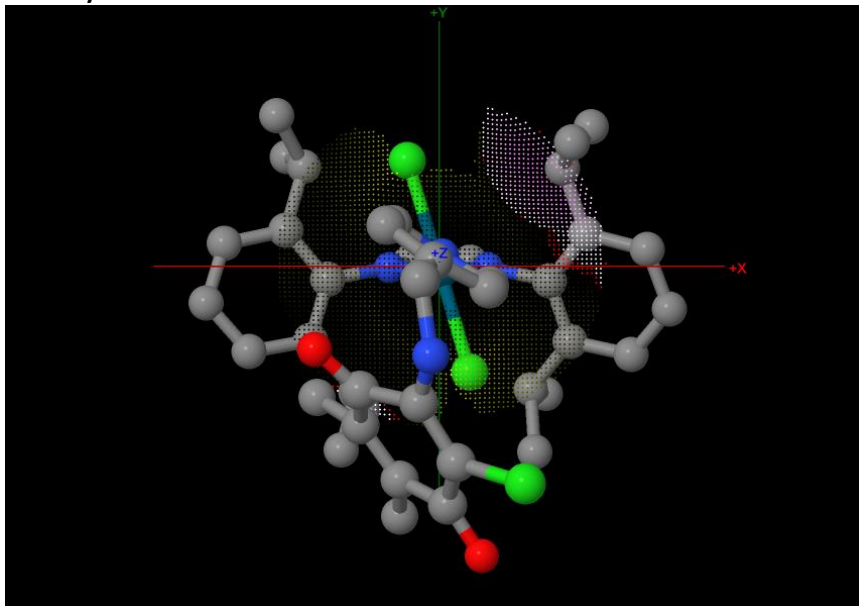
- IPrCl<sub>2</sub>Py<sub>5</sub>:



%V Free	%V Buried	% V Tot/V Ex
60.9	39.1	99.9

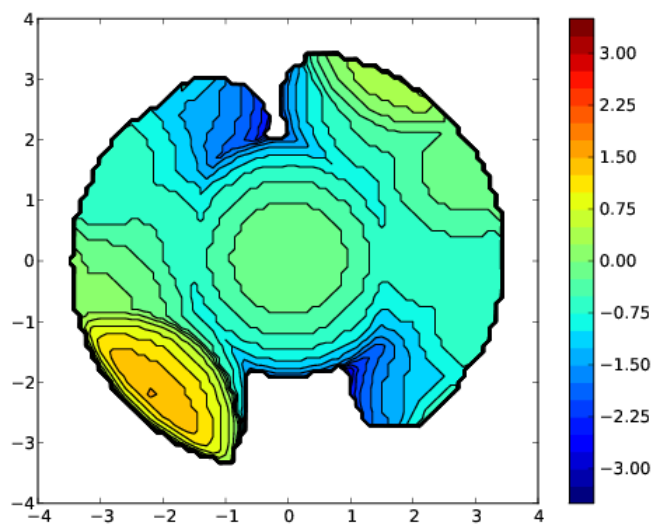
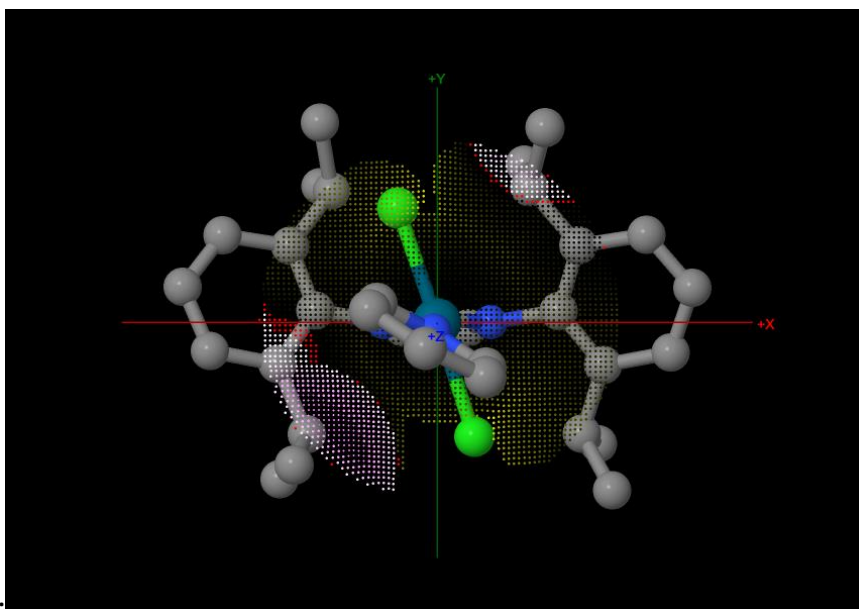
Quadrant	V f	V b	V t	%V f	%V b
SW	21.7	23.1	44.9	48.5	51.5
NW	29.8	15.0	44.9	66.5	33.5
NE	25.4	19.5	44.9	56.6	43.4
SE	32.3	12.5	44.9	72.1	27.9

▪ IPrCl2Py6:



%V Free	%V Buried	% V Tot/V Ex
62.0	38.0	99.9

Quadrant	V f	V b	V t	%V f	%V b
SW	26.7	18.2	44.9	59.5	40.5
NW	32.2	12.7	44.9	71.7	28.3
NE	22.5	22.3	44.9	50.2	49.8
SE	29.9	14.9	44.9	66.8	33.2

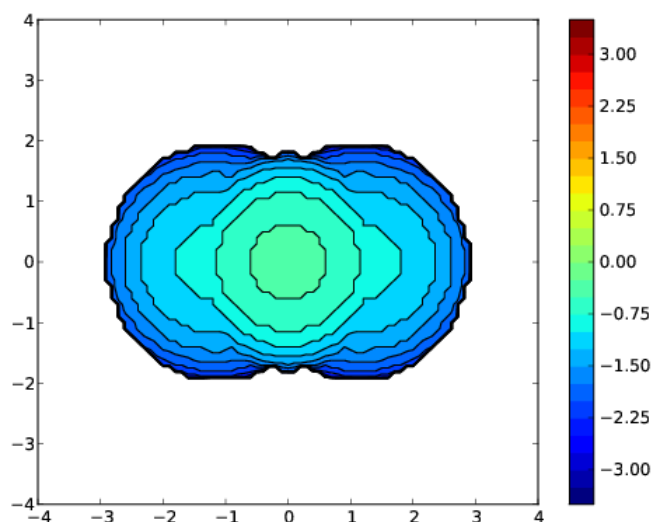
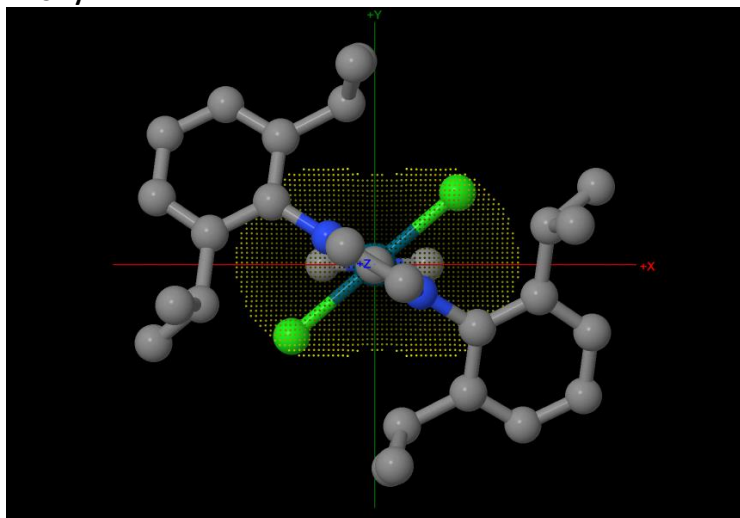


%V Free	%V Buried	% V Tot/V Ex
61.9	38.1	99.9

Quadrant	V f	V b	V t	%V f	%V b
SW	22.9	22.0	44.9	51.0	49.0
NW	30.3	14.6	44.9	67.5	32.5
NE	25.8	19.1	44.9	57.5	42.5
SE	32.2	12.7	44.9	71.8	28.2

Steric maps (xy plane). The metal is at the centre, whereas the N atom of the pyridine ring is on the z axis and 2 Å below the xy plane described by the metal and both halide atoms. The isocontour curves of the steric maps are given in Å.

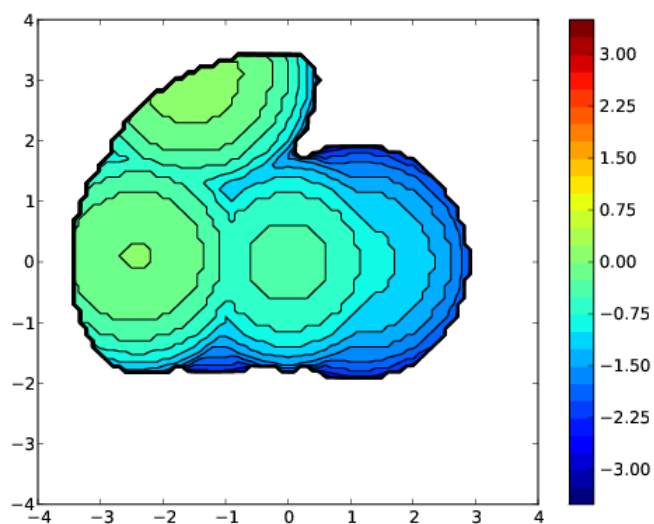
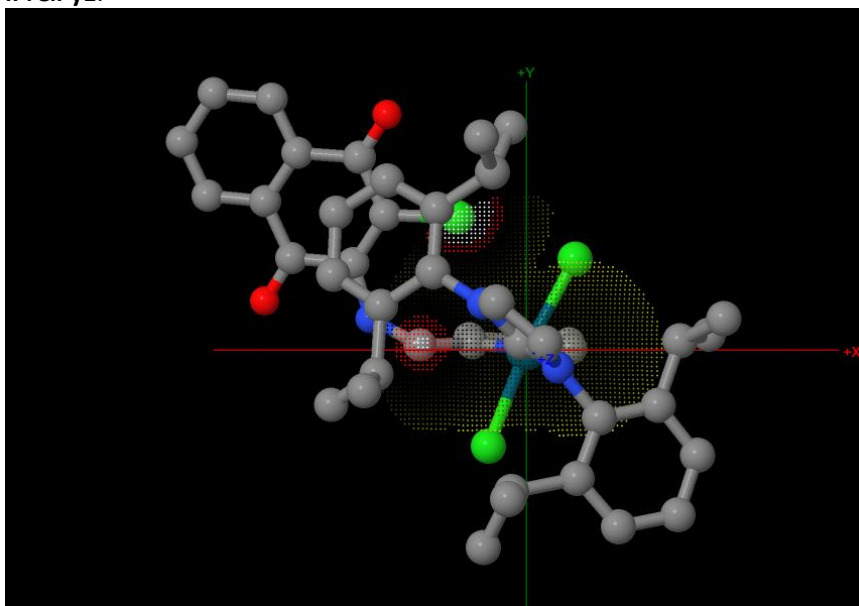
▪ IPrClPy:



%V Free	%V Buried	% V Tot/V Ex
80.5	19.5	99.9

Quadrant	V f	V b	V t	%V f	%V b
SW	36.1	8.7	44.9	80.5	19.5
NW	36.1	8.7	44.9	80.5	19.5
NE	36.1	8.7	44.9	80.5	19.5
SE	36.1	8.7	44.9	80.5	19.5

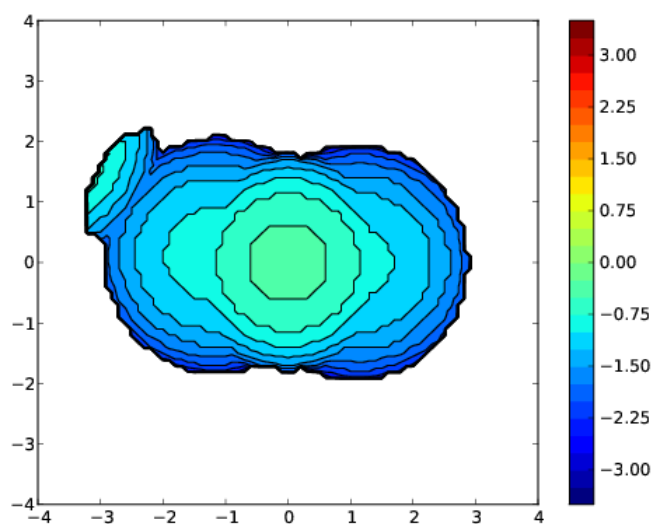
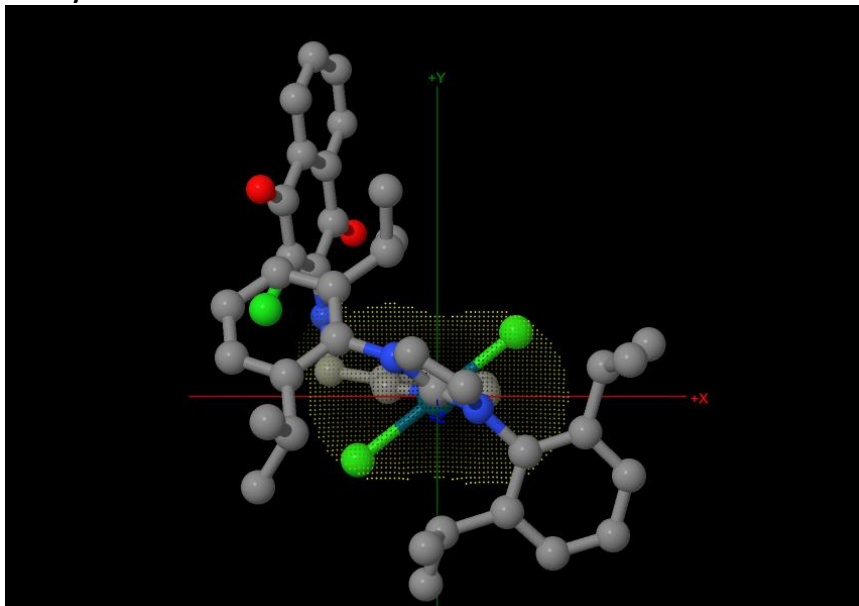
- IPrCIPy1:



%V Free	%V Buried	% V Tot/V Ex
72.0	28.0	99.9

Quadrant	V f	V b	V t	%V f	%V b
SW	32.5	12.4	44.9	72.3	27.7
NW	25.1	19.8	44.9	55.8	44.2
NE	35.5	9.3	44.9	79.2	20.8
SE	36.2	8.7	44.9	80.6	19.4

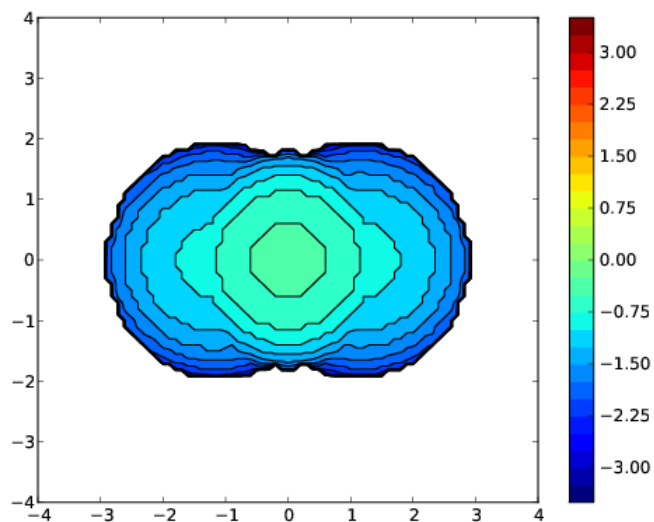
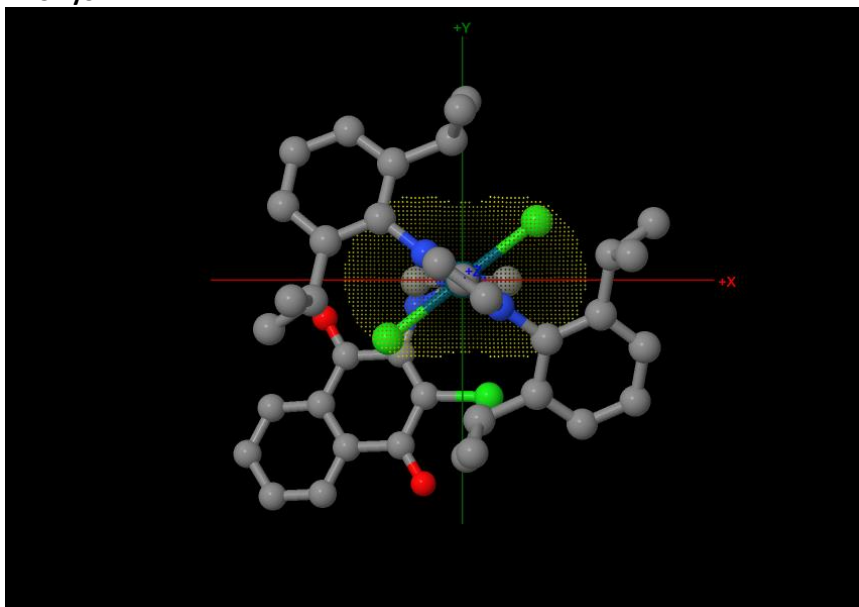
- IPrClPy2:



%V Free	%V Buried	% V Tot/V Ex
80.1	19.9	99.9

Quadrant	V f	V b	V t	%V f	%V b
SW	36.3	8.5	44.9	81.0	19.0
NW	35.0	9.9	44.9	77.9	22.1
NE	36.2	8.6	44.9	80.7	19.3
SE	36.2	8.6	44.9	80.7	19.3

- IPrClPy3:

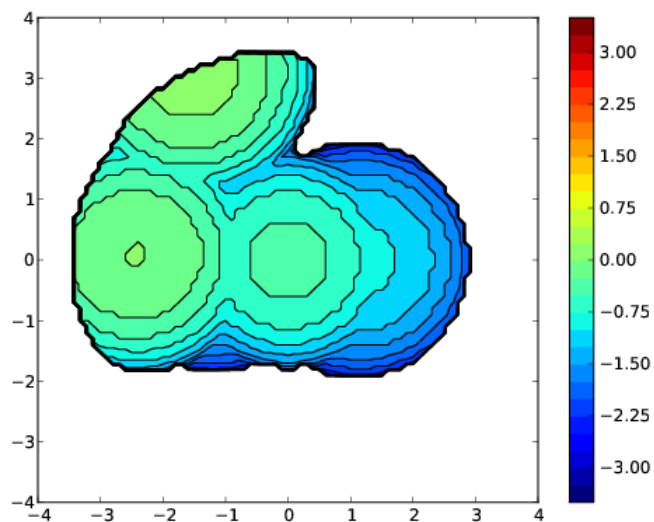
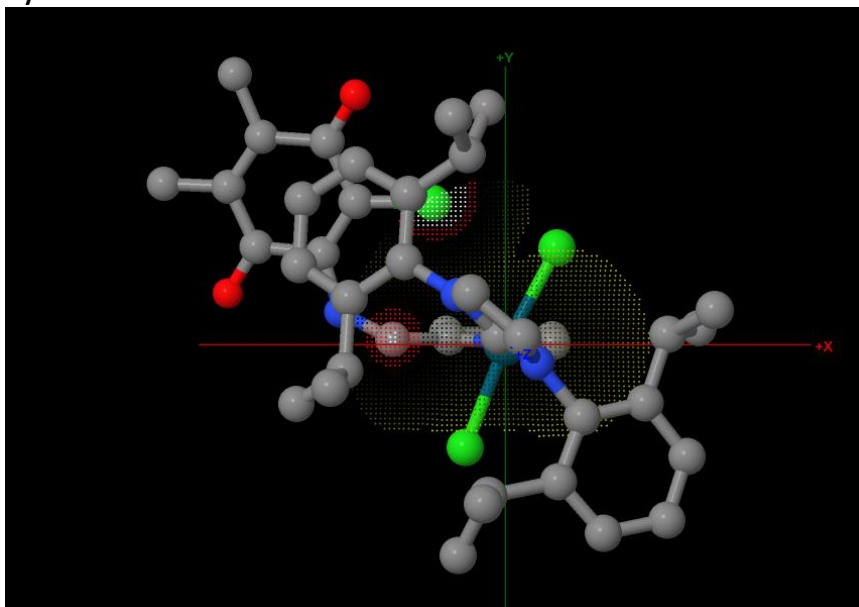


%V Free	%V Buried	% V Tot/V Ex
80.6	19.4	99.9

Quadrant	V f	V b	V t	%V f	%V b
SW	36.1	8.7	44.9	80.5	19.5
NW	36.2	8.7	44.9	80.7	19.3
NE	36.2	8.7	44.9	80.6	19.4
SE	36.2	8.7	44.9	80.6	19.4

-

IPrCIPy4:

**%V Free****%V Buried****% V Tot/V Ex**

72.1

27.9

99.9

**Quadrant****V f****V b****V t****%V f****%V b**

SW

32.5

12.4

44.9

72.4

27.6

NW

25.2

19.7

44.9

56.2

43.8

NE

35.6

9.3

44.9

79.3

20.7

SE

36.2

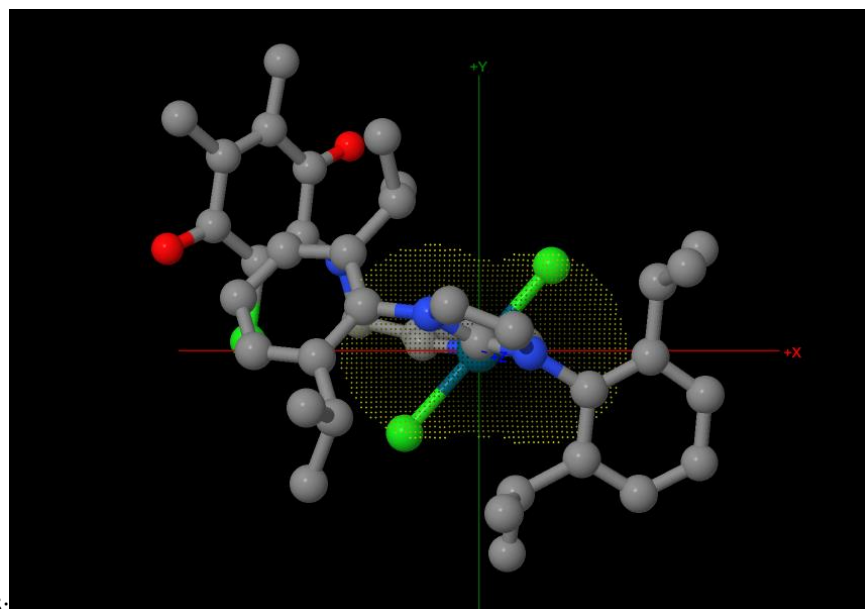
8.7

44.9

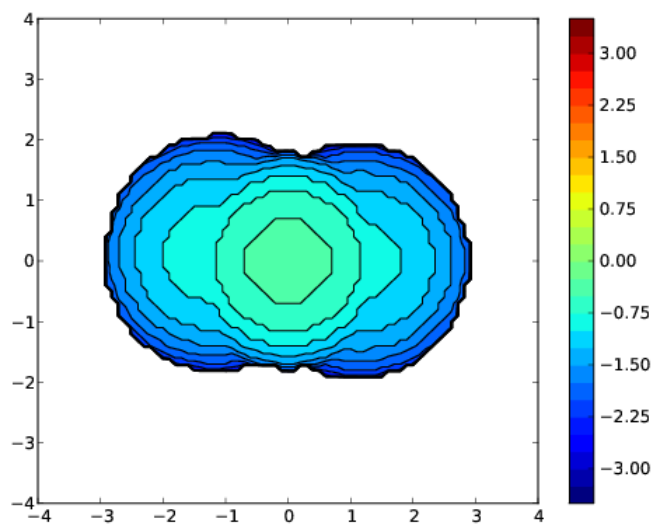
80.6

19.4





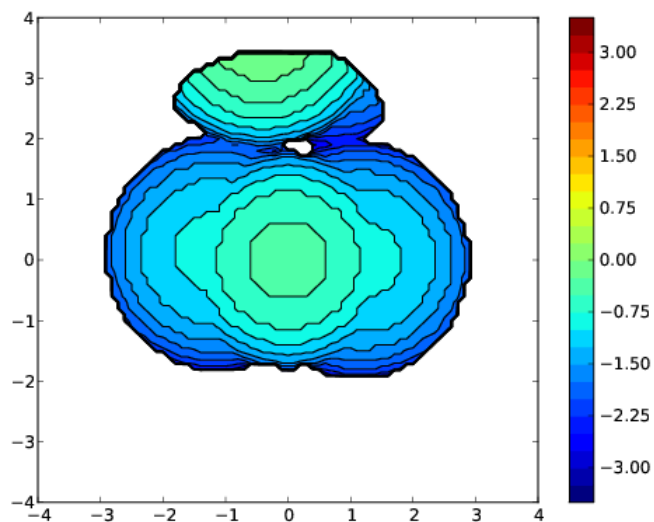
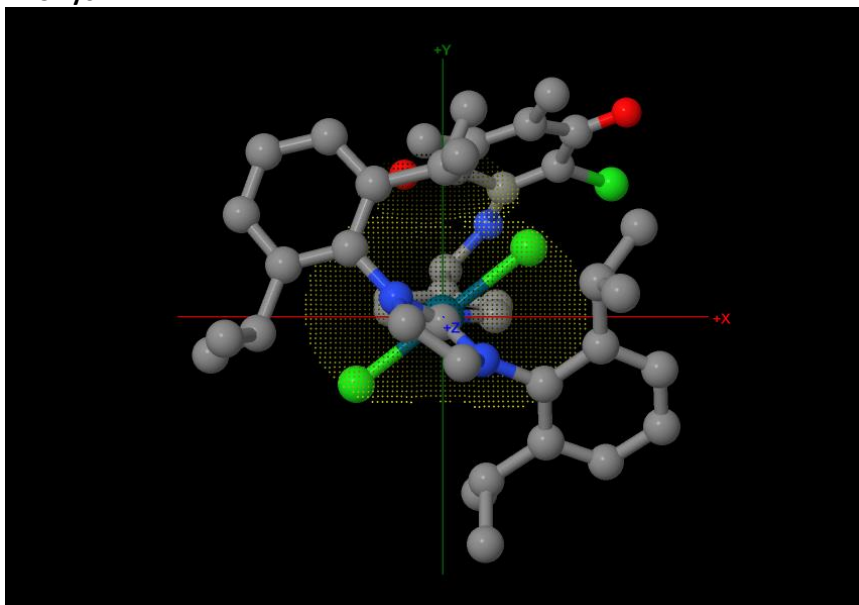
▪ IPrCIPy5:



%V Free	%V Buried	% V Tot/V Ex
80.2	19.8	99.9

Quadrant	V f	V b	V t	%V f	%V b
SW	36.3	8.6	44.9	80.9	19.1
NW	35.4	9.5	44.9	78.9	21.1
NE	36.1	8.8	44.9	80.4	19.6
SE	36.1	8.8	44.9	80.4	19.6

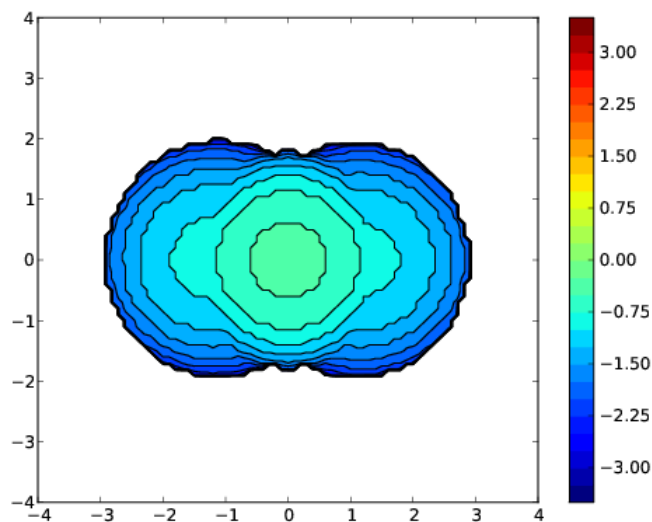
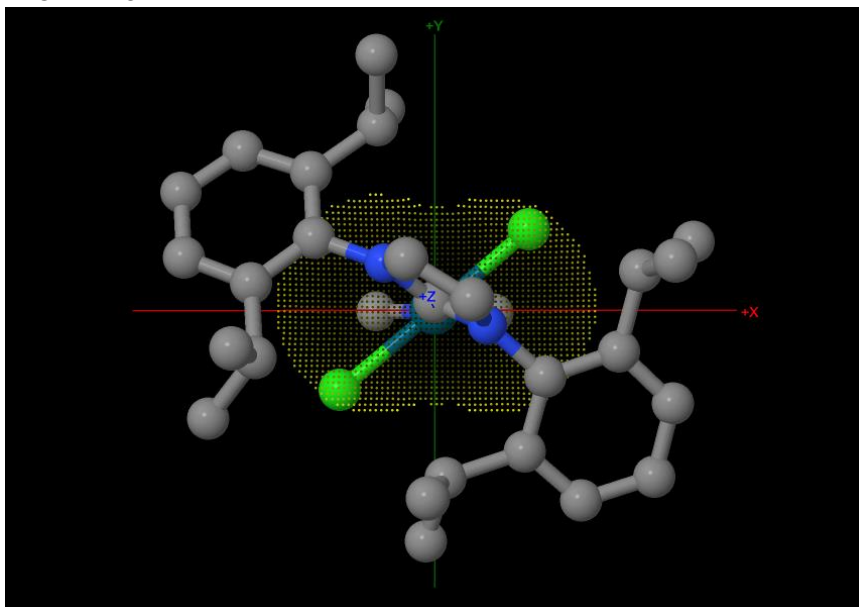
- IPrClPy6:



%V Free	%V Buried	% V Tot/V Ex
77.7	22.3	99.9

Quadrant	V f	V b	V t	%V f	%V b
SW	36.5	8.4	44.9	81.3	18.7
NW	32.7	12.1	44.9	72.9	27.1
NE	34.2	10.7	44.9	76.3	23.7
SE	36.1	8.8	44.9	80.5	19.5

▪ **IPrCl<sub>2</sub>PEPPSI:**

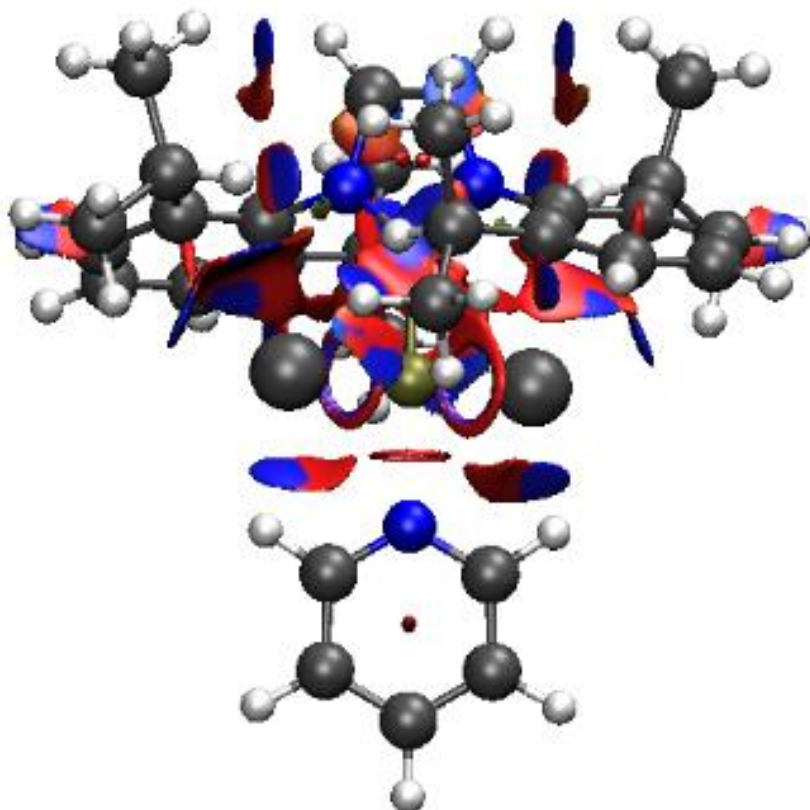


%V Free	%V Buried	% V Tot/V Ex
80.5	19.5	99.9

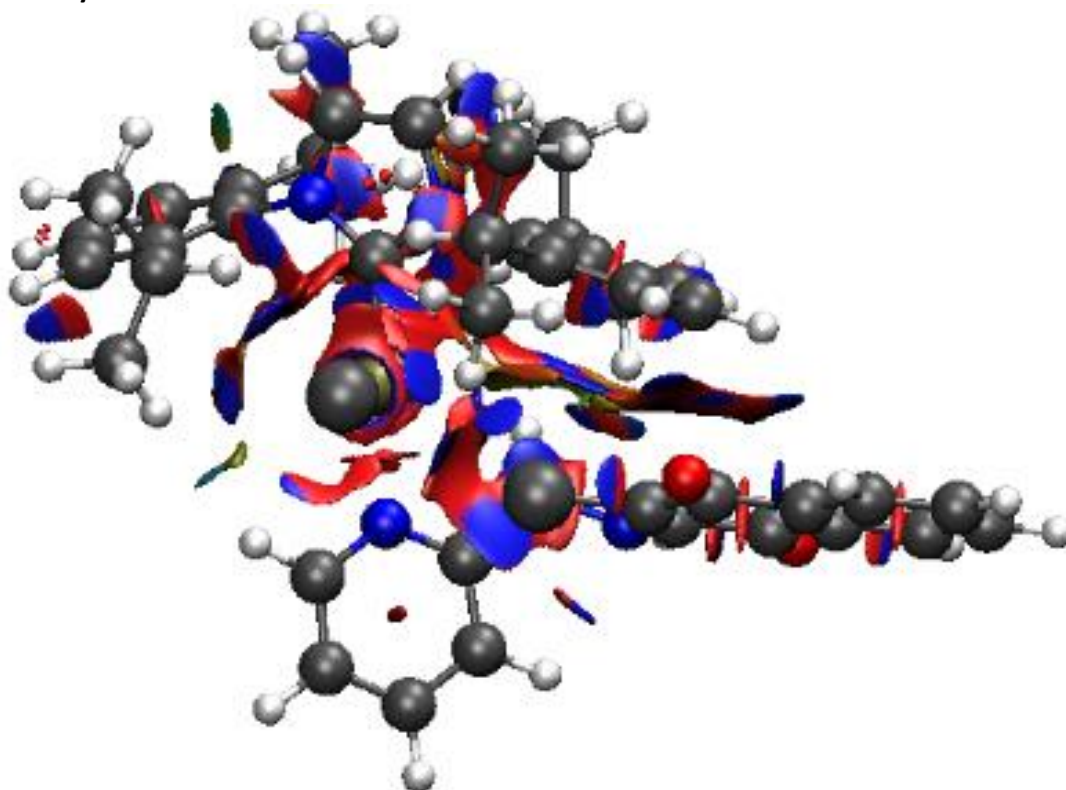
Quadrant	V f	V b	V t	%V f	%V b
SW	36.2	8.7	44.9	80.6	19.4
NW	36.0	8.9	44.9	80.2	19.8
NE	36.2	8.7	44.9	80.6	19.4
SE	36.2	8.7	44.9	80.6	19.4

## NCI plots

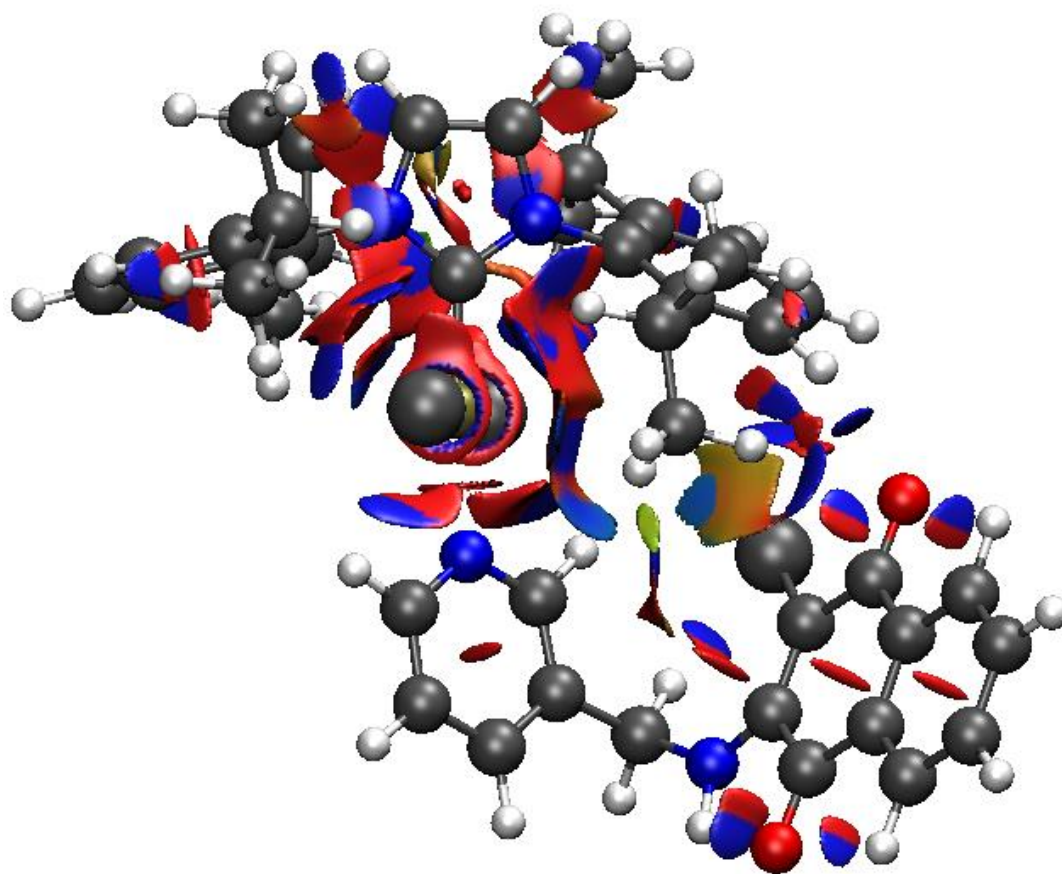
- IPrCl<sub>2</sub>Py:



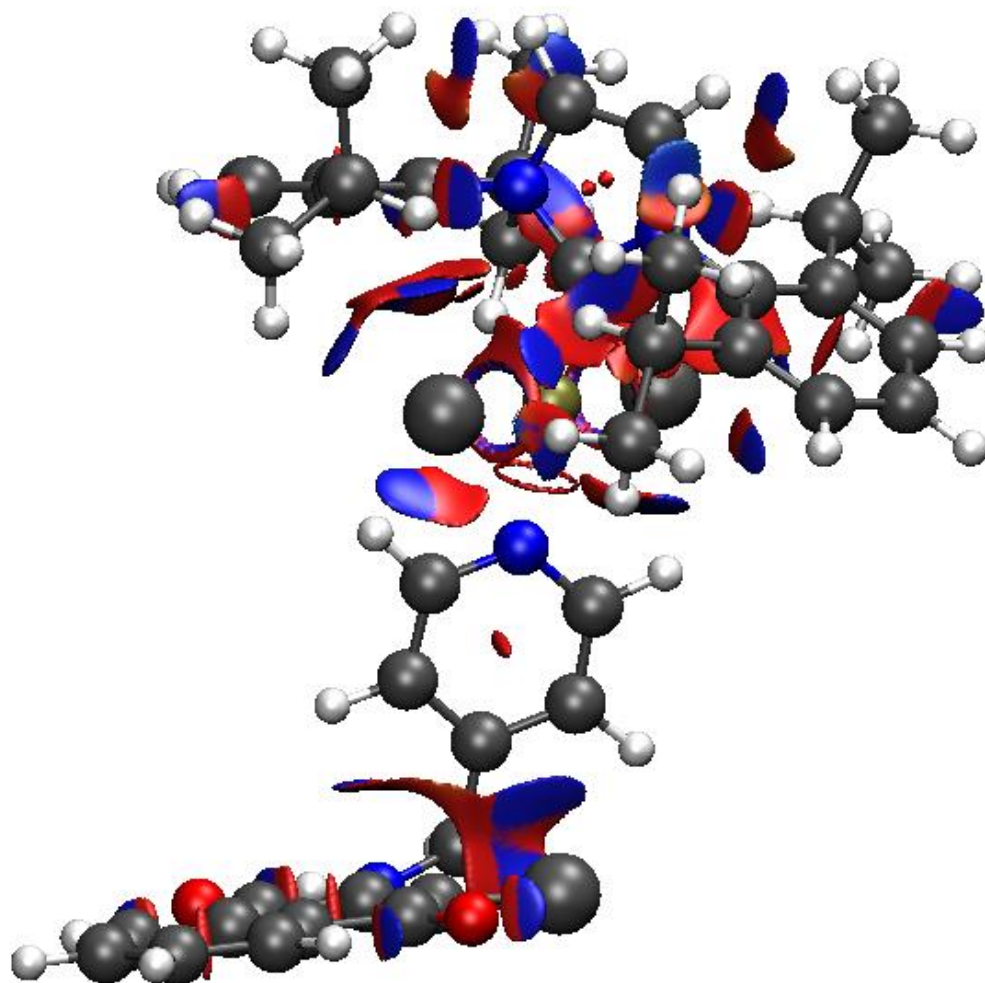
- IPrCl<sub>2</sub>Py<sub>1</sub>



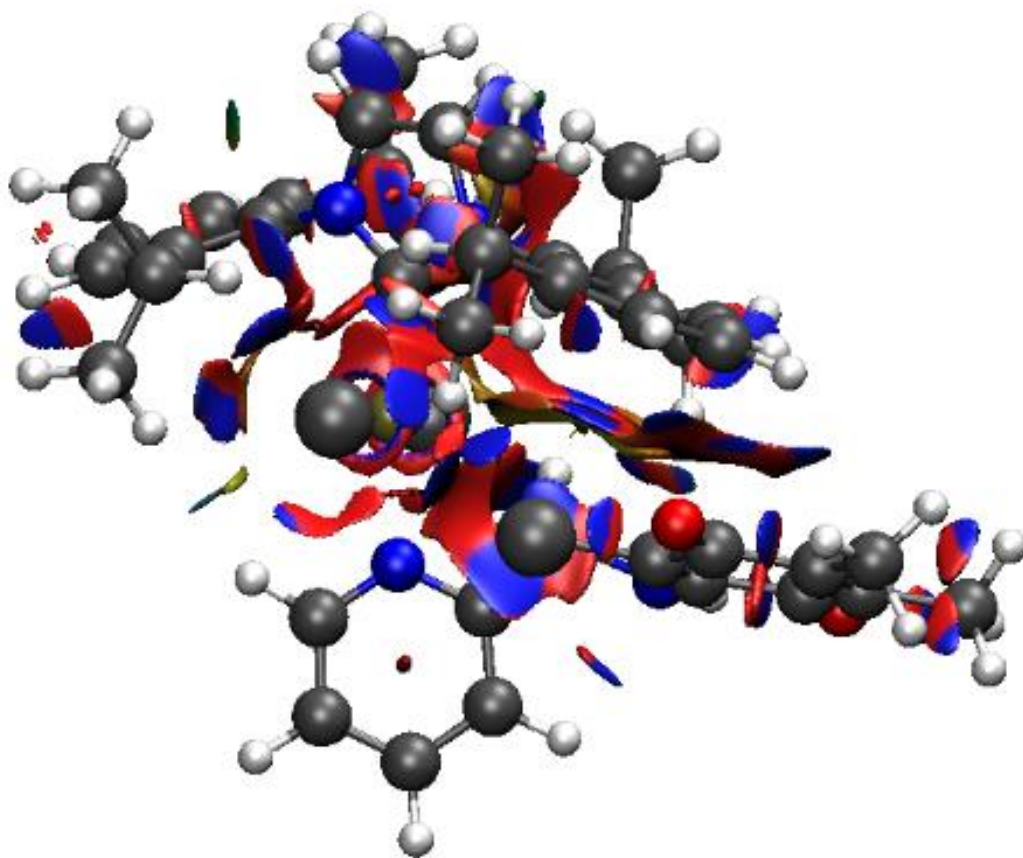
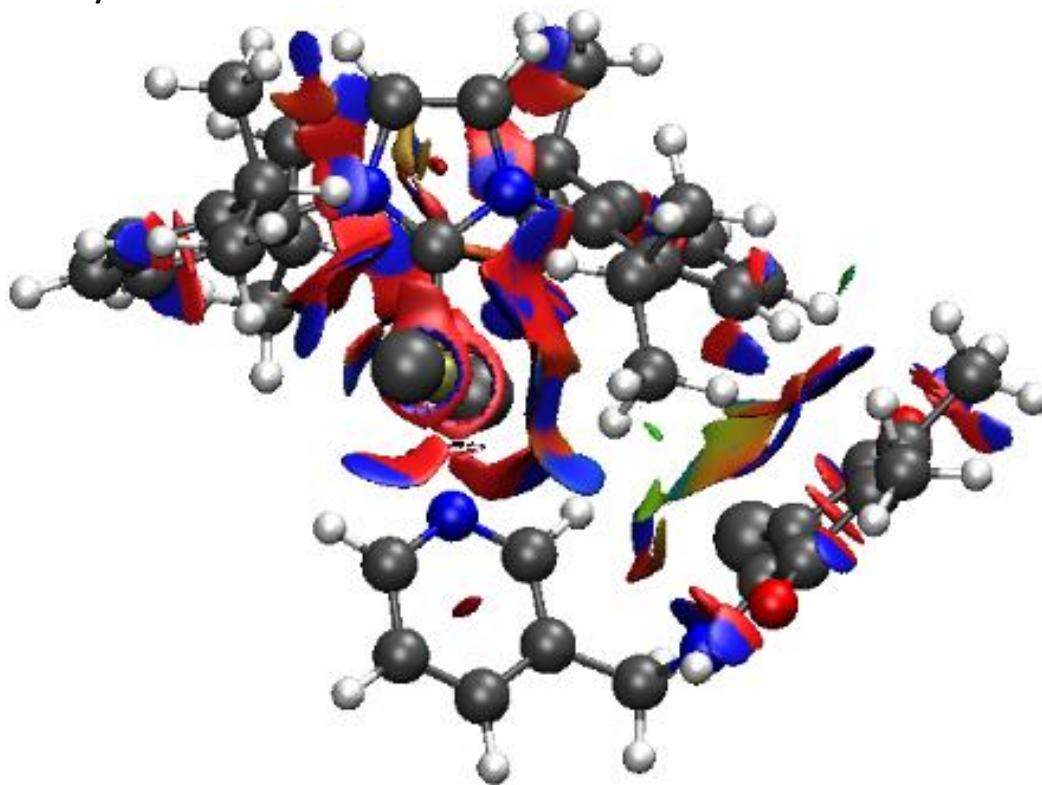
▪ IPrCl<sub>2</sub>Py<sub>2</sub>

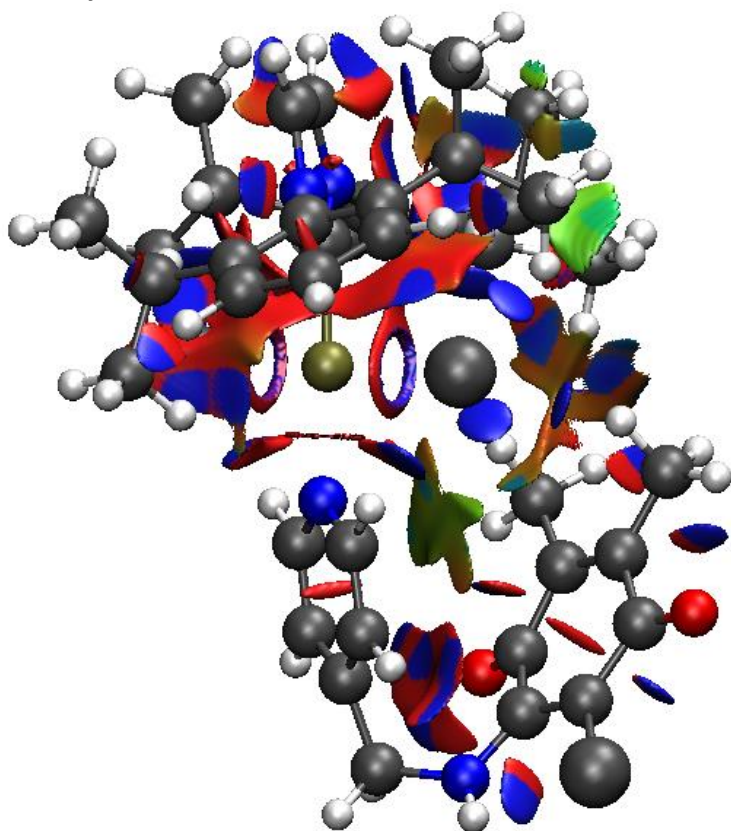
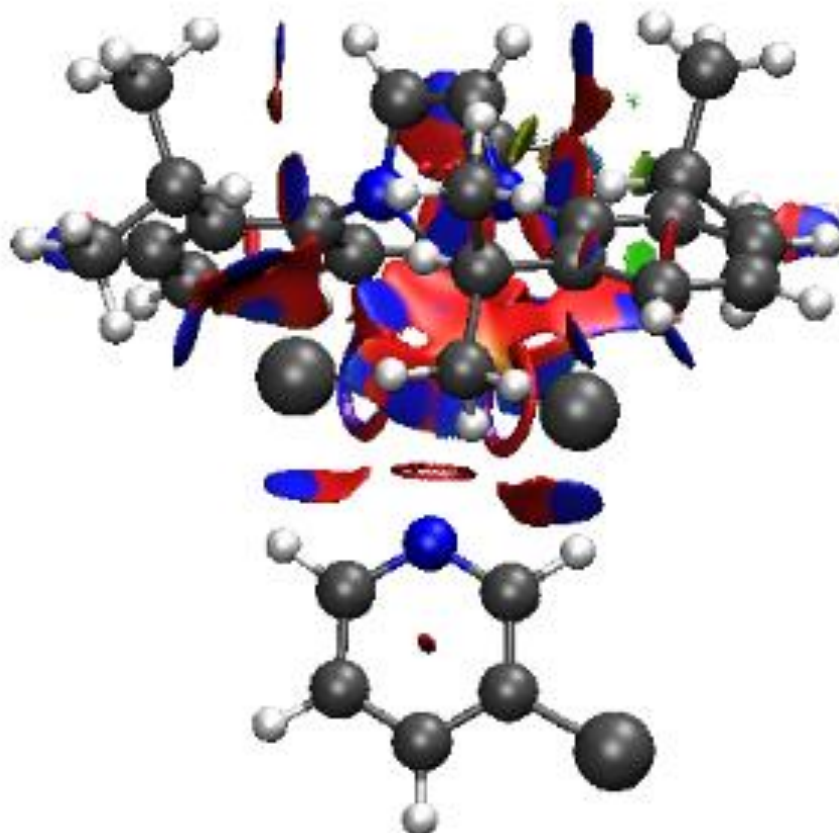


▪ IPrCl<sub>2</sub>Py<sub>3</sub>





▪ IPrCl<sub>2</sub>Py<sub>4</sub>▪ IPrCl<sub>2</sub>Py<sub>5</sub>

▪ IPrCl<sub>2</sub>Py6▪ IPrCl<sub>2</sub>PEPPI



**xyz coordinates of all computed species  
BP86-d3/def2SVP (PCM)****XYZ Cartesian Coordinates:**

32

**Py1** SCF Done: -1335.75751090 A.U.

N	-4.248024	-0.045686	-0.570639
C	-5.072698	0.277808	0.429312
C	-3.064458	-0.593755	-0.267528
C	-4.763186	0.076076	1.778751
C	-2.664149	-0.845660	1.050727
C	-3.530549	-0.501117	2.090814
H	-6.033121	0.725567	0.147477
H	-5.471443	0.364812	2.558066
H	-1.693686	-1.299051	1.256540
H	-3.244855	-0.681136	3.130216
C	-2.195197	-0.939086	-1.467528
H	-2.638248	-1.808829	-1.977211
H	-2.240505	-0.104877	-2.179212
N	-0.823927	-1.291180	-1.157725
H	-0.589596	-2.282969	-1.151938
C	0.212052	-0.533779	-0.751975
C	1.424972	-1.405051	-0.433471
C	0.314675	0.831964	-0.582473
C	2.670902	-0.757122	0.022104
C	1.531706	1.501809	-0.113385
C	2.724057	0.639675	0.179799
Cl	-1.015915	1.928706	-0.910289
O	1.596924	2.716896	0.038794
O	1.323394	-2.614804	-0.563346
C	3.909616	1.238013	0.617024
C	5.032762	0.452378	0.893555
C	3.798210	-1.543171	0.300803
C	4.978538	-0.938215	0.735652
H	3.934531	2.322321	0.734884
H	5.955983	0.927021	1.234196
H	5.857399	-1.549439	0.952324
H	3.731696	-2.624697	0.171457

32

**Py2** SCF Done: -1335.75336813 A.U.

N	-3.682046	0.241627	1.965073
C	-4.495510	-0.820439	1.936804
C	-3.028774	0.557994	0.842702
C	-4.694226	-1.603259	0.795083
C	-3.147796	-0.157097	-0.360364

C	-4.006286	-1.263717	-0.371136
H	-5.021092	-1.063740	2.867693
H	-5.374423	-2.457294	0.821973
H	-2.371902	1.434048	0.886639
H	-4.137386	-1.850977	-1.284677
C	-2.335487	0.226337	-1.583705
H	-2.837567	-0.137947	-2.491322
H	-2.247934	1.312849	-1.668042
N	-1.005321	-0.379262	-1.565212
H	-0.981646	-1.374980	-1.790811
C	0.130432	-0.002611	-0.948812
C	1.095449	-1.182622	-0.827212
C	0.532859	1.226181	-0.463043
C	2.399417	-0.977974	-0.165504
C	1.813774	1.456587	0.212579
C	2.741726	0.286294	0.347034
Cl	-0.438728	2.679723	-0.631287
O	2.138349	2.555242	0.649926
O	0.750993	-2.264379	-1.275735
C	3.974220	0.460658	0.983881
C	3.289041	-2.054927	-0.041071
C	4.517670	-1.872976	0.595617
C	4.858696	-0.614933	1.108328
H	3.000841	-3.026321	-0.446199
H	5.210563	-2.711481	0.694285
H	5.819913	-0.471690	1.607516
H	4.224620	1.447805	1.375182
32			
<b>Py3</b> SCF Done: -1335.75529681 A.U.			
N	-4.585309	-0.099587	1.993467
C	-3.444109	-0.793050	2.058416
C	-4.955012	0.356163	0.789485
C	-2.633924	-1.060979	0.949990
C	-4.216277	0.147538	-0.376821
C	-3.022100	-0.581666	-0.305141
H	-3.147021	-1.161477	3.047566
H	-1.711925	-1.632490	1.072025
H	-5.890125	0.926955	0.745497
H	-4.566316	0.558104	-1.327408
C	-2.214561	-0.848399	-1.563258
H	-2.670803	-1.696337	-2.097875
H	-2.284118	0.016222	-2.236124
N	-0.829504	-1.209678	-1.329626
H	-0.593988	-2.199810	-1.381167

C	0.196093	-0.479070	-0.850672
C	1.400464	-1.367828	-0.552278
C	0.293711	0.874678	-0.605599
C	2.629847	-0.749758	-0.016950
C	1.494222	1.514455	-0.055106
C	2.675267	0.634527	0.229460
Cl	-1.016752	1.993380	-0.936590
O	1.553649	2.718777	0.165806
O	1.304706	-2.567118	-0.760528
C	3.843537	1.203828	0.745022
C	3.748188	-1.552101	0.250938
C	4.911315	-0.976074	0.764414
C	4.957479	0.401780	1.011456
H	3.688249	-2.623380	0.051961
H	5.782999	-1.600119	0.973371
H	5.867207	0.853498	1.413921
H	3.862641	2.278685	0.930993
32			
<b>Py3isom</b> SCF Done: -1335.75529681 A.U.			
N	-4.585311	-0.099584	1.993466
C	-3.444112	-0.793051	2.058416
C	-4.955011	0.356167	0.789485
C	-2.633926	-1.060980	0.949991
C	-4.216276	0.147539	-0.376821
C	-3.022100	-0.581667	-0.305140
H	-3.147025	-1.161476	3.047567
H	-1.711929	-1.632493	1.072027
H	-5.890123	0.926961	0.745495
H	-4.566314	0.558106	-1.327409
C	-2.214560	-0.848401	-1.563257
H	-2.670803	-1.696339	-2.097875
H	-2.284117	0.016220	-2.236123
N	-0.829504	-1.209680	-1.329623
H	-0.593988	-2.199812	-1.381164
C	0.196094	-0.479072	-0.850671
C	1.400465	-1.367829	-0.552276
C	0.293712	0.874677	-0.605600
C	2.629848	-0.749757	-0.016949
C	1.494221	1.514455	-0.055105
C	2.675266	0.634527	0.229461
Cl	-1.016752	1.993378	-0.936594
O	1.553647	2.718777	0.165809
O	1.304708	-2.567119	-0.760526
C	3.843536	1.203829	0.745022

C	4.957479	0.401783	1.011455
C	3.748190	-1.552099	0.250938
C	4.911316	-0.976072	0.764413
H	3.862640	2.278686	0.930993
H	5.867207	0.853501	1.413920
H	5.783001	-1.600116	0.973370
H	3.688252	-2.623379	0.051961
32			
<b>Py4</b> SCF Done: -1260.78521839 A.U.			
N	-3.860423	-0.023635	-0.730020
C	-4.744316	0.328389	0.207778
C	-2.701710	-0.569771	-0.339593
C	-4.521807	0.158198	1.578552
C	-2.386762	-0.790869	1.006989
C	-3.314818	-0.416904	1.981662
H	-5.682202	0.773790	-0.144889
H	-5.276045	0.469223	2.304329
H	-1.433589	-1.243091	1.283905
H	-3.096306	-0.572611	3.041114
C	-1.760581	-0.947740	-1.473866
H	-2.187623	-1.813553	-2.003618
H	-1.740067	-0.120596	-2.195317
N	-0.420685	-1.321157	-1.070140
H	-0.204575	-2.315908	-1.027668
C	0.604493	-0.566222	-0.632090
C	1.797609	-1.437309	-0.236847
C	0.722461	0.795088	-0.483998
C	3.040880	-0.808556	0.254746
C	1.942131	1.425524	0.022347
C	3.111390	0.540350	0.380209
Cl	-0.567154	1.922319	-0.876052
O	2.038460	2.640783	0.160536
O	1.680172	-2.649558	-0.340234
C	4.349687	1.219790	0.881373
H	4.607991	0.861573	1.892093
H	5.212004	0.981585	0.236248
H	4.216416	2.307151	0.912119
C	4.188085	-1.713469	0.607114
H	4.475840	-1.588121	1.663988
H	3.929224	-2.765476	0.437664
H	5.078802	-1.468642	0.005348
32			
<b>Py5</b> SCF Done: -1260.78118999 A.U.			
N	-3.411390	0.634613	1.793849

C	-4.312503	-0.354457	1.810243
C	-2.674023	0.789294	0.689679
C	-4.517946	-1.222051	0.732713
C	-2.791698	-0.022820	-0.450285
C	-3.741875	-1.051294	-0.414935
H	-4.906329	-0.465151	2.725199
H	-5.270833	-2.010835	0.794135
H	-1.945264	1.607755	0.695431
H	-3.874504	-1.709122	-1.278895
C	-1.883674	0.174401	-1.650207
H	-2.370773	-0.221256	-2.552953
H	-1.686883	1.236803	-1.819104
N	-0.620624	-0.544931	-1.499454
H	-0.680252	-1.556421	-1.625081
C	0.506018	-0.209284	-0.842228
C	1.354703	-1.447371	-0.538898
C	0.992749	1.012560	-0.439795
C	2.641085	-1.307883	0.174161
C	2.253381	1.158405	0.289723
C	3.058704	-0.083347	0.581879
Cl	0.187283	2.536013	-0.786642
O	2.671097	2.252098	0.656154
O	0.927196	-2.534925	-0.896519
C	4.345839	0.100952	1.327074
H	5.198395	-0.250234	0.721476
H	4.503648	1.154416	1.584551
H	4.350472	-0.500978	2.250988
C	3.433990	-2.558152	0.433511
H	3.571944	-2.716231	1.516004
H	2.933884	-3.438948	0.013488
H	4.441931	-2.480890	-0.005978
32			
<b>PySisom</b> SCF Done: -1260.78167494 A.U.			
N	-4.742561	-1.127499	0.548212
C	-4.570723	-0.384544	1.646671
C	-3.882906	-0.953645	-0.460585
C	-3.545556	0.558753	1.780812
C	-2.817701	-0.040943	-0.437309
C	-2.654887	0.732105	0.721225
H	-5.282975	-0.541909	2.465194
H	-3.452422	1.145472	2.697306
H	-4.043031	-1.571561	-1.353627
H	-1.846754	1.464361	0.785359
C	-1.862115	0.064803	-1.610793

H	-2.318490	-0.390063	-2.502027
H	-1.651815	1.111900	-1.846509
N	-0.610964	-0.645778	-1.364937
H	-0.666793	-1.663211	-1.427832
C	0.530706	-0.260253	-0.767636
C	1.407904	-1.472943	-0.437336
C	1.014061	0.985042	-0.436620
C	2.723600	-1.283032	0.206424
C	2.305484	1.181395	0.221251
C	3.144909	-0.034346	0.527959
Cl	0.151977	2.479904	-0.776515
O	2.722095	2.296100	0.520885
O	0.978531	-2.582050	-0.717795
C	3.543737	-2.509826	0.492236
H	3.743223	-2.604168	1.572487
H	3.031468	-3.417394	0.151332
H	4.524891	-2.449800	-0.006669
C	4.465503	0.202480	1.195632
H	4.519619	-0.340115	2.154275
H	5.290290	-0.182293	0.572465
H	4.626756	1.270679	1.379760
32			
<b>Py6</b> SCF Done: -1260.78075052 A.U.			
N	-4.403360	0.532404	1.608751
C	-3.386028	-0.295407	1.871497
C	-4.574898	0.902620	0.333410
C	-2.511193	-0.783621	0.896110
C	-3.755509	0.474671	-0.713862
C	-2.692812	-0.393540	-0.435656
H	-3.251234	-0.593281	2.918194
H	-1.695995	-1.454032	1.176550
H	-5.407619	1.585596	0.127350
H	-3.940024	0.825092	-1.732513
C	-1.804033	-0.910117	-1.552297
H	-2.271063	-1.810617	-1.981583
H	-1.749778	-0.162571	-2.353323
N	-0.473273	-1.314600	-1.126452
H	-0.325802	-2.315078	-1.035052
C	0.544894	-0.563336	-0.646476
C	0.469743	0.948225	-0.718742
C	1.675646	-1.123188	-0.094641
C	1.618257	1.752482	-0.223613
C	2.810446	-0.351778	0.394864
C	2.716722	1.148937	0.296129

Cl	1.795932	-2.868678	0.048598
O	3.807807	-0.880479	0.877125
O	-0.525187	1.485230	-1.179654
C	3.886946	1.937186	0.802749
H	4.307443	2.569405	0.002867
H	3.576486	2.620738	1.610716
H	4.672181	1.272634	1.181449
C	1.500135	3.247913	-0.321405
H	0.544072	3.541469	-0.770702
H	1.577341	3.712764	0.675407
H	2.318719	3.666487	-0.929787
32			
<b>Py6isom</b> SCF Done: -1260.78300323 A.U.			
N	-4.338332	0.004328	1.806959
C	-3.223702	-0.719669	1.951974
C	-4.620199	0.451048	0.576123
C	-2.355135	-1.027739	0.899625
C	-3.817504	0.203344	-0.539133
C	-2.651639	-0.557846	-0.383795
H	-2.998576	-1.080371	2.962744
H	-1.459108	-1.622627	1.086443
H	-5.533899	1.047122	0.466351
H	-4.095881	0.608566	-1.515341
C	-1.776371	-0.866720	-1.585961
H	-2.219329	-1.714360	-2.132147
H	-1.786666	-0.012871	-2.276215
N	-0.416186	-1.250794	-1.263466
H	-0.196311	-2.245463	-1.275640
C	0.588336	-0.521600	-0.738045
C	1.765559	-1.411426	-0.340367
C	0.696202	0.829476	-0.515710
C	2.980040	-0.810781	0.249174
C	1.884999	1.431063	0.092983
C	3.034975	0.527406	0.465146
Cl	-0.560547	1.979422	-0.942913
O	1.970180	2.636938	0.299367
O	1.658378	-2.615698	-0.520221
C	4.113069	-1.732938	0.602308
H	4.330712	-1.689736	1.682397
H	3.877523	-2.770123	0.335483
H	5.037468	-1.435076	0.080993
C	4.239161	1.176738	1.077035
H	4.456543	0.740245	2.066110
H	5.133023	1.000870	0.454991

H	4.090216	2.256843	1.187595
11			
<b>PEPPSIorg</b> SCF Done: -707.581006065 A.U.			
N	1.538468	-1.249499	-0.000003
C	2.222035	-0.099090	-0.000014
C	0.205281	-1.194926	0.000017
C	1.606109	1.156725	0.000005
C	-0.495639	0.018643	0.000000
C	0.211559	1.222843	0.000004
H	3.314982	-0.175271	-0.000010
H	2.206927	2.068457	0.000010
H	-0.346655	-2.141002	0.000003
H	-0.317390	2.177548	0.000006
Cl	-2.242542	0.011270	-0.000004
66			
<b>IPr</b> SCF Done: -1287.27374544 A.U.			
Pd	-0.000052	0.000005	-1.899259
N	1.075663	-0.000029	0.912082
C	5.096296	0.000048	-0.332054
N	-1.075661	-0.000003	0.912116
C	4.430908	-1.210389	-0.129899
C	3.090163	-1.237109	0.281321
C	2.445017	-0.000001	0.483336
C	3.090154	1.237130	0.281446
C	4.430880	1.210457	-0.129829
C	2.367246	2.565311	0.469292
C	3.038389	3.433034	1.546013
C	2.237040	3.316589	-0.866426
C	2.367306	-2.565325	0.469129
C	3.038525	-3.433045	1.545797
C	2.237073	-3.316565	-0.866601
C	0.679263	-0.000089	2.245565
C	-0.679221	0.000014	2.245587
C	-2.445024	-0.000003	0.483406
C	-3.090143	1.237116	0.281378
C	-4.430880	1.210421	-0.129866
C	-5.096287	-0.000005	-0.332030
C	-4.430893	-1.210426	-0.129806
C	-3.090174	-1.237122	0.281491
C	-2.367248	2.565313	0.469165
C	-3.038521	3.433122	1.545726
C	-2.236868	3.316463	-0.866601
C	-2.367274	-2.565310	0.469309
C	-3.038497	-3.433108	1.545918



C	-2.236943	-3.316494	-0.866449
C	-0.000013	-0.000023	0.058540
H	6.141386	0.000072	-0.652392
H	4.960702	-2.150900	-0.298636
H	4.960650	2.150990	-0.298529
H	1.346547	2.347866	0.814788
H	4.062462	3.718840	1.255367
H	3.096418	2.899604	2.508149
H	2.465221	4.361104	1.702988
H	1.651794	4.241001	-0.732493
H	1.724678	2.690126	-1.614805
H	3.224458	3.596784	-1.268586
H	1.346602	-2.347935	0.814644
H	3.096498	-2.899656	2.507961
H	4.062633	-3.718721	1.255140
H	2.465452	-4.361178	1.702729
H	1.724683	-2.690089	-1.614953
H	1.651826	-4.240980	-0.732666
H	3.224468	-3.596759	-1.268819
H	1.397596	-0.000149	3.060042
H	-1.397529	0.000059	3.060087
H	-4.960652	2.150941	-0.298617
H	-6.141370	-0.000010	-0.652391
H	-4.960673	-2.150949	-0.298528
H	-1.346580	2.347901	0.814775
H	-4.062599	3.718808	1.254974
H	-2.465433	4.361249	1.702640
H	-3.096581	2.899798	2.507921
H	-1.724432	2.689918	-1.614864
H	-1.651601	4.240866	-0.732674
H	-3.224217	3.596665	-1.268928
H	-1.346605	-2.347878	0.814903
H	-3.096607	-2.899743	2.508085
H	-2.465337	-4.361185	1.702877
H	-4.062546	-3.718900	1.255171
H	-3.224323	-3.596666	-1.268720
H	-1.651703	-4.240913	-0.732529
H	-1.724515	-2.689974	-1.614736
68			
<b>IPrCI2</b> SCF Done: -2207.54082013 A.U.			
Pd	0.000045	0.000094	-1.753361
N	1.083889	-0.033178	0.991349
C	5.109813	-0.170996	-0.230809
N	-1.083914	0.033133	0.991315

C	4.393633	-1.357338	-0.068988
C	3.051524	-1.341790	0.337786
Cl	-0.216380	-2.310792	-1.950209
C	2.464089	-0.079069	0.565052
C	3.164475	1.138110	0.428370
C	4.504238	1.060441	0.020394
C	2.530034	2.480249	0.775092
C	2.823482	2.847226	2.242690
C	2.967227	3.616919	-0.158784
C	2.295796	-2.640559	0.593894
C	2.536974	-3.121415	2.037734
C	2.636631	-3.749450	-0.410007
C	0.678436	-0.022172	2.322239
C	-0.678500	0.022121	2.322217
C	-2.464107	0.079012	0.564989
C	-3.051586	1.341719	0.337739
C	-4.393698	1.357227	-0.069022
C	-5.109838	0.170864	-0.230864
C	-4.504222	-1.060556	0.020325
C	-3.164461	-1.138185	0.428313
C	-2.295923	2.640522	0.593865
C	-2.536953	3.121232	2.037778
C	-2.636999	3.749471	-0.409891
C	-2.529985	-2.480295	0.775087
C	-2.823592	-2.847330	2.242641
C	-2.966977	-3.616973	-0.158872
C	0.000002	0.000000	0.177920
H	6.154619	-0.206973	-0.549589
H	4.888864	-2.311146	-0.256496
H	5.084877	1.976311	-0.099060
H	1.441841	2.375356	0.659574
H	3.907688	2.966043	2.403050
H	2.464154	2.077184	2.940891
H	2.332725	3.798043	2.506133
H	2.370101	4.518481	0.050503
H	2.812506	3.345923	-1.212382
H	4.025715	3.885656	-0.012389
H	1.222692	-2.433716	0.480170
H	2.236965	-2.364734	2.777824
H	3.604021	-3.346245	2.199807
H	1.959637	-4.038355	2.238444
H	2.509142	-3.400549	-1.444555
H	1.962029	-4.606538	-0.257876
H	3.667429	-4.117884	-0.284238

H	1.392704	-0.047804	3.138312
H	-1.392793	0.047751	3.138269
H	-4.888961	2.311022	-0.256513
H	-6.154649	0.206811	-0.549630
H	-5.084838	-1.976442	-0.099119
H	-1.222816	2.433786	0.479982
H	-3.603997	3.345960	2.200008
H	-1.959665	4.038202	2.238494
H	-2.236785	2.364508	2.777760
H	-2.509631	3.400670	-1.444487
H	-1.962449	4.606603	-0.257785
H	-3.667812	4.117801	-0.283940
H	-1.441786	-2.375327	0.659704
H	-2.464398	-2.077288	2.940908
H	-2.332811	-3.798125	2.506120
H	-3.907810	-2.966217	2.402863
H	-4.025464	-3.885789	-0.012622
H	-2.369814	-4.518496	0.050474
H	-2.812137	-3.345944	-1.212445
Cl	0.216492	2.311001	-1.949881

68

**IPrCl<sub>2</sub>isomer** SCF Done: -2207.52781155 A.U.

Pd	-0.219394	0.756354	1.308844
N	-1.052159	-0.435776	-1.267025
C	-5.050258	-0.117619	-0.005314
N	1.104856	-0.372245	-1.169512
C	-4.417945	-1.360157	0.005625
C	-3.086967	-1.498628	-0.417057
Cl	0.558591	-1.184666	2.321766
C	-2.432173	-0.335244	-0.862819
C	-3.043878	0.936028	-0.889953
C	-4.369807	1.019963	-0.445860
C	-2.276412	2.178110	-1.333020
C	-3.151851	3.200579	-2.074966
C	-1.587469	2.857496	-0.139375
C	-2.403475	-2.860048	-0.374392
C	-3.073632	-3.847235	-1.345319
C	-2.350242	-3.419794	1.057079
C	-0.588178	-0.872546	-2.502374
C	0.770305	-0.828174	-2.441033
C	2.452819	-0.158264	-0.700164
C	2.972265	1.151307	-0.729096
C	4.287164	1.331483	-0.273626
C	5.042009	0.252495	0.184323

C	4.498198	-1.033192	0.199864
C	3.187809	-1.270724	-0.237176
C	2.183587	2.339666	-1.267039
C	2.756099	2.805772	-2.617277
C	2.115896	3.496823	-0.257600
C	2.610087	-2.681655	-0.240927
C	3.038183	-3.442378	-1.510262
C	2.980822	-3.485498	1.014100
C	-0.016811	-0.119488	-0.455460
H	-6.085309	-0.031631	0.334186
H	-4.963837	-2.238581	0.356395
H	-4.881384	1.983339	-0.441714
H	-1.489575	1.859891	-2.034579
H	-3.878517	3.684314	-1.403963
H	-3.708209	2.721891	-2.894907
H	-2.520937	3.994561	-2.502638
H	-1.104875	3.803947	-0.425736
H	-0.714059	2.254908	0.238002
H	-2.272580	3.036259	0.699044
H	-1.362178	-2.733732	-0.704616
H	-3.077603	-3.457046	-2.375334
H	-4.118176	-4.046125	-1.055381
H	-2.536100	-4.808881	-1.344775
H	-1.812331	-2.733116	1.727712
H	-1.820442	-4.386056	1.064329
H	-3.360346	-3.590018	1.463124
H	-1.264544	-1.168104	-3.298687
H	1.527451	-1.060544	-3.182766
H	4.727318	2.330731	-0.284287
H	6.065192	0.413533	0.532901
H	5.103479	-1.865282	0.563108
H	1.151105	2.012475	-1.454057
H	3.793111	3.161760	-2.505256
H	2.154863	3.634507	-3.024486
H	2.756730	1.987312	-3.354137
H	1.718761	3.161426	0.712892
H	1.460979	4.296057	-0.639035
H	3.108754	3.939707	-0.081100
H	1.513860	-2.589577	-0.247892
H	2.732607	-2.920979	-2.429128
H	2.588144	-4.448074	-1.526191
H	4.134038	-3.558505	-1.540127
H	4.052335	-3.740923	1.036873
H	2.420301	-4.433705	1.027501

H	2.734039	-2.927443	1.928179
Cl	-0.518926	2.001790	3.317658
79			
<b>IPrCl2Py</b> SCF Done: -2455.70111635 A.U.			
Pd	0.000094	1.149433	-0.000020
N	-1.070545	-1.667646	0.146290
C	-5.050000	-0.421934	0.747145
N	1.070233	-1.667837	-0.146157
C	-4.160965	-0.452359	1.822066
C	-2.833399	-0.870676	1.649841
Cl	0.908934	1.180783	2.180359
C	-2.435433	-1.242012	0.347179
C	-3.315251	-1.238924	-0.756497
C	-4.633418	-0.818889	-0.523357
C	-2.892750	-1.727409	-2.137888
C	-3.251636	-3.215498	-2.317314
C	-3.496627	-0.901108	-3.282980
C	-1.892390	-1.001117	2.841690
C	-2.018861	-2.405635	3.462269
C	-2.094316	0.087231	3.902732
C	-0.671799	-2.999831	0.097410
C	0.671263	-2.999951	-0.097175
C	2.435183	-1.242435	-0.347125
C	2.833160	-0.871246	-1.649827
C	4.160786	-0.453155	-1.822129
C	5.049868	-0.422802	-0.747244
C	4.633273	-0.819607	0.523298
C	3.315046	-1.239417	0.756514
C	1.892090	-1.001604	-2.841635
C	2.018268	-2.406202	-3.462093
C	2.094204	0.086613	-3.902770
C	2.892522	-1.727745	2.137951
C	3.251244	-3.215862	2.317478
C	3.496520	-0.901425	3.282964
C	-0.000089	-0.843610	0.000030
H	-6.080717	-0.093238	0.903198
H	-4.508888	-0.155003	2.812377
H	-5.346164	-0.801116	-1.349319
H	-1.800291	-1.621399	-2.206137
H	-4.343521	-3.358305	-2.263314
H	-2.794441	-3.851113	-1.545740
H	-2.909185	-3.577654	-3.300225
H	-3.035032	-1.197714	-4.238330
H	-3.315547	0.171936	-3.134207

H	-4.581493	-1.067754	-3.381371
H	-0.863588	-0.887567	2.476614
H	-1.807551	-3.195315	2.725169
H	-3.036800	-2.571193	3.852420
H	-1.308720	-2.522991	4.296975
H	-2.045592	1.091193	3.455733
H	-1.298531	0.017842	4.660474
H	-3.057749	-0.016485	4.427513
H	-1.376851	-3.816062	0.210960
H	1.376179	-3.816310	-0.210646
H	4.508719	-0.155920	-2.812472
H	6.080632	-0.094280	-0.903358
H	5.346055	-0.801897	1.349230
H	0.863322	-0.887818	-2.476540
H	3.036169	-2.571993	-3.852244
H	1.308091	-2.523491	-4.296777
H	1.806815	-3.195777	-2.724920
H	2.045721	1.090618	-3.455841
H	1.298363	0.017346	-4.660465
H	3.057587	-0.017357	-4.427593
H	1.800078	-1.621603	2.206219
H	2.793976	-3.851480	1.545949
H	2.908762	-3.577914	3.300416
H	4.343112	-3.358792	2.263477
H	4.581370	-1.068186	3.381344
H	3.034913	-1.197903	4.238349
H	3.315556	0.171627	3.134110
Cl	-0.908816	1.180890	-2.180368
N	0.000345	3.281892	-0.000053
C	1.106929	3.962962	0.347731
C	-1.106064	3.963226	-0.347877
C	1.149576	5.356169	0.352651
C	-1.148346	5.356444	-0.352888
C	0.000708	6.068249	-0.000145
H	1.970616	3.364630	0.641724
H	-1.969912	3.365102	-0.641820
H	2.072288	5.866149	0.634108
H	-2.070928	5.866645	-0.634373
H	0.000851	7.160639	-0.000184
100			
<b>IPrCl2Py1</b> SCF Done: -3543.35915652 A.U.			
Pd	1.255823	0.951043	0.151892
N	1.318681	-1.981345	-0.393118
C	-2.882630	-2.200082	-0.661851

N	3.339317	-1.242794	-0.181474
C	-2.250992	-2.490720	0.545629
C	-0.854779	-2.427919	0.665701
Cl	1.035069	0.499160	2.460301
C	-0.123323	-2.052570	-0.481208
C	-0.734982	-1.767290	-1.723141
C	-2.133912	-1.842041	-1.783267
C	0.086636	-1.466211	-2.970987
C	0.474548	-2.773935	-3.687920
C	-0.611209	-0.510755	-3.947028
C	-0.170105	-2.816691	1.970890
C	0.047626	-4.341190	2.026652
C	-0.927167	-2.341830	3.218554
C	2.164751	-3.074570	-0.552645
C	3.433444	-2.611942	-0.415296
C	4.479660	-0.374879	-0.003396
C	5.099907	0.166805	-1.150407
C	6.203817	1.007589	-0.944815
C	6.667819	1.286350	0.340958
C	6.047943	0.716751	1.453297
C	4.942058	-0.133977	1.308084
C	4.649114	-0.193496	-2.561914
C	5.438056	-1.409721	-3.085090
C	4.760999	0.974218	-3.551892
C	4.328388	-0.831368	2.516224
C	5.068339	-2.153288	2.797251
C	4.291835	0.047409	3.772843
C	2.039644	-0.851931	-0.160659
H	-3.972054	-2.250495	-0.729915
H	-2.857506	-2.750799	1.413345
H	-2.647444	-1.621228	-2.719757
H	1.010558	-0.966611	-2.651021
H	-0.424938	-3.311199	-4.031264
H	1.041303	-3.450019	-3.031467
H	1.100463	-2.556761	-4.568719
H	0.097317	-0.196530	-4.728790
H	-0.971556	0.393195	-3.436994
H	-1.467222	-0.987664	-4.451235
H	0.813024	-2.324825	1.988571
H	0.638108	-4.707985	1.174597
H	-0.919635	-4.870366	2.016510
H	0.578902	-4.620014	2.951127
H	-1.134805	-1.266120	3.166564
H	-0.318315	-2.535203	4.116149

H	-1.881466	-2.877152	3.349533
H	1.786381	-4.071332	-0.752881
H	4.388714	-3.123935	-0.459259
H	6.711555	1.449402	-1.803459
H	7.527754	1.947260	0.476865
H	6.435939	0.931212	2.450179
H	3.585837	-0.467575	-2.510487
H	6.513011	-1.174180	-3.152894
H	5.086466	-1.690836	-4.091068
H	5.328155	-2.287827	-2.432827
H	4.259504	1.871398	-3.164096
H	4.279325	0.700257	-4.503943
H	5.810509	1.222690	-3.778011
H	3.284727	-1.070448	2.271892
H	5.049041	-2.825505	1.926408
H	4.601655	-2.682811	3.643733
H	6.123986	-1.963189	3.052688
H	5.300029	0.239438	4.174195
H	3.716131	-0.459806	4.562860
H	3.803042	1.010639	3.568033
Cl	1.644650	1.607058	-2.093443
N	0.241646	2.800298	0.465878
C	0.817941	3.748087	1.224959
C	-0.992617	3.002891	-0.036664
C	0.186270	4.952686	1.520296
C	-1.689691	4.185337	0.226251
C	-1.096508	5.172272	1.011899
H	1.812194	3.518398	1.612665
H	0.692018	5.693722	2.140851
H	-2.692618	4.311696	-0.182744
H	-1.629116	6.101631	1.226090
C	-1.565114	1.917475	-0.927818
H	-1.113192	2.040830	-1.923202
H	-1.228715	0.933472	-0.575326
N	-3.005235	1.930914	-1.088069
H	-3.366273	2.267147	-1.978800
C	-3.920220	1.200576	-0.413516
C	-5.208617	1.041150	-1.202872
C	-3.825336	0.627916	0.835101
C	-6.267975	0.165407	-0.658883
C	-4.834195	-0.285012	1.380042
C	-6.081825	-0.488589	0.573819
Cl	-2.438293	0.878633	1.867836
O	-4.678754	-0.874727	2.444273



O	-5.317538	1.623413	-2.270868
C	-7.080758	-1.336318	1.061579
C	-8.256934	-1.529462	0.330341
C	-7.448845	-0.028494	-1.388606
C	-8.442532	-0.875433	-0.893935
H	-6.920299	-1.835582	2.018284
H	-9.033374	-2.193429	0.717423
H	-9.361702	-1.028857	-1.463586
H	-7.569204	0.487224	-2.342773
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<b>IPrCl2Py1isomer</b> SCF Done: -3543.35805660 A.U.			
Pd	-1.243574	0.171855	-0.990466
N	-1.448410	0.251950	1.970689
C	2.620225	1.337972	2.185215
N	-3.363177	-0.330202	1.154460
C	2.262874	-0.009525	2.130970
C	0.915387	-0.398812	2.079940
Cl	-0.962622	-2.166912	-1.131745
C	-0.055863	0.626957	2.074648
C	0.274716	1.996721	2.157878
C	1.637732	2.326345	2.205609
C	-0.791292	3.080660	2.260499
C	-1.136737	3.351159	3.738147
C	-0.398566	4.389810	1.562619
C	0.524365	-1.871479	2.107372
C	0.363636	-2.347464	3.563882
C	1.499045	-2.774751	1.343349
C	-2.301330	0.056058	3.051918
C	-3.506207	-0.303174	2.539357
C	-4.421656	-0.683267	0.238532
C	-5.195460	0.354989	-0.322909
C	-6.217307	-0.013452	-1.210285
C	-6.459777	-1.354259	-1.510377
C	-5.691561	-2.359000	-0.922011
C	-4.653103	-2.049383	-0.030987
C	-4.992052	1.811548	0.077100
C	-5.880899	2.157669	1.287067
C	-5.228983	2.798472	-1.072658
C	-3.863343	-3.157506	0.656920
C	-4.596640	-3.634112	1.925716
C	-3.567018	-4.350288	-0.262959
C	-2.100497	0.014572	0.799989
H	3.674190	1.622924	2.203882
H	3.045250	-0.769903	2.128718

H	1.938737	3.373458	2.254255
H	-1.693309	2.705515	1.756575
H	-0.254432	3.732205	4.278343
H	-1.480616	2.445021	4.256886
H	-1.935297	4.106907	3.812828
H	-1.265231	5.069018	1.534839
H	-0.078806	4.206548	0.527752
H	0.409134	4.914761	2.097742
H	-0.448863	-1.969544	1.607782
H	-0.380125	-1.749008	4.110927
H	1.321057	-2.273201	4.105655
H	0.036802	-3.399626	3.589544
H	1.643602	-2.418377	0.314805
H	1.093739	-3.797360	1.291531
H	2.481897	-2.838429	1.836790
H	-1.972543	0.184613	4.077667
H	-4.447615	-0.536478	3.025130
H	-6.838561	0.757833	-1.667898
H	-7.261388	-1.619409	-2.204540
H	-5.904377	-3.402574	-1.158852
H	-3.943821	1.934293	0.380858
H	-6.948133	2.054771	1.029776
H	-5.705125	3.197029	1.608872
H	-5.676496	1.499209	2.144725
H	-4.628467	2.531519	-1.954348
H	-4.932073	3.811265	-0.758397
H	-6.289487	2.844455	-1.368598
H	-2.892797	-2.736028	0.955306
H	-4.773545	-2.813543	2.635751
H	-4.005772	-4.407191	2.443228
H	-5.575651	-4.069875	1.666417
H	-4.478272	-4.922120	-0.501682
H	-2.871499	-5.041698	0.238831
H	-3.099571	-4.019675	-1.200584
Cl	-1.664954	2.502541	-1.074989
N	-0.088223	0.394183	-2.768244
C	-0.593645	0.040335	-3.962032
C	1.161234	0.893831	-2.686935
C	0.128291	0.174730	-5.144114
C	1.943639	1.055936	-3.833155
C	1.424267	0.693848	-5.074925
H	-1.607611	-0.364762	-3.957133
H	-0.320123	-0.124609	-6.092460
H	2.953498	1.454405	-3.732636

H	2.024558	0.812871	-5.979823
C	1.643167	1.289137	-1.306224
H	1.097027	2.195087	-1.003625
H	1.346421	0.511215	-0.590364
N	3.063216	1.576805	-1.188314
H	3.293498	2.560291	-1.085264
C	4.026915	0.734782	-0.745348
C	3.830321	-0.751844	-0.927098
C	5.207708	1.179803	-0.188305
C	4.826813	-1.666605	-0.318496
C	6.248667	0.313276	0.362524
C	5.991213	-1.161106	0.290305
Cl	5.458143	2.901380	0.019045
O	7.264328	0.752278	0.890051
O	2.877719	-1.170154	-1.564552
C	6.922282	-2.045310	0.843494
C	6.694730	-3.423935	0.796999
C	4.608012	-3.050102	-0.372624
C	5.537894	-3.926935	0.189032
H	7.819439	-1.634293	1.309075
H	7.423341	-4.109657	1.235657
H	5.361994	-5.004219	0.152139
H	3.702777	-3.422079	-0.853903

112

**IPrCl2Py1isomer+DMF** SCF Done: -3791.72541478 A.U.

Pd	-0.941618	-0.530511	0.245448
N	-0.558423	2.357031	-0.332643
C	3.572427	1.857077	-1.030563
N	-2.668527	1.972154	-0.057991
C	3.129412	2.281990	0.219896
C	1.761091	2.447463	0.487038
Cl	-0.472954	-0.012391	2.504358
C	0.858330	2.175346	-0.561717
C	1.280522	1.763990	-1.849107
C	2.657531	1.596611	-2.051788
C	0.293470	1.572751	-2.995595
C	-0.010710	2.919604	-3.680158
C	0.748981	0.542034	-4.035564
C	1.303545	2.962931	1.845517
C	1.416869	4.498143	1.903682
C	2.069291	2.322852	3.012613
C	-1.205536	3.585904	-0.423383
C	-2.529066	3.345209	-0.246356
C	-3.952748	1.315502	0.030670

C	-4.631284	1.022152	-1.173583
C	-5.901929	0.439965	-1.066090
C	-6.459639	0.153282	0.179661
C	-5.764005	0.452065	1.349737
C	-4.495369	1.048325	1.303726
C	-4.055024	1.374196	-2.541764
C	-4.582947	2.740203	-3.020734
C	-4.325438	0.302187	-3.607022
C	-3.768884	1.447231	2.580775
C	-4.162921	2.876229	2.999049
C	-3.987868	0.456208	3.731892
C	-1.456861	1.363032	-0.090635
H	4.640997	1.725759	-1.213302
H	3.859867	2.482486	1.004393
H	3.026733	1.258368	-3.020305
H	-0.642660	1.189364	-2.570206
H	0.900508	3.337756	-4.138717
H	-0.404972	3.662291	-2.972204
H	-0.762353	2.781856	-4.474360
H	-0.076713	0.331483	-4.732416
H	1.040344	-0.407573	-3.564987
H	1.599981	0.905719	-4.633732
H	0.246543	2.687524	1.967087
H	0.832046	4.986238	1.110056
H	2.466609	4.815087	1.788754
H	1.051893	4.873945	2.873203
H	2.036668	1.226942	2.947303
H	1.609622	2.621664	3.968036
H	3.122331	2.645456	3.041663
H	-0.666802	4.507898	-0.614430
H	-3.382606	4.014630	-0.239595
H	-6.463689	0.203908	-1.971054
H	-7.448454	-0.308304	0.238019
H	-6.213765	0.216803	2.315001
H	-2.963439	1.446323	-2.434809
H	-5.676422	2.705363	-3.157016
H	-4.127038	3.009988	-3.987161
H	-4.359839	3.545481	-2.306713
H	-3.993673	-0.686755	-3.264983
H	-3.772013	0.547250	-4.527553
H	-5.393024	0.246613	-3.873652
H	-2.692277	1.444404	2.366217
H	-3.940018	3.609722	2.209219
H	-3.611313	3.177127	3.904743

H	-5.241560	2.935716	3.220574
H	-5.009305	0.523296	4.142081
H	-3.291030	0.682710	4.554097
H	-3.817839	-0.577631	3.398711
Cl	-1.611734	-1.235751	-1.923105
N	-0.112569	-2.466284	0.582322
C	-0.734173	-3.353442	1.379477
C	1.080005	-2.771952	0.032333
C	-0.191210	-4.606550	1.652063
C	1.682229	-4.010148	0.265852
C	1.040733	-4.939827	1.083350
H	-1.690841	-3.039613	1.804302
H	-0.728539	-5.299210	2.301567
H	2.650627	-4.222631	-0.187853
H	1.499261	-5.912251	1.277387
C	1.698270	-1.718094	-0.862669
H	1.098133	-1.671694	-1.783126
H	1.587401	-0.735806	-0.386012
N	3.079420	-1.942436	-1.250179
H	3.215900	-2.272233	-2.200845
C	4.182452	-1.396693	-0.686538
C	4.124021	-0.971853	0.763341
C	5.381324	-1.280614	-1.359518
C	5.291600	-0.246372	1.321698
C	6.583189	-0.649315	-0.817543
C	6.473315	-0.098116	0.571850
Cl	5.477882	-1.808417	-3.027496
O	7.620218	-0.536108	-1.461736
O	3.144857	-1.234302	1.441215
C	7.561828	0.583861	1.124931
C	7.473603	1.120339	2.412769
C	5.211677	0.281338	2.617408
C	6.298524	0.969349	3.159696
H	8.469977	0.687348	0.529021
H	8.325002	1.657832	2.836717
H	6.230371	1.388615	4.165901
H	4.286992	0.154809	3.181152
O	-3.910508	-2.535821	1.934255
N	-5.221293	-2.967246	0.097445
C	-5.313450	-2.982842	-1.350578
H	-5.469024	-4.010707	-1.720635
H	-6.153856	-2.358123	-1.693655
H	-4.385383	-2.584436	-1.783126
C	-6.368644	-3.436624	0.850410

H	-6.146695	-3.357721	1.921450
H	-7.256728	-2.826070	0.617055
H	-6.595245	-4.487149	0.600965
C	-4.098418	-2.544890	0.718095
H	-3.326050	-2.197744	0.000993
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<b>IPrCl2Py2</b> SCF Done: -3543.35530411 A.U.			
Pd	-1.168573	0.960998	0.102061
N	-1.485361	-1.971367	0.634941
C	2.204047	-2.034685	2.668657
N	-3.187231	-1.233134	-0.472597
C	2.167329	-2.224230	1.287552
C	0.952824	-2.231745	0.588236
Cl	-0.263305	0.609435	-2.056245
C	-0.225348	-2.030056	1.338927
C	-0.226182	-1.878442	2.742410
C	1.019607	-1.879646	3.387925
C	-1.519855	-1.785138	3.543454
C	-1.986905	-3.191112	3.968816
C	-1.413945	-0.870156	4.770945
C	0.916263	-2.518324	-0.907730
C	0.793321	-4.034119	-1.154998
C	2.120866	-1.945127	-1.663556
C	-2.328187	-3.057716	0.425449
C	-3.400459	-2.593186	-0.265743
C	-4.105838	-0.370961	-1.178124
C	-5.070479	0.336701	-0.428966
C	-5.949005	1.170018	-1.136922
C	-5.874296	1.279234	-2.525795
C	-4.926155	0.547290	-3.240649
C	-4.019327	-0.299008	-2.585193
C	-5.215208	0.146354	1.076202
C	-6.211471	-0.990704	1.373809
C	-5.617208	1.428274	1.816163
C	-3.035985	-1.150042	-3.380828
C	-3.700083	-2.469248	-3.820514
C	-2.448837	-0.419378	-4.596353
C	-2.009673	-0.846157	0.081844
H	3.169055	-1.998600	3.177462
H	3.100688	-2.368850	0.745342
H	1.065130	-1.752434	4.470471
H	-2.286095	-1.350433	2.885795
H	-1.243588	-3.660915	4.633947
H	-2.132853	-3.858220	3.107160

H	-2.942508	-3.129989	4.514502
H	-2.412818	-0.725013	5.212238
H	-1.018092	0.116875	4.495432
H	-0.772587	-1.305342	5.554324
H	0.023067	-2.031656	-1.322179
H	-0.100574	-4.456529	-0.672123
H	1.674070	-4.565691	-0.758079
H	0.725760	-4.243602	-2.234967
H	2.250894	-0.876207	-1.445070
H	1.966282	-2.048575	-2.748790
H	3.056357	-2.469833	-1.415174
H	-2.086050	-4.052766	0.783131
H	-4.291603	-3.097153	-0.624429
H	-6.708501	1.736457	-0.596023
H	-6.568450	1.935083	-3.057553
H	-4.892791	0.633574	-4.327788
H	-4.234670	-0.148342	1.473439
H	-7.216342	-0.738037	0.996740
H	-6.286694	-1.161541	2.460041
H	-5.903826	-1.936744	0.903652
H	-4.934922	2.255520	1.573387
H	-5.566635	1.259520	2.903236
H	-6.648092	1.737872	1.579997
H	-2.193696	-1.391454	-2.717166
H	-4.076759	-3.048416	-2.965062
H	-2.977948	-3.100148	-4.363756
H	-4.551644	-2.270026	-4.491940
H	-3.202552	-0.258953	-5.384092
H	-1.640376	-1.023775	-5.037489
H	-2.025670	0.552208	-4.306392
Cl	-2.099191	1.426559	2.223149
N	-0.170420	2.842033	0.173428
C	-0.791905	3.979579	0.523799
C	1.146259	2.864430	-0.090937
C	-0.105206	5.189912	0.612650
C	1.914779	4.025328	-0.007437
C	1.264186	5.213388	0.347879
H	-1.856530	3.904081	0.749001
H	-0.643674	6.097936	0.888456
H	1.587218	1.915441	-0.392110
H	1.824444	6.149772	0.416426
C	3.410432	3.998494	-0.263373
H	3.688255	4.882413	-0.856712
H	3.946442	4.083528	0.691225

N	3.875547	2.833435	-0.991005
H	3.905133	2.910504	-2.007659
C	4.298406	1.628160	-0.568797
C	4.762140	0.776056	-1.748533
C	4.321940	1.073262	0.694948
C	5.314511	-0.566554	-1.485279
C	4.935467	-0.222827	0.994331
C	5.406039	-1.046133	-0.166805
Cl	3.646247	1.883356	2.097979
O	5.044642	-0.650999	2.138664
O	4.650620	1.232712	-2.874810
C	5.914120	-2.327578	0.065797
C	5.725791	-1.367716	-2.559165
C	6.225758	-2.648657	-2.319989
C	6.318799	-3.127685	-1.007194
H	5.640347	-0.974538	-3.573373
H	6.542215	-3.275810	-3.156194
H	6.708050	-4.130881	-0.818909
H	5.975932	-2.686570	1.094086
100			
<b>IPrCl2Py2isomer</b> SCF Done: -3543.34876074 A.U.			
Pd	0.952458	-0.797627	-0.206634
N	2.291029	1.628371	0.984361
C	-1.223066	3.673309	2.096774
N	3.743020	0.317324	0.064086
C	-0.474798	4.111827	1.005061
C	0.676268	3.426350	0.591379
Cl	0.022827	0.724590	-1.756263
C	1.062912	2.297004	1.346471
C	0.328978	1.831529	2.456742
C	-0.829203	2.540896	2.808444
C	0.799844	0.650376	3.293703
C	1.693381	1.138523	4.448693
C	-0.356435	-0.218494	3.806351
C	1.474374	3.931682	-0.607400
C	2.327442	5.154936	-0.222199
C	0.585504	4.264708	-1.816163
C	3.545698	2.181094	1.227778
C	4.455445	1.365907	0.638465
C	4.349623	-0.733673	-0.717516
C	5.071716	-1.749263	-0.056194
C	5.657868	-2.744160	-0.853819
C	5.523440	-2.728366	-2.241009
C	4.812381	-1.703950	-2.868073



C	4.216270	-0.675851	-2.124137
C	5.272578	-1.763614	1.455307
C	6.644705	-1.167210	1.825240
C	5.129802	-3.165517	2.068019
C	3.527283	0.495219	-2.818137
C	4.513804	1.664608	-3.000274
C	2.871494	0.120008	-4.152066
C	2.410144	0.470826	0.281424
H	-2.125681	4.214794	2.390185
H	-0.796611	4.999687	0.457887
H	-1.427937	2.207541	3.657110
H	1.414883	0.003276	2.657492
H	1.131747	1.800643	5.128461
H	2.563931	1.699005	4.072681
H	2.067259	0.283069	5.034731
H	0.038970	-1.157423	4.223463
H	-1.058729	-0.465304	2.996170
H	-0.928454	0.281336	4.604986
H	2.153158	3.126609	-0.924798
H	3.010669	4.939244	0.611978
H	1.682698	5.995430	0.083100
H	2.934084	5.486665	-1.080231
H	-0.045105	3.407134	-2.084949
H	1.216065	4.514252	-2.684595
H	-0.061449	5.135504	-1.623040
H	3.667470	3.099342	1.792115
H	5.534905	1.436724	0.564385
H	6.226544	-3.546177	-0.380175
H	5.982903	-3.517680	-2.841500
H	4.730859	-1.700582	-3.955646
H	4.486443	-1.136232	1.899904
H	7.458086	-1.783596	1.408222
H	6.768805	-1.136418	2.919792
H	6.774994	-0.145022	1.441657
H	4.185724	-3.635816	1.761803
H	5.138447	-3.093599	3.167448
H	5.963922	-3.825405	1.779888
H	2.714798	0.847732	-2.170863
H	4.939116	1.990296	-2.038963
H	4.002470	2.530072	-3.452449
H	5.348296	1.374995	-3.660181
H	3.614761	-0.109749	-4.932636
H	2.264031	0.963350	-4.514850
H	2.207879	-0.751266	-4.040818

Cl	1.771176	-2.357420	1.373558
N	-0.649491	-2.121650	-0.627890
C	-0.949522	-2.537803	-1.868894
C	-1.488988	-2.396712	0.381163
C	-2.117533	-3.249917	-2.138746
C	-2.703749	-3.057230	0.194674
C	-3.015472	-3.494772	-1.098488
H	-0.244325	-2.272248	-2.658141
H	-2.325383	-3.582874	-3.156733
H	-1.192729	-2.043698	1.368514
H	-3.961948	-4.006084	-1.292791
C	-3.682814	-3.184566	1.345145
H	-3.910409	-4.243863	1.530238
H	-3.237783	-2.774555	2.260832
N	-4.969144	-2.542414	1.059965
H	-5.759996	-3.171736	0.961500
C	-5.173529	-1.307169	0.545728
C	-4.107460	-0.247057	0.719096
C	-6.364163	-0.925741	-0.040782
C	-4.202141	0.967530	-0.122965
C	-6.584292	0.354133	-0.715908
C	-5.403722	1.274563	-0.791374
Cl	-7.692127	-2.067452	-0.105251
O	-7.652128	0.649798	-1.240827
O	-3.214947	-0.404254	1.535955
C	-5.492036	2.444657	-1.549687
C	-3.096041	1.820268	-0.230443
C	-3.185620	2.974679	-1.012620
C	-4.382610	3.289875	-1.664524
H	-2.168417	1.566533	0.281874
H	-2.316150	3.625537	-1.111506
H	-4.451750	4.196781	-2.269912
H	-6.433870	2.673025	-2.051274

108

**IPrCl2Py2isomer+K3PO4** SCF Done: -5985.59231782 A.U.

Pd	2.009497	-0.773715	0.435561
N	4.785357	-0.100894	-0.372696
C	5.883244	-4.150357	-0.765795
N	3.668037	1.738049	-0.167514
C	5.712522	-3.600033	0.503671
C	5.342704	-2.255843	0.666648
Cl	2.003184	0.285662	2.554919
C	5.145969	-1.492943	-0.501360
C	5.310613	-2.020868	-1.802081

C	5.687886	-3.366745	-1.904293
C	5.132566	-1.173501	-3.058668
C	6.492334	-0.655393	-3.566552
C	4.404669	-1.913709	-4.191553
C	5.225821	-1.661037	2.064650
C	6.623708	-1.424396	2.663572
C	4.352074	-2.518593	2.991718
C	5.688560	0.936899	-0.568691
C	4.986739	2.089833	-0.454178
C	2.646499	2.749600	-0.018894
C	1.701559	2.924284	-1.060290
C	0.808193	4.000018	-0.942471
C	0.868495	4.878055	0.142794
C	1.809116	4.680348	1.153052
C	2.713170	3.605186	1.103521
C	1.678204	2.020046	-2.290413
C	2.841113	2.340205	-3.250895
C	0.347872	2.055854	-3.053411
C	3.736205	3.436081	2.223942
C	4.847988	4.497833	2.121014
C	3.092859	3.484429	3.620196
C	3.542358	0.384841	-0.106081
H	6.175231	-5.198425	-0.870419
H	5.880187	-4.221231	1.385673
H	5.828262	-3.812232	-2.890592
H	4.510345	-0.306714	-2.791029
H	7.137354	-1.498138	-3.864906
H	7.032673	-0.077367	-2.803905
H	6.351876	-0.006472	-4.446060
H	4.173240	-1.208045	-5.005575
H	3.462480	-2.352924	-3.837642
H	5.026418	-2.714278	-4.623552
H	4.732175	-0.683840	1.986236
H	7.226203	-0.762222	2.021493
H	7.171806	-2.374126	2.778080
H	6.542794	-0.956055	3.657993
H	3.359895	-2.686658	2.546850
H	4.207516	-2.004830	3.954660
H	4.811361	-3.497505	3.202502
H	6.738786	0.755234	-0.768825
H	5.289719	3.124984	-0.563317
H	0.057143	4.167115	-1.713623
H	0.170377	5.716835	0.202687
H	1.842460	5.371210	1.997640

H	1.816830	0.987658	-1.944178
H	2.747759	3.364561	-3.647843
H	2.827641	1.640582	-4.102087
H	3.823945	2.253280	-2.767438
H	-0.524182	1.908571	-2.396944
H	0.346047	1.265107	-3.820945
H	0.204833	3.012475	-3.582254
H	4.191796	2.441411	2.116983
H	5.359230	4.476576	1.147668
H	5.605718	4.336387	2.904365
H	4.432693	5.510015	2.255686
H	2.679314	4.479977	3.847255
H	3.852216	3.263211	4.387243
H	2.291437	2.739297	3.711954
Cl	1.828231	-1.674778	-1.759001
N	0.454040	-2.103497	1.039730
C	0.414037	-3.398269	0.661753
C	-0.628335	-1.562040	1.610504
C	-0.733159	-4.168816	0.830797
C	-1.843460	-2.239846	1.748945
C	-1.889474	-3.574972	1.354408
H	1.312412	-3.798758	0.190771
H	-0.727757	-5.215119	0.520010
H	-0.548086	-0.522845	1.908894
H	-2.825533	-4.132690	1.429512
C	-3.006898	-1.406730	2.223875
H	-2.872186	-1.174121	3.293504
H	-2.957534	-0.455617	1.675057
N	-4.344364	-1.966091	2.066663
H	-4.793630	-2.236687	2.936010
C	-5.222149	-1.552857	1.116817
C	-4.704707	-1.319412	-0.286823
C	-6.581371	-1.480119	1.346408
C	-5.680662	-0.827298	-1.302951
C	-7.560535	-0.993629	0.387760
C	-7.041937	-0.670818	-0.979430
Cl	-7.202259	-1.832309	2.960725
O	-8.748118	-0.826358	0.667279
O	-3.625986	-1.807548	-0.621309
C	-7.944462	-0.216687	-1.952949
C	-7.501330	0.076855	-3.244051
C	-5.247744	-0.557246	-2.608247
C	-6.149417	-0.100369	-3.571672
H	-8.993641	-0.105506	-1.674100

H	-8.207334	0.434883	-3.997343
H	-5.797387	0.121601	-4.582123
H	-4.194994	-0.676363	-2.850663
O	-1.666958	0.756830	0.295045
P	-2.947626	1.541942	-0.176155
O	-3.048157	1.515166	-1.742032
K	-0.787630	2.440491	1.995251
O	-4.268108	0.865869	0.433906
O	-2.899371	3.016940	0.373478
K	-1.405283	-0.740690	-1.804661
K	-5.564592	2.734229	-0.996368
100			
<b>IPrCl2Py3</b> SCF Done: -3543.34340332 A.U.			
Pd	1.275754	-0.157111	-0.461417
N	3.936914	-0.538171	0.906221
C	3.424139	-4.692110	1.391518
N	3.621825	1.537374	0.394700
C	2.809042	-3.807445	2.277829
C	2.968895	-2.420683	2.141870
Cl	0.175256	0.787263	1.405864
C	3.761185	-1.962261	1.067172
C	4.408584	-2.831991	0.163250
C	4.220201	-4.209210	0.353057
C	5.326528	-2.323581	-0.943208
C	6.793940	-2.322330	-0.472108
C	5.196425	-3.120839	-2.249494
C	2.379743	-1.461138	3.168588
C	3.379162	-1.240630	4.320140
C	1.013113	-1.904615	3.704396
C	5.057434	0.159059	1.347354
C	4.864740	1.460762	1.015732
C	3.051281	2.761592	-0.115164
C	3.168226	3.027277	-1.496957
C	2.603836	4.219787	-1.972800
C	1.967591	5.109607	-1.106671
C	1.889644	4.830589	0.257561
C	2.428961	3.649231	0.788674
C	3.951147	2.107160	-2.426096
C	5.432080	2.530183	-2.463027
C	3.366789	2.027598	-3.841503
C	2.385999	3.388251	2.290306
C	3.560267	4.094191	2.996054
C	1.057453	3.806025	2.937817
C	3.047942	0.307918	0.322897

H	3.287699	-5.769426	1.516194
H	2.203048	-4.203093	3.094195
H	4.703043	-4.916315	-0.323306
H	5.031476	-1.288219	-1.167444
H	7.126451	-3.348173	-0.242802
H	6.941893	-1.714497	0.431734
H	7.450292	-1.920135	-1.260768
H	5.755160	-2.613216	-3.051921
H	4.146045	-3.200051	-2.560412
H	5.615661	-4.135476	-2.154133
H	2.217894	-0.493619	2.676843
H	4.342509	-0.855151	3.952446
H	3.574961	-2.184536	4.855476
H	2.977576	-0.513090	5.044216
H	0.312445	-2.112304	2.881972
H	0.579217	-1.102837	4.321562
H	1.085689	-2.804191	4.336785
H	5.877436	-0.334217	1.857796
H	5.492757	2.333917	1.155189
H	2.670764	4.462433	-3.034332
H	1.535277	6.034087	-1.498117
H	1.399465	5.544135	0.921812
H	3.904763	1.089753	-2.017532
H	5.538928	3.547784	-2.874004
H	6.013318	1.841495	-3.097634
H	5.880465	2.523361	-1.457713
H	2.296522	1.774143	-3.815086
H	3.884684	1.241482	-4.412401
H	3.488789	2.971897	-4.396337
H	2.490347	2.303915	2.440088
H	4.536000	3.781366	2.597821
H	3.549075	3.872473	4.075521
H	3.484260	5.187088	2.872298
H	0.941213	4.901491	2.965005
H	1.023809	3.450363	3.979997
H	0.203387	3.372521	2.400258
Cl	2.326353	-1.115908	-2.349161
N	-0.621488	-0.661379	-1.289585
C	-1.614543	0.242721	-1.332909
C	-0.858229	-1.903748	-1.750739
C	-2.877928	-0.061172	-1.833391
C	-2.098283	-2.287122	-2.247965
C	-3.142770	-1.354755	-2.293698
H	-1.388008	1.232249	-0.933403

H	-3.648751	0.710254	-1.845106
H	-0.019905	-2.600951	-1.716875
H	-2.245906	-3.315206	-2.584834
C	-4.500786	-1.758488	-2.835831
H	-4.461198	-1.718648	-3.935705
H	-4.703593	-2.804675	-2.570230
N	-5.593243	-0.898378	-2.428961
H	-5.942928	-0.231876	-3.115967
C	-6.144808	-0.701846	-1.214484
C	-7.135973	0.458031	-1.253186
C	-5.938137	-1.358277	-0.020110
C	-7.844593	0.833930	-0.013853
C	-6.613916	-0.995859	1.232137
C	-7.590872	0.140696	1.183703
Cl	-4.839973	-2.718174	0.137478
O	-6.405394	-1.588229	2.284448
O	-7.305952	1.042380	-2.311576
C	-8.263499	0.514036	2.351126
C	-8.765620	1.890956	-0.036591
C	-9.433852	2.257173	1.132866
C	-9.181669	1.568265	2.325932
H	-8.944471	2.414263	-0.977322
H	-10.151458	3.080393	1.116166
H	-9.703877	1.854619	3.241851
H	-8.055229	-0.033482	3.271542

100

**IPrCl2Py3del2** SCF Done: -3543.34548320 A.U.

Pd	-1.263378	0.331165	-1.038093
N	-1.860598	0.243694	1.829689
C	1.929376	2.027366	2.312227
N	-3.577879	-0.555905	0.785574
C	1.820063	0.640502	2.218301
C	0.569435	0.016823	2.103246
Cl	-0.746572	-1.972088	-1.188527
C	-0.569103	0.850360	2.071024
C	-0.496295	2.253747	2.215430
C	0.781834	2.821372	2.330721
C	-1.748169	3.119480	2.304624
C	-2.227450	3.215989	3.766809
C	-1.566808	4.526704	1.720303
C	0.455712	-1.501441	2.081635
C	0.298014	-2.037780	3.517569
C	1.630487	-2.187628	1.374421
C	-2.773439	-0.145263	2.803007

C	-3.855467	-0.640950	2.148252
C	-4.495943	-0.956462	-0.253854
C	-5.320301	0.033576	-0.832391
C	-6.204218	-0.376487	-1.841042
C	-6.270457	-1.711933	-2.240139
C	-5.460713	-2.670660	-1.631798
C	-4.553102	-2.317521	-0.621655
C	-5.319903	1.472528	-0.328458
C	-6.339849	1.633782	0.815134
C	-5.572319	2.507268	-1.431730
C	-3.723589	-3.384972	0.083066
C	-4.536234	-4.033357	1.220424
C	-3.190499	-4.462978	-0.871307
C	-2.351534	-0.015058	0.586844
H	2.921771	2.480898	2.370539
H	2.723682	0.033716	2.232091
H	0.883043	3.903004	2.428753
H	-2.533886	2.624566	1.715142
H	-1.465639	3.712522	4.390176
H	-2.426139	2.228487	4.206605
H	-3.156173	3.806111	3.828438
H	-2.542136	5.036585	1.673289
H	-1.155269	4.483105	0.702950
H	-0.905763	5.148298	2.345679
H	-0.450804	-1.763732	1.520219
H	-0.577795	-1.602431	4.022420
H	1.189002	-1.799882	4.122020
H	0.174435	-3.132971	3.507824
H	1.797849	-1.760774	0.375599
H	1.416819	-3.260512	1.250359
H	2.563816	-2.105877	1.950823
H	-2.569221	-0.037947	3.862935
H	-4.794379	-1.038155	2.518975
H	-6.857463	0.356527	-2.316529
H	-6.967086	-2.009679	-3.028039
H	-5.536882	-3.712667	-1.946450
H	-4.321729	1.688436	0.075065
H	-7.363199	1.433958	0.456526
H	-6.311179	2.660985	1.213599
H	-6.133202	0.943419	1.646618
H	-4.871806	2.373900	-2.268817
H	-5.424306	3.521184	-1.028234
H	-6.602053	2.456791	-1.820991
H	-2.847422	-2.887430	0.522378



H	-4.882286	-3.293052	1.956316
H	-3.924204	-4.779060	1.753285
H	-5.425304	-4.546666	0.818289
H	-3.997553	-5.104723	-1.260038
H	-2.484512	-5.117066	-0.335227
H	-2.657316	-4.010855	-1.718938
Cl	-2.009233	2.572364	-1.144827
N	0.347048	0.770636	-2.394768
C	0.823404	-0.081489	-3.320551
C	1.136685	1.777263	-1.978942
C	2.124774	0.003296	-3.806697
C	2.451404	1.921839	-2.410747
C	2.983043	0.997676	-3.315343
H	0.151580	-0.880666	-3.636005
H	2.472598	-0.732592	-4.534932
H	0.703259	2.466088	-1.252229
H	3.061392	2.727688	-2.002798
C	4.466609	0.973899	-3.638200
H	4.627684	0.714389	-4.693216
H	4.923370	1.952595	-3.456393
N	5.129540	-0.065808	-2.844990
H	5.088407	-0.997754	-3.259642
C	5.193554	-0.158062	-1.494667
C	5.151644	-1.605942	-1.023057
C	5.298522	0.842098	-0.554157
C	5.182480	-1.884981	0.427929
C	5.246956	0.602023	0.895091
C	5.211789	-0.824454	1.351739
Cl	5.552407	2.516763	-0.995929
O	5.236722	1.516836	1.710994
O	5.086732	-2.490041	-1.862240
C	5.218274	-1.103740	2.722117
C	5.159014	-3.211865	0.878253
C	5.164898	-3.482987	2.247490
C	5.193957	-2.428391	3.168385
H	5.128788	-4.017223	0.142739
H	5.141327	-4.516734	2.598755
H	5.196012	-2.639560	4.240086
H	5.239440	-0.270309	3.425679
100			
<b>IPrCl2Py3isomer</b> SCF Done: -3543.34264700 A.U.			
Pd	0.984576	-0.011027	-0.757349
N	3.151767	-0.834387	1.134437
C	2.509604	-4.963810	0.576906

N	3.226583	1.301630	0.807235
C	1.604588	-4.221675	1.334059
C	1.786660	-2.844516	1.536459
Cl	-0.283821	1.092469	0.911134
C	2.914529	-2.246045	0.942119
C	3.846161	-2.969392	0.162606
C	3.618918	-4.342819	0.000531
C	5.079243	-2.317115	-0.456551
C	6.323744	-2.563905	0.417585
C	5.347344	-2.777640	-1.897445
C	0.809111	-2.066785	2.406224
C	1.033153	-2.391569	3.893739
C	-0.651759	-2.301797	1.995133
C	4.127696	-0.331174	1.989290
C	4.183484	1.007466	1.775140
C	3.047519	2.611712	0.227791
C	3.568312	2.837538	-1.068491
C	3.396680	4.116837	-1.615399
C	2.755947	5.128106	-0.897525
C	2.275778	4.881726	0.387172
C	2.406362	3.616738	0.981574
C	4.356262	1.765796	-1.816087
C	5.828458	1.761888	-1.361459
C	4.257908	1.879752	-3.341507
C	1.913784	3.388840	2.406245
C	2.935922	3.926307	3.426292
C	0.532799	4.010227	2.667097
C	2.579632	0.170878	0.420824
H	2.351071	-6.035859	0.434420
H	0.743558	-4.719973	1.784104
H	4.318152	-4.937175	-0.590336
H	4.901915	-1.232698	-0.497875
H	6.550984	-3.641445	0.468930
H	6.187534	-2.202464	1.446920
H	7.200972	-2.050872	-0.008675
H	6.157741	-2.172431	-2.334846
H	4.451393	-2.656817	-2.520741
H	5.669113	-3.830660	-1.938629
H	1.002308	-0.995666	2.269370
H	2.066245	-2.163999	4.201657
H	0.846451	-3.458537	4.100102
H	0.349750	-1.799273	4.523952
H	-0.796753	-2.106074	0.922209
H	-1.311733	-1.617838	2.548165

H	-0.981734	-3.331550	2.208839
H	4.687411	-0.972605	2.661531
H	4.818982	1.773056	2.206422
H	3.778963	4.332779	-2.613713
H	2.637257	6.119336	-1.342579
H	1.788021	5.686427	0.939939
H	3.928473	0.788828	-1.560353
H	6.319625	2.716206	-1.614011
H	6.380193	0.948762	-1.860880
H	5.919756	1.610773	-0.275490
H	3.209495	1.937303	-3.671458
H	4.709480	0.990190	-3.806843
H	4.792269	2.761981	-3.729801
H	1.809530	2.304081	2.550808
H	3.929808	3.472505	3.301012
H	2.597590	3.721557	4.454923
H	3.053675	5.017158	3.318186
H	0.572835	5.111405	2.673707
H	0.161920	3.692861	3.654889
H	-0.193473	3.687631	1.908713
Cl	2.212527	-1.102930	-2.455309
N	-0.806879	-0.314738	-1.862784
C	-1.715799	0.663939	-2.014017
C	-1.131033	-1.564106	-2.241649
C	-2.992716	0.419745	-2.508894
C	-2.392765	-1.888349	-2.729990
C	-3.363127	-0.887901	-2.847885
H	-1.415889	1.661587	-1.690957
H	-3.704777	1.243270	-2.584063
H	-0.355644	-2.322515	-2.123321
H	-2.624199	-2.927144	-2.971354
C	-4.784503	-1.215161	-3.262525
H	-4.927689	-0.941059	-4.318830
H	-4.952955	-2.296184	-3.176842
N	-5.785041	-0.464497	-2.507845
H	-6.313133	0.221651	-3.038159
C	-5.839657	-0.293788	-1.164486
C	-5.156668	-1.301783	-0.267365
C	-6.556193	0.726134	-0.571482
C	-5.047193	-0.983555	1.177430
C	-6.580911	1.003129	0.865634
C	-5.742731	0.109043	1.728168
Cl	-7.432780	1.854853	-1.584327
O	-7.215529	1.933889	1.348605

O	-4.719083	-2.341118	-0.731916
C	-5.643275	0.372108	3.097618
C	-4.255347	-1.798248	1.997513
C	-4.149830	-1.521734	3.362229
C	-4.846205	-0.438569	3.912016
H	-3.720771	-2.637246	1.549580
H	-3.522466	-2.150547	3.997598
H	-4.766255	-0.223617	4.980148
H	-6.193626	1.220436	3.507615
112			
<b>IPrCl2Py3isomer+DMF</b> SCF Done: -3791.70848389 A.U.			
Pd	-1.083205	-0.405461	-0.508480
N	-1.383992	2.131308	0.928307
C	2.030984	3.693726	-0.997443
N	-3.204869	0.995431	1.209086
C	2.187139	2.775764	0.038388
C	1.076017	2.242991	0.711976
Cl	-0.840943	-1.569541	1.542374
C	-0.199730	2.667794	0.292884
C	-0.390481	3.606691	-0.748550
C	0.754605	4.109523	-1.380682
C	-1.773591	4.109792	-1.151919
C	-2.082244	5.451585	-0.460216
C	-1.958211	4.240991	-2.670804
C	1.291046	1.288260	1.878299
C	1.842118	2.051945	3.096294
C	2.211515	0.120412	1.497748
C	-2.145755	2.821823	1.865147
C	-3.291306	2.114235	2.036242
C	-4.296090	0.073102	0.999254
C	-5.062690	0.214982	-0.183162
C	-6.132917	-0.671570	-0.362429
C	-6.441262	-1.635358	0.598981
C	-5.685935	-1.730897	1.764990
C	-4.592437	-0.880867	1.993642
C	-4.791559	1.331600	-1.188564
C	-5.429500	2.653631	-0.718291
C	-5.238767	1.009329	-2.619080
C	-3.816565	-0.972430	3.302159
C	-4.594692	-0.283035	4.438758
C	-3.471094	-2.418821	3.688150
C	-2.022328	0.992282	0.544161
H	2.912786	4.091791	-1.505757
H	3.191639	2.473121	0.335988

H	0.647664	4.836451	-2.187646
H	-2.514746	3.376393	-0.805769
H	-1.376669	6.229577	-0.795236
H	-2.006127	5.380466	0.634469
H	-3.102525	5.785848	-0.708699
H	-3.011929	4.471615	-2.896408
H	-1.694237	3.304189	-3.179288
H	-1.349637	5.058105	-3.090317
H	0.320812	0.858292	2.158753
H	1.172249	2.875627	3.390541
H	2.833537	2.482532	2.878315
H	1.951702	1.373325	3.957709
H	1.795814	-0.456654	0.661828
H	2.344254	-0.564660	2.348979
H	3.205620	0.479859	1.204173
H	-1.803806	3.749639	2.311609
H	-4.164056	2.305601	2.651339
H	-6.742532	-0.605559	-1.264064
H	-7.281829	-2.314799	0.437027
H	-5.945931	-2.482523	2.512309
H	-3.705539	1.479412	-1.239581
H	-6.527349	2.562702	-0.674780
H	-5.180675	3.466753	-1.419323
H	-5.074614	2.952885	0.278056
H	-4.825308	0.053075	-2.969005
H	-4.879813	1.797097	-3.299217
H	-6.336040	0.969142	-2.713329
H	-2.862972	-0.445261	3.161880
H	-4.814581	0.770496	4.209630
H	-4.014835	-0.312224	5.375425
H	-5.556121	-0.792020	4.618090
H	-4.369307	-3.001945	3.947546
H	-2.813918	-2.421409	4.572501
H	-2.941820	-2.927946	2.871159
Cl	-1.540315	0.654970	-2.575414
N	0.426177	-1.656466	-1.421350
C	0.764789	-2.865465	-0.936952
C	1.307514	-1.012229	-2.210170
C	2.015084	-3.432540	-1.163365
C	2.578060	-1.512768	-2.477893
C	2.969148	-2.732955	-1.913573
H	0.021573	-3.373123	-0.325948
H	2.245523	-4.404770	-0.722465
H	0.982588	-0.051817	-2.612390

H	3.267869	-0.929716	-3.088444
C	4.405152	-3.215916	-1.990699
H	4.434262	-4.308191	-2.101759
H	4.926386	-2.766753	-2.840373
N	5.115119	-2.911457	-0.739276
H	5.030151	-3.640522	-0.035381
C	5.338130	-1.682692	-0.203053
C	5.551068	-0.499452	-1.120283
C	5.469931	-1.483769	1.156667
C	5.670658	0.848470	-0.505724
C	5.705411	-0.187641	1.798133
C	5.770006	1.000818	0.889271
Cl	5.256907	-2.835443	2.248049
O	5.794607	-0.059269	3.012750
O	5.621750	-0.655001	-2.328474
C	5.896478	2.279362	1.440751
C	5.917113	3.402872	0.608712
C	5.698440	1.976927	-1.336634
C	5.817531	3.252135	-0.779857
H	5.967244	2.375211	2.525236
H	6.006030	4.400265	1.044891
H	5.830535	4.130652	-1.428457
H	5.620772	1.838188	-2.416041
O	-1.339830	-5.128389	-1.551522
N	-2.989975	-3.530080	-1.573487
C	-3.698693	-2.513872	-2.327441
H	-4.780133	-2.728274	-2.351505
H	-3.552352	-1.525419	-1.867769
H	-3.319810	-2.474114	-3.358045
C	-3.372488	-3.700538	-0.182128
H	-2.781379	-4.514926	0.252990
H	-3.182141	-2.776047	0.382976
H	-4.445629	-3.940144	-0.107183
C	-2.001079	-4.268395	-2.124179
H	-1.829819	-4.006932	-3.194413
100			
<b>IPrCl2Py3del2Isomer</b> SCF Done: -3543.34402124 A.U.			
Pd	-0.775808	-0.650810	-0.416744
N	-2.658197	1.687007	-0.011758
C	-0.197889	4.906742	-1.173800
N	-3.557322	-0.179925	0.605209
C	-0.440571	4.664655	0.178775
C	-1.209203	3.568287	0.593960
Cl	0.426956	0.368466	1.342148

C	-1.740043	2.728226	-0.412316
C	-1.481535	2.927123	-1.782965
C	-0.699287	4.036882	-2.140398
C	-2.032795	2.013199	-2.868068
C	-3.121506	2.723112	-3.690474
C	-0.908646	1.468876	-3.763564
C	-1.467262	3.341482	2.080854
C	-2.544897	4.304635	2.612867
C	-0.187005	3.465338	2.923217
C	-3.956810	1.978597	0.399656
C	-4.514751	0.809863	0.801299
C	-3.749071	-1.562552	0.974820
C	-4.550172	-2.386489	0.155912
C	-4.720792	-3.719843	0.558371
C	-4.118143	-4.206724	1.717539
C	-3.343462	-3.363844	2.515290
C	-3.147730	-2.019025	2.169420
C	-5.260607	-1.864462	-1.088215
C	-6.719638	-1.489929	-0.762117
C	-5.226259	-2.855407	-2.261963
C	-2.391780	-1.077315	3.100332
C	-3.366500	-0.426772	4.100234
C	-1.218311	-1.745571	3.826195
C	-2.413901	0.354869	0.098392
H	0.399359	5.771318	-1.473957
H	-0.026469	5.343277	0.926711
H	-0.490270	4.226531	-3.195233
H	-2.497669	1.142971	-2.389095
H	-2.717325	3.603765	-4.216378
H	-3.948123	3.063964	-3.046732
H	-3.537904	2.038849	-4.447547
H	-1.308685	0.710771	-4.453744
H	-0.125338	0.990453	-3.156454
H	-0.441203	2.264816	-4.365468
H	-1.831297	2.311061	2.203228
H	-3.496229	4.207050	2.070725
H	-2.210532	5.350792	2.517134
H	-2.742296	4.108002	3.679047
H	0.611018	2.826860	2.522225
H	-0.391742	3.152366	3.959643
H	0.177945	4.504351	2.962636
H	-4.355355	2.986658	0.361993
H	-5.492843	0.590542	1.214996
H	-5.334116	-4.389288	-0.047028

H	-4.260175	-5.251056	2.007293
H	-2.894123	-3.756692	3.428430
H	-4.730460	-0.958202	-1.415495
H	-7.283155	-2.380599	-0.438655
H	-7.219327	-1.076769	-1.653238
H	-6.791185	-0.743013	0.041369
H	-4.201287	-3.195459	-2.462034
H	-5.611614	-2.367886	-3.171775
H	-5.860734	-3.736363	-2.073191
H	-1.955015	-0.273271	2.496053
H	-4.173269	0.114757	3.582582
H	-2.833941	0.293494	4.742562
H	-3.830910	-1.187890	4.748952
H	-1.554142	-2.483469	4.572577
H	-0.629820	-0.982616	4.358503
H	-0.547942	-2.251145	3.114709
Cl	-1.942275	-1.620887	-2.229736
N	0.981901	-1.731086	-0.964770
C	1.751610	-2.295345	-0.016659
C	1.423936	-1.720851	-2.234108
C	3.016456	-2.801247	-0.293519
C	2.684023	-2.198755	-2.586366
C	3.526823	-2.713869	-1.596331
H	1.355190	-2.291595	0.999062
H	3.622557	-3.198497	0.522704
H	0.753244	-1.285424	-2.976095
H	3.025464	-2.098809	-3.617764
C	4.989117	-3.020705	-1.869342
H	5.173313	-4.101592	-1.782439
H	5.250011	-2.715908	-2.890855
N	5.865492	-2.366842	-0.886125
H	6.356008	-2.993537	-0.255264
C	5.617406	-1.134899	-0.370174
C	4.971915	-0.107329	-1.271755
C	5.985319	-0.731805	0.892669
C	4.293628	1.035116	-0.621475
C	5.535275	0.520308	1.518202
C	4.576821	1.352743	0.719786
Cl	6.880718	-1.831142	1.918978
O	5.855633	0.838483	2.656371
O	5.010845	-0.246777	-2.482312
C	3.936099	2.441443	1.318814
C	3.371095	1.795219	-1.350404
C	2.710575	2.859478	-0.734772



C	2.997368	3.184606	0.595763
H	3.165309	1.525927	-2.387915
H	1.959810	3.427980	-1.284576
H	2.472540	4.013575	1.074920
H	4.169760	2.680685	2.357572
100			
<b>IPrCl2Py4</b> SCF Done: -3468.38664971 A.U.			
Pd	1.028468	0.951424	0.166108
N	1.195028	-1.972250	-0.399446
C	-2.996025	-2.310289	-0.701900
N	3.188605	-1.168440	-0.169476
C	-2.364690	-2.598855	0.506062
C	-0.971540	-2.498915	0.636527
Cl	0.797639	0.465083	2.466139
C	-0.243202	-2.088491	-0.500183
C	-0.854149	-1.806571	-1.743446
C	-2.249958	-1.919188	-1.814036
C	-0.032282	-1.467830	-2.981592
C	0.413402	-2.755848	-3.700727
C	-0.755920	-0.535762	-3.961443
C	-0.285094	-2.885558	1.941437
C	-0.024974	-4.403988	1.978446
C	-1.063351	-2.448881	3.190021
C	2.077849	-3.036093	-0.557902
C	3.329528	-2.532626	-0.408855
C	4.298231	-0.263136	0.015822
C	4.905946	0.300165	-1.127570
C	5.979310	1.177994	-0.915270
C	6.426286	1.471547	0.373283
C	5.820053	0.880375	1.481893
C	4.744648	-0.007460	1.329966
C	4.475039	-0.073791	-2.541840
C	5.304356	-1.264964	-3.060233
C	4.557108	1.096522	-3.531609
C	4.147641	-0.726326	2.533767
C	4.928931	-2.023804	2.816803
C	4.074789	0.148554	3.791412
C	1.876619	-0.820882	-0.155516
H	-4.083363	-2.386350	-0.778125
H	-2.969029	-2.886510	1.366642
H	-2.763610	-1.700281	-2.750853
H	0.868282	-0.934422	-2.649744
H	-0.461054	-3.325536	-4.056264
H	0.999100	-3.413043	-3.041887

H	1.039558	-2.509907	-4.573749
H	-0.051362	-0.190183	-4.733487
H	-1.158532	0.350784	-3.452473
H	-1.586442	-1.043702	-4.477858
H	0.683681	-2.366636	1.972432
H	0.580213	-4.742721	1.125086
H	-0.976902	-4.959886	1.955496
H	0.508755	-4.680207	2.902290
H	-1.299639	-1.378600	3.150559
H	-0.455376	-2.637548	4.089231
H	-2.003295	-3.012089	3.307283
H	1.734348	-4.043807	-0.765834
H	4.301415	-3.012738	-0.448172
H	6.476304	1.637719	-1.770772
H	7.262294	2.161452	0.514301
H	6.194811	1.107398	2.481062
H	3.420357	-0.380538	-2.496854
H	6.371741	-0.995833	-3.122194
H	4.967267	-1.557119	-4.068022
H	5.218351	-2.145878	-2.408299
H	4.026426	1.978101	-3.147042
H	4.089791	0.807741	-4.486436
H	5.599913	1.376729	-3.751576
H	3.113698	-0.999132	2.283447
H	4.936160	-2.694691	1.944724
H	4.475285	-2.569798	3.659900
H	5.976471	-1.799881	3.078175
H	5.073706	0.373841	4.198619
H	3.512167	-0.379182	4.577404
H	3.555120	1.095279	3.585544
Cl	1.426611	1.651892	-2.065128
N	-0.056591	2.759506	0.486617
C	0.474474	3.721354	1.260740
C	-1.291437	2.920178	-0.029801
C	-0.205446	4.898909	1.558104
C	-2.035101	4.073782	0.233617
C	-1.488993	5.075181	1.034941
H	1.471906	3.525945	1.658827
H	0.264575	5.652722	2.191240
H	-3.036691	4.166019	-0.187592
H	-2.058369	5.982308	1.249916
C	-1.812174	1.821279	-0.936271
H	-1.346714	1.964747	-1.922708
H	-1.449262	0.847348	-0.581406

N	-3.248455	1.786470	-1.120630
H	-3.606765	2.097769	-2.021108
C	-4.145624	1.030685	-0.448386
C	-5.421829	0.809548	-1.246980
C	-4.052682	0.468918	0.798773
C	-6.475033	-0.083460	-0.714456
C	-5.059071	-0.462973	1.308940
C	-6.299371	-0.697541	0.483020
Cl	-2.687477	0.740267	1.858084
O	-4.914669	-1.054988	2.373873
O	-5.527709	1.367645	-2.329421
C	-7.325593	-1.632521	1.047784
H	-8.285995	-1.110730	1.196700
H	-7.525007	-2.461006	0.348012
H	-6.993961	-2.046760	2.006748
C	-7.707014	-0.283408	-1.550881
H	-8.612712	-0.001112	-0.989651
H	-7.661991	0.312757	-2.470143
H	-7.823313	-1.344660	-1.826797
100			
<b>IPrCl2Py4isomer</b> SCF Done: -3468.38538542 A.U.			
Pd	1.073189	-0.232001	0.962918
N	1.321078	0.944720	-1.752689
C	-2.785736	1.897073	-1.654762
N	3.250946	0.187776	-1.140817
C	-2.374874	0.639384	-2.096888
C	-1.013710	0.304086	-2.161352
Cl	0.895901	-2.462801	0.209533
C	-0.084125	1.285338	-1.750870
C	-0.468516	2.576806	-1.329903
C	-1.843182	2.854840	-1.284882
C	0.554207	3.656982	-0.998880
C	0.907382	4.463317	-2.264311
C	0.100554	4.605036	0.119463
C	-0.564011	-1.038852	-2.723809
C	-0.346908	-0.927733	-4.245222
C	-1.522911	-2.188790	-2.395531
C	2.200464	1.197027	-2.800574
C	3.414313	0.727083	-2.414205
C	4.315101	-0.418362	-0.376477
C	5.020765	0.387189	0.543027
C	6.049168	-0.224206	1.275054
C	6.362644	-1.570749	1.087141
C	5.660987	-2.335145	0.154767

C	4.619832	-1.777806	-0.602573
C	4.738710	1.878558	0.681991
C	5.621825	2.679353	-0.294034
C	4.901485	2.399032	2.115348
C	3.903869	-2.602197	-1.666758
C	4.678314	-2.552244	-2.998063
C	3.666399	-4.059231	-1.245911
C	1.965883	0.322095	-0.728737
H	-3.850130	2.131667	-1.588872
H	-3.126385	-0.092842	-2.395016
H	-2.185035	3.834615	-0.949237
H	1.464392	3.152923	-0.644088
H	0.017597	4.988025	-2.649578
H	1.293225	3.823539	-3.070577
H	1.676356	5.218693	-2.035127
H	0.939065	5.254266	0.417171
H	-0.225632	4.044910	1.006344
H	-0.720044	5.263633	-0.207970
H	0.398748	-1.291466	-2.259180
H	0.386698	-0.148207	-4.498994
H	-1.292151	-0.680199	-4.756054
H	0.021121	-1.883927	-4.651105
H	-1.715478	-2.249939	-1.316445
H	-1.078412	-3.145100	-2.712251
H	-2.485921	-2.087782	-2.921356
H	1.882524	1.680276	-3.718212
H	4.374455	0.729599	-2.919017
H	6.618854	0.361850	1.997709
H	7.167812	-2.027459	1.668407
H	5.928994	-3.383193	0.012635
H	3.689052	2.048715	0.407349
H	6.689749	2.544900	-0.054773
H	5.389416	3.754749	-0.228976
H	5.468121	2.363176	-1.336698
H	4.302882	1.806224	2.821894
H	4.552273	3.441837	2.172251
H	5.952961	2.386826	2.444902
H	2.913950	-2.150618	-1.824516
H	4.813561	-1.523153	-3.360745
H	4.140309	-3.116896	-3.776712
H	5.678745	-3.000739	-2.881415
H	4.606129	-4.633032	-1.200909
H	3.016496	-4.556954	-1.983085
H	3.171236	-4.112403	-0.266639

Cl	1.377603	1.912933	1.921372
N	-0.110258	-0.730589	2.663788
C	0.404099	-1.468367	3.662439
C	-1.381657	-0.288875	2.738238
C	-0.331106	-1.799019	4.796700
C	-2.178022	-0.582647	3.848114
C	-1.649925	-1.344587	4.888750
H	1.436679	-1.800648	3.537144
H	0.124920	-2.400299	5.584428
H	-3.205085	-0.217606	3.873064
H	-2.260749	-1.584301	5.762161
C	-1.873625	0.554981	1.580306
H	-1.376780	1.535044	1.641335
H	-1.525587	0.103877	0.641407
N	-3.306539	0.793189	1.530871
H	-3.590649	1.739598	1.764023
C	-4.212060	0.117966	0.780677
C	-3.945032	-1.332094	0.443608
C	-5.397921	0.666122	0.358854
C	-4.871862	-2.045765	-0.471225
C	-6.351261	-0.034251	-0.496845
C	-6.012287	-1.446569	-0.898823
Cl	-5.758596	2.343031	0.721954
O	-7.377710	0.497829	-0.905555
O	-2.980709	-1.894511	0.938762
C	-6.990199	-2.152138	-1.789036
H	-6.500770	-2.482537	-2.720254
H	-7.376956	-3.061568	-1.299046
H	-7.833555	-1.498836	-2.041053
C	-4.519677	-3.456896	-0.849136
H	-4.410224	-3.551769	-1.941531
H	-3.582296	-3.771868	-0.376515
H	-5.318214	-4.154033	-0.546826

112

**IPrCl2Py4isomer+DMF** SCF Done: -3716.75249972 A.U.

Pd	0.792279	0.512466	0.253547
N	0.453914	-2.403680	-0.229161
C	-3.736861	-2.051802	-0.563471
N	2.563520	-1.947451	-0.101314
C	-3.170744	-2.460347	0.641972
C	-1.779573	-2.579267	0.787240
Cl	0.407861	0.021736	2.531601
C	-0.982938	-2.275729	-0.336880
C	-1.530521	-1.879964	-1.581109

C	-2.925310	-1.760963	-1.660936
C	-0.654156	-1.648389	-2.807716
C	-0.312120	-2.985038	-3.494707
C	-1.263523	-0.676553	-3.825785
C	-1.186522	-3.081940	2.097877
C	-1.233648	-4.621052	2.154122
C	-1.872688	-2.483288	3.334556
C	1.133929	-3.613100	-0.339786
C	2.457465	-3.327603	-0.253818
C	3.828165	-1.249562	-0.081658
C	4.444555	-0.955845	-1.318483
C	5.697100	-0.327847	-1.274733
C	6.295712	0.001378	-0.058698
C	5.661311	-0.300449	1.144951
C	4.413731	-0.940895	1.162832
C	3.821944	-1.351839	-2.653998
C	4.362560	-2.715446	-3.125860
C	4.025043	-0.298476	-3.752384
C	3.756208	-1.343090	2.476020
C	4.223162	-2.748209	2.900301
C	3.982455	-0.323768	3.600558
C	1.333444	-1.376970	-0.067256
H	-4.821003	-1.955593	-0.649184
H	-3.820971	-2.687997	1.487396
H	-3.390920	-1.435886	-2.591571
H	0.284851	-1.193116	-2.467048
H	-1.226364	-3.477632	-3.864733
H	0.196589	-3.681618	-2.813758
H	0.355266	-2.810737	-4.354267
H	-0.508607	-0.412290	-4.581851
H	-1.604303	0.254022	-3.350615
H	-2.121012	-1.119801	-4.357450
H	-0.135004	-2.763677	2.129935
H	-0.704018	-5.084057	1.308801
H	-2.276418	-4.978338	2.131036
H	-0.769485	-4.985634	3.084709
H	-1.892731	-1.386555	3.280339
H	-1.317793	-2.769592	4.242032
H	-2.903943	-2.852116	3.453319
H	0.614697	-4.555171	-0.479021
H	3.330850	-3.969987	-0.287537
H	6.211584	-0.088415	-2.206448
H	7.268260	0.499679	-0.050145
H	6.142203	-0.031359	2.086034

H	2.737268	-1.445592	-2.499827
H	5.449015	-2.658987	-3.304458
H	3.877027	-3.014774	-4.068878
H	4.185070	-3.511168	-2.388874
H	3.689720	0.691618	-3.417257
H	3.437866	-0.573965	-4.642887
H	5.078981	-0.228903	-4.066089
H	2.672294	-1.385687	2.307747
H	3.999037	-3.502973	2.131055
H	3.720104	-3.055340	3.831787
H	5.311211	-2.761332	3.079303
H	5.024213	-0.335766	3.961976
H	3.337019	-0.568847	4.458643
H	3.747645	0.695005	3.260340
Cl	1.370207	1.188975	-1.952437
N	-0.050399	2.442288	0.592784
C	0.583382	3.343034	1.364779
C	-1.263146	2.728778	0.077576
C	0.031804	4.590170	1.646980
C	-1.875322	3.959777	0.322952
C	-1.222126	4.902777	1.115504
H	1.557498	3.046179	1.760931
H	0.579468	5.294238	2.275228
H	-2.860002	4.155913	-0.102326
H	-1.688005	5.869809	1.318780
C	-1.890626	1.662949	-0.796258
H	-1.323453	1.636104	-1.738151
H	-1.735571	0.682887	-0.327256
N	-3.290077	1.850076	-1.129615
H	-3.474066	2.172260	-2.074820
C	-4.360557	1.290020	-0.515397
C	-4.241540	0.870979	0.933849
C	-5.583516	1.148387	-1.124201
C	-5.372889	0.150187	1.571594
C	-6.739351	0.529997	-0.481677
C	-6.560909	0.028052	0.927821
Cl	-5.781556	1.633795	-2.797574
O	-7.812446	0.389392	-1.059289
O	-3.231435	1.147196	1.561052
O	3.820682	2.645184	1.780969
N	4.980217	3.085587	-0.153348
C	4.969613	3.066741	-1.604321
H	5.056827	4.089982	-2.008144
H	5.808639	2.466719	-1.992101

H	4.030243	2.621453	-1.959971
C	6.155918	3.622118	0.504918
H	6.015486	3.558168	1.590716
H	7.051943	3.046139	0.219134
H	6.316357	4.675650	0.219290
C	3.923971	2.630107	0.554951
H	3.121930	2.229373	-0.098289
C	-5.157712	-0.358427	2.968840
H	-5.717620	0.252709	3.697582
H	-5.522648	-1.391706	3.071716
H	-4.097031	-0.328770	3.242976
C	-7.745488	-0.633697	1.566348
H	-7.538185	-1.702095	1.750006
H	-7.968184	-0.182918	2.546723
H	-8.630095	-0.556820	0.923517
108			
<b>IPrCl2Py4isomer+K3PO4</b> SCF Done: -5910.62855915 A.U.			
Pd	-1.498647	0.652894	0.283468
N	-4.316848	-0.148261	0.114495
C	-5.421746	3.879712	-0.442600
N	-3.146357	-1.962577	0.215393
C	-5.057132	3.432297	0.826875
C	-4.699040	2.093347	1.045776
Cl	-1.135557	-0.152893	2.489342
C	-4.708779	1.230284	-0.068417
C	-5.088027	1.648819	-1.363728
C	-5.446095	2.994836	-1.521586
C	-5.160551	0.685110	-2.544826
C	-6.589791	0.129731	-2.704569
C	-4.697320	1.304117	-3.872240
C	-4.388216	1.595872	2.451787
C	-5.697403	1.307119	3.209257
C	-3.484378	2.553608	3.239230
C	-5.220563	-1.199228	0.209018
C	-4.488229	-2.338791	0.258478
C	-2.090777	-2.945907	0.161230
C	-1.469036	-3.189114	-1.086507
C	-0.534109	-4.232950	-1.143842
C	-0.242383	-5.006269	-0.018006
C	-0.871807	-4.742475	1.199377
C	-1.808663	-3.701725	1.320741
C	-1.839014	-2.397352	-2.337491
C	-3.112890	-2.966244	-2.991406
C	-0.694113	-2.296731	-3.352327



C	-2.507154	-3.462361	2.655974
C	-3.577822	-4.539354	2.915253
C	-1.522858	-3.401801	3.835545
C	-3.035569	-0.611104	0.138452
H	-5.697452	4.926759	-0.591973
H	-5.060338	4.132345	1.664064
H	-5.743727	3.360482	-2.505558
H	-4.485800	-0.156829	-2.330151
H	-7.293955	0.944648	-2.939764
H	-6.950607	-0.369272	-1.794601
H	-6.627265	-0.601301	-3.528280
H	-4.629085	0.518436	-4.641666
H	-3.709635	1.772491	-3.769463
H	-5.409305	2.059090	-4.242725
H	-3.840531	0.648633	2.367905
H	-6.316248	0.570283	2.672980
H	-6.294511	2.226211	3.329049
H	-5.481929	0.906121	4.213048
H	-2.562959	2.772475	2.680156
H	-3.196878	2.094290	4.197492
H	-3.987890	3.506389	3.467927
H	-6.292543	-1.036170	0.231359
H	-4.787724	-3.379999	0.302531
H	-0.025089	-4.448493	-2.083029
H	0.485478	-5.818335	-0.090592
H	-0.634691	-5.356352	2.070354
H	-2.059118	-1.368020	-2.027619
H	-2.944056	-3.996869	-3.345271
H	-3.400760	-2.349622	-3.858400
H	-3.964840	-2.982162	-2.295537
H	0.220249	-1.938595	-2.856658
H	-0.969788	-1.584173	-4.146363
H	-0.485631	-3.262372	-3.841880
H	-3.002219	-2.482289	2.603103
H	-4.325704	-4.585677	2.110325
H	-4.108709	-4.333609	3.858537
H	-3.114826	-5.536489	2.996915
H	-1.031948	-4.372178	4.011810
H	-2.063089	-3.135988	4.758156
H	-0.749676	-2.639770	3.667489
Cl	-1.714611	1.311612	-1.989764
N	-0.248698	2.398761	0.583955
C	-0.967952	3.526609	0.396633
C	1.038296	2.493838	0.973808

C	-0.440322	4.797031	0.589580
C	1.635016	3.744171	1.182194
C	0.895382	4.906732	0.989134
H	-2.004499	3.394113	0.081889
H	-1.068302	5.674390	0.428424
H	2.679371	3.780859	1.489350
H	1.352165	5.886322	1.148252
C	1.784819	1.202584	1.193663
H	1.218190	0.647046	1.955199
H	1.753762	0.597016	0.271935
N	3.142767	1.342568	1.676741
H	3.266706	1.260544	2.680537
C	4.286854	1.305095	0.962434
C	4.228858	1.499326	-0.537811
C	5.520844	1.127683	1.546330
C	5.510682	1.389756	-1.308451
C	6.764710	1.034727	0.806498
C	6.701185	1.231961	-0.676786
Cl	5.604177	0.783947	3.283791
O	7.839415	0.750927	1.353925
O	3.251930	2.076169	-1.037993
O	1.512771	-0.935433	-1.113777
P	2.969914	-1.382950	-1.511680
O	3.251101	-1.029692	-3.001895
K	1.581443	-2.131763	1.171731
O	3.992262	-0.597800	-0.539976
O	3.214562	-2.891878	-1.145722
K	1.433641	1.034832	-2.851762
K	5.741057	-2.405878	-0.143967
C	5.334497	1.472003	-2.792529
H	4.825082	2.408480	-3.071838
H	6.282611	1.404922	-3.338991
H	4.673135	0.639117	-3.095015
C	8.019909	1.136633	-1.404256
H	8.151252	0.138075	-1.858801
H	8.097394	1.875183	-2.215209
H	8.851881	1.287687	-0.704892
100			
<b>IPrCl2Py5</b> SCF Done: -3468.38287060 A.U.			
Pd	-0.997801	-0.837369	-0.470854
N	-1.421156	2.039283	0.253682
C	2.440582	3.019641	-1.120041
N	-3.188063	0.888163	0.725973
C	2.271544	2.465095	0.148246

C	0.996807	2.149473	0.638287
Cl	-0.673339	-1.607920	1.740980
C	-0.102807	2.404683	-0.208559
C	0.031094	2.990506	-1.485831
C	1.330916	3.291222	-1.919834
C	-1.176137	3.338024	-2.350025
C	-1.621792	4.791263	-2.093807
C	-0.932991	3.123479	-3.850904
C	0.814669	1.622316	2.055583
C	0.647832	2.795548	3.039351
C	1.942891	0.685754	2.501786
C	-2.336650	2.923201	0.815268
C	-3.451201	2.202663	1.101306
C	-4.126973	-0.198399	0.872270
C	-4.860053	-0.605209	-0.263886
C	-5.765237	-1.663769	-0.099849
C	-5.938710	-2.275669	1.142162
C	-5.213580	-1.838600	2.250267
C	-4.287136	-0.790352	2.143442
C	-4.738750	0.123402	-1.597028
C	-5.727388	1.303649	-1.648740
C	-4.914133	-0.794594	-2.812534
C	-3.538552	-0.293174	3.375419
C	-4.401171	0.710289	4.165273
C	-3.075962	-1.429316	4.299749
C	-1.940086	0.784257	0.201571
H	3.447874	3.227752	-1.485964
H	3.145480	2.274704	0.770627
H	1.479345	3.736857	-2.904565
H	-1.995873	2.665567	-2.056760
H	-0.825135	5.495313	-2.385698
H	-1.857544	4.975989	-1.036250
H	-2.519865	5.028439	-2.686898
H	-1.881067	3.237249	-4.400424
H	-0.541019	2.116630	-4.047524
H	-0.229154	3.864951	-4.262232
H	-0.107905	1.029075	2.083069
H	-0.205827	3.434134	2.764443
H	1.551922	3.426677	3.053754
H	0.475654	2.420162	4.061236
H	2.099548	-0.117590	1.767860
H	1.684222	0.214508	3.461808
H	2.894817	1.220528	2.643168
H	-2.108344	3.973260	0.962473

H	-4.403448	2.499470	1.527400
H	-6.350390	-2.010490	-0.952728
H	-6.651021	-3.097925	1.248307
H	-5.368683	-2.322682	3.215816
H	-3.723973	0.534787	-1.668680
H	-6.768647	0.946115	-1.587121
H	-5.611720	1.861237	-2.592451
H	-5.561774	2.007029	-0.818404
H	-4.246618	-1.667216	-2.750615
H	-4.663057	-0.243447	-3.731860
H	-5.950429	-1.154811	-2.916780
H	-2.633466	0.224286	3.025385
H	-4.709440	1.568969	3.551984
H	-3.843157	1.097582	5.033108
H	-5.316167	0.221965	4.539271
H	-3.923723	-1.913384	4.810870
H	-2.413411	-1.025312	5.081815
H	-2.518376	-2.191732	3.739258
Cl	-1.326706	-0.179394	-2.715921
N	0.129915	-2.489453	-1.172792
C	-0.324938	-3.350107	-2.095834
C	1.390849	-2.602755	-0.724953
C	0.481049	-4.371139	-2.599498
C	2.273773	-3.572933	-1.194799
C	1.796690	-4.480091	-2.149499
H	-1.349276	-3.201336	-2.440681
H	0.078300	-5.062145	-3.341628
H	1.696741	-1.885934	0.035905
H	2.451766	-5.262634	-2.542010
C	3.712956	-3.629826	-0.717042
H	3.930828	-4.648078	-0.360179
H	4.382510	-3.449131	-1.569626
N	4.035617	-2.722468	0.366429
H	4.010625	-3.100789	1.312469
C	4.474970	-1.448999	0.341174
C	4.875535	-0.974690	1.737083
C	4.565979	-0.549908	-0.693711
C	5.467762	0.367001	1.918490
C	5.177131	0.769130	-0.529962
C	5.623820	1.186325	0.848902
Cl	3.976352	-0.884877	-2.313621
O	5.313070	1.544617	-1.471239
O	4.687469	-1.733972	2.675390
C	6.207858	2.559533	0.987673

H	7.180696	2.523483	1.503531
H	6.334294	3.034333	0.008119
H	5.549857	3.196704	1.603993
C	5.852436	0.775200	3.312203
H	5.322869	1.695085	3.609661
H	5.616045	-0.014565	4.035091
H	6.930839	0.995980	3.372231
100			
<b>IPrCl2Py5isomer</b> SCF Done: -3468.37447725 A.U.			
Pd	-0.604644	-0.705122	-0.237842
N	-2.261788	1.851996	-0.315334
C	0.611576	4.769031	-1.299236
N	-3.409404	0.138886	0.332258
C	0.157808	4.649320	0.014482
C	-0.755423	3.650422	0.378124
Cl	0.566023	0.344290	1.532045
C	-1.202415	2.777583	-0.640553
C	-0.730432	2.848519	-1.965195
C	0.182884	3.869014	-2.271965
C	-1.179328	1.883465	-3.053596
C	-2.025699	2.598804	-4.119628
C	0.023006	1.155323	-3.675818
C	-1.252571	3.560997	1.818500
C	-2.281283	4.666611	2.120634
C	-0.105228	3.610218	2.839956
C	-3.570740	2.289200	-0.124829
C	-4.286579	1.217534	0.296082
C	-3.774893	-1.174713	0.807929
C	-4.552024	-2.013072	-0.019005
C	-4.892613	-3.277110	0.486659
C	-4.473611	-3.684995	1.752004
C	-3.718847	-2.827639	2.553888
C	-3.360416	-1.547764	2.107471
C	-5.063206	-1.572510	-1.386283
C	-6.510992	-1.054268	-1.282146
C	-4.981471	-2.681975	-2.446148
C	-2.628585	-0.575854	3.027696
C	-3.639966	0.307442	3.782996
C	-1.662660	-1.260689	4.001037
C	-2.161279	0.523766	-0.053053
H	1.319576	5.559219	-1.561064
H	0.519395	5.347125	0.772085
H	0.562824	3.957961	-3.291827
H	-1.809976	1.110181	-2.597057

H	-1.444403	3.378236	-4.639191
H	-2.908468	3.079806	-3.668781
H	-2.377411	1.879536	-4.877048
H	-0.322157	0.391996	-4.389767
H	0.614011	0.646836	-2.899399
H	0.688495	1.848917	-4.214534
H	-1.747921	2.587372	1.944640
H	-3.142981	4.630365	1.438564
H	-1.819245	5.662837	2.024003
H	-2.660723	4.567085	3.150430
H	0.643539	2.837531	2.621558
H	-0.499798	3.429115	3.852720
H	0.391828	4.593329	2.852862
H	-3.860221	3.318499	-0.306721
H	-5.328115	1.122924	0.582648
H	-5.493678	-3.954730	-0.121947
H	-4.744696	-4.677307	2.121574
H	-3.415148	-3.157077	3.548298
H	-4.419296	-0.749977	-1.730230
H	-7.186091	-1.860588	-0.951166
H	-6.863575	-0.697291	-2.263314
H	-6.609793	-0.225740	-0.566268
H	-3.973099	-3.115177	-2.487161
H	-5.218992	-2.266445	-3.438557
H	-5.705980	-3.489003	-2.251160
H	-2.012244	0.086101	2.407400
H	-4.293973	0.857928	3.089728
H	-3.111785	1.046990	4.406762
H	-4.280061	-0.303057	4.441250
H	-2.190246	-1.847797	4.769976
H	-1.062603	-0.499195	4.522272
H	-0.968738	-1.929052	3.468988
Cl	-1.619178	-1.726341	-2.114112
N	0.950507	-2.140514	-0.355485
C	0.947416	-3.163170	0.513947
C	1.955221	-2.024200	-1.236285
C	1.965621	-4.115316	0.530399
C	3.037385	-2.910123	-1.268220
C	3.028281	-3.979400	-0.362303
H	0.108172	-3.212466	1.211050
H	1.924848	-4.939551	1.244075
H	1.899944	-1.183162	-1.928224
H	3.853379	-4.696548	-0.350636
C	4.239152	-2.629656	-2.151043

H	4.658020	-3.569256	-2.535002
H	3.957198	-2.008106	-3.006860
N	5.315031	-1.974787	-1.386036
H	5.963109	-2.629424	-0.955231
C	5.127424	-0.849713	-0.637819
C	4.255107	0.255270	-1.192329
C	5.770843	-0.602742	0.546360
C	3.834413	1.360765	-0.296268
C	5.472463	0.557576	1.397554
C	4.411928	1.511131	0.921756
Cl	6.897353	-1.775326	1.195901
O	6.027412	0.726392	2.476375
O	3.909909	0.219087	-2.364353
C	4.010080	2.615215	1.852242
H	4.159556	3.602505	1.384474
H	2.934715	2.534916	2.082238
H	4.582878	2.573940	2.786053
C	2.779957	2.294157	-0.806126
H	2.529000	2.083597	-1.851285
H	1.863143	2.191309	-0.203557
H	3.099238	3.344155	-0.727300

112

**IPrCl2Py5isomer+DMF** SCF Done: -3716.73637653 A.U.

Pd	-0.830145	-0.211288	-0.300214
N	-1.806171	2.501769	0.477591
C	1.696367	4.498973	-0.752132
N	-3.398695	1.062730	0.729224
C	1.699784	3.760842	0.430163
C	0.555082	3.070763	0.857746
Cl	-0.816845	-1.074470	1.906760
C	-0.594649	3.160365	0.049518
C	-0.630329	3.898197	-1.155957
C	0.542853	4.565117	-1.535317
C	-1.892257	4.015963	-2.006049
C	-2.645859	5.322579	-1.690185
C	-1.615863	3.925858	-3.514568
C	0.571080	2.304429	2.172738
C	0.444626	3.272420	3.362426
C	1.809869	1.406887	2.307341
C	-2.874649	3.183806	1.050336
C	-3.878966	2.284443	1.195065
C	-4.239019	-0.108968	0.643352
C	-4.769542	-0.454780	-0.620363
C	-5.669246	-1.527759	-0.668086

C	-6.026362	-2.221779	0.487669
C	-5.483406	-1.861543	1.718880
C	-4.575602	-0.796755	1.828129
C	-4.438082	0.338414	-1.879515
C	-5.401144	1.528903	-2.043394
C	-4.400213	-0.527706	-3.144696
C	-4.039639	-0.392142	3.197162
C	-5.097786	0.402774	3.985172
C	-3.557540	-1.595388	4.022434
C	-2.116264	1.189452	0.296174
H	2.599510	5.028658	-1.065985
H	2.603116	3.727384	1.040457
H	0.555982	5.146586	-2.458767
H	-2.546796	3.169975	-1.749907
H	-2.026378	6.196760	-1.950027
H	-2.911087	5.406076	-0.626939
H	-3.577512	5.379529	-2.276103
H	-2.569926	3.866478	-4.062720
H	-1.024755	3.032115	-3.754264
H	-1.082195	4.814951	-3.887345
H	-0.299960	1.638466	2.194524
H	-0.477289	3.871876	3.294609
H	1.298796	3.968922	3.398666
H	0.420062	2.714421	4.312739
H	1.939506	0.773847	1.416848
H	1.702423	0.747340	3.181884
H	2.730585	1.994899	2.443174
H	-2.815921	4.238249	1.297743
H	-4.890437	2.396188	1.570041
H	-6.099936	-1.827096	-1.624304
H	-6.732683	-3.053178	0.425876
H	-5.771740	-2.414717	2.614497
H	-3.426782	0.747237	-1.766980
H	-6.438189	1.180026	-2.181030
H	-5.121206	2.129164	-2.924643
H	-5.380452	2.192138	-1.165053
H	-3.766687	-1.413372	-2.987671
H	-3.981389	0.055997	-3.979079
H	-5.404794	-0.863576	-3.450213
H	-3.165013	0.253468	3.034149
H	-5.432246	1.300238	3.444502
H	-4.691857	0.725677	4.957555
H	-5.986894	-0.219811	4.178569
H	-4.392075	-2.250879	4.319342



H	-3.074219	-1.243293	4.947954
H	-2.825251	-2.188481	3.459238
Cl	-0.834398	0.601190	-2.524263
N	0.677564	-1.615690	-0.838280
C	0.568563	-2.916636	-0.522859
C	1.792125	-1.173504	-1.445508
C	1.588522	-3.825050	-0.801486
C	2.857451	-2.015084	-1.770137
C	2.747589	-3.369015	-1.427913
H	-0.362763	-3.221973	-0.050712
H	1.464319	-4.875340	-0.532840
H	1.830591	-0.109677	-1.678153
H	3.562567	-4.062047	-1.652894
C	4.087128	-1.480676	-2.480356
H	4.202198	-2.011901	-3.436958
H	3.963441	-0.416905	-2.708653
N	5.327529	-1.709032	-1.747285
H	5.831267	-2.556124	-1.994564
C	5.876078	-1.027507	-0.717561
C	5.237205	0.254139	-0.222072
C	7.016656	-1.459337	-0.074380
C	5.977348	1.093710	0.754875
C	7.699506	-0.701745	0.964330
C	7.113726	0.636190	1.338063
Cl	7.758978	-2.977433	-0.552319
O	8.718866	-1.106771	1.516033
O	4.128686	0.577891	-0.621080
O	-2.449123	-2.979348	-1.403188
N	-3.630901	-4.455255	-0.101997
C	-4.660317	-5.474871	-0.041954
H	-4.229135	-6.454691	0.226051
H	-5.419425	-5.214177	0.714113
H	-5.157511	-5.567745	-1.017687
C	-2.886358	-4.184847	1.115487
H	-2.377970	-3.216759	1.036483
H	-3.579890	-4.143371	1.968341
H	-2.138805	-4.974165	1.310433
C	-3.342461	-3.806082	-1.250891
H	-4.021778	-4.095706	-2.084287
C	5.384274	2.430733	1.099165
H	6.119716	3.235321	0.938869
H	4.496318	2.635176	0.490833
H	5.094569	2.473170	2.162200
C	7.848458	1.434515	2.372392

H	8.715597	0.880775	2.750726
H	8.194858	2.392807	1.949365
H	7.185580	1.686791	3.216516
100			
<b>IPrCl2Py6</b> SCF Done: -3468.36980263 A.U.			
Pd	0.639805	-0.060896	-0.827276
N	3.177864	-0.855671	0.605760
C	1.793995	-4.725986	1.538965
N	3.163160	1.254674	0.136453
C	1.438206	-3.642643	2.344794
C	1.899629	-2.349325	2.063872
Cl	-0.520638	0.888454	1.005505
C	2.717096	-2.188702	0.918610
C	3.115840	-3.267186	0.103394
C	2.632165	-4.541302	0.441037
C	4.089108	-3.095268	-1.056521
C	5.522755	-3.435891	-0.605812
C	3.708062	-3.925146	-2.291116
C	1.593685	-1.185613	3.003344
C	2.754876	-0.964078	3.992096
C	0.271484	-1.331029	3.764110
C	4.426307	-0.353948	0.964235
C	4.419823	0.969287	0.662038
C	2.686041	2.593973	-0.117127
C	2.682333	3.085859	-1.436117
C	2.216156	4.394942	-1.634815
C	1.777431	5.172303	-0.563765
C	1.799289	4.659209	0.734271
C	2.251824	3.357740	0.990820
C	3.215973	2.271133	-2.605780
C	4.635971	2.736815	-2.975011
C	2.278563	2.304268	-3.820668
C	2.315907	2.832086	2.421991
C	3.591876	3.332034	3.126412
C	1.077273	3.185409	3.258494
C	2.406684	0.128531	0.073101
H	1.422486	-5.725785	1.777969
H	0.798005	-3.811100	3.211414
H	2.917627	-5.402312	-0.165588
H	4.059744	-2.039079	-1.359102
H	5.593199	-4.493190	-0.301237
H	5.846176	-2.822495	0.248091
H	6.235116	-3.271014	-1.430355
H	4.364745	-3.659679	-3.134989

H	2.670339	-3.727519	-2.592913
H	3.827692	-5.006121	-2.113753
H	1.490983	-0.280438	2.391565
H	3.710355	-0.790554	3.477332
H	2.877916	-1.840089	4.650111
H	2.551928	-0.085266	4.625656
H	-0.562673	-1.540431	3.082944
H	0.044606	-0.390581	4.289555
H	0.313241	-2.129737	4.522394
H	5.190986	-0.979446	1.412052
H	5.181913	1.733266	0.774135
H	2.204192	4.813532	-2.642957
H	1.418985	6.189705	-0.740146
H	1.457628	5.282629	1.562410
H	3.281012	1.221890	-2.290855
H	4.634265	3.788762	-3.305586
H	5.042824	2.122657	-3.794868
H	5.320007	2.654941	-2.115259
H	1.264819	1.981227	-3.539870
H	2.646737	1.616847	-4.597742
H	2.215542	3.309208	-4.268132
H	2.364628	1.735319	2.375473
H	4.504339	3.052618	2.580254
H	3.660887	2.907641	4.141108
H	3.578192	4.430733	3.216093
H	1.020703	4.264609	3.473379
H	1.124994	2.662498	4.227350
H	0.156025	2.875750	2.747445
Cl	1.734829	-1.056387	-2.671614
N	-1.221773	-0.283667	-1.835243
C	-2.114366	0.722068	-1.854397
C	-1.594271	-1.489412	-2.298217
C	-3.430037	0.535425	-2.262586
C	-2.897906	-1.756153	-2.708935
C	-3.859228	-0.742146	-2.649291
H	-1.769717	1.687588	-1.482685
H	-4.130426	1.370464	-2.206471
H	-0.826482	-2.264781	-2.300940
H	-3.170374	-2.771572	-3.000870
C	-5.338345	-1.032235	-2.833669
H	-5.703638	-0.569205	-3.762326
H	-5.495804	-2.115616	-2.915674
N	-6.139245	-0.466203	-1.739136
H	-6.766507	0.287126	-2.004264

C	-5.707941	-0.402734	-0.450877
C	-4.837972	-1.525569	0.069645
C	-6.063451	0.568486	0.446459
C	-4.000730	-1.277383	1.268494
C	-5.417876	0.712917	1.757365
C	-4.288760	-0.232513	2.083888
Cl	-7.176356	1.834381	-0.029794
O	-5.725473	1.607658	2.535604
O	-4.837505	-2.598509	-0.511818
C	-3.490870	0.055479	3.320160
H	-3.464775	-0.819415	3.990367
H	-2.446482	0.275699	3.041998
H	-3.907259	0.910050	3.866363
C	-2.861543	-2.223787	1.513313
H	-2.931395	-3.101149	0.858653
H	-1.911600	-1.702175	1.304998
H	-2.826514	-2.561013	2.560187

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**IPrCl2Py6del2** SCF Done: -3468.37217479 A.U.

Pd	-0.891559	-0.269416	-0.891728
N	-2.164247	1.317924	1.273918
C	0.354931	4.638551	0.632031
N	-3.343221	-0.456952	0.900755
C	0.864564	3.498683	1.251439
C	0.054005	2.376264	1.485137
Cl	-0.222327	-1.999684	0.581060
C	-1.287930	2.447543	1.063286
C	-1.832919	3.587026	0.427537
C	-0.980794	4.681620	0.229135
C	-3.296424	3.667897	0.001495
C	-4.126697	4.432383	1.050349
C	-3.489825	4.297127	-1.386533
C	0.627912	1.165098	2.207384
C	0.810763	1.465659	3.705826
C	1.942160	0.685476	1.575523
C	-3.158639	1.284792	2.246595
C	-3.905521	0.177670	2.005882
C	-3.916042	-1.616269	0.259080
C	-4.605016	-1.421745	-0.962107
C	-5.162465	-2.554344	-1.571480
C	-5.057855	-3.815739	-0.982534
C	-4.396168	-3.970545	0.233783
C	-3.805915	-2.875485	0.884484
C	-4.808222	-0.031210	-1.557862

C	-6.001892	0.675626	-0.886934
C	-4.964509	-0.028252	-3.082657
C	-3.132022	-3.066678	2.238592
C	-4.184356	-3.132683	3.362152
C	-2.230282	-4.309970	2.286290
C	-2.262032	0.234938	0.457873
H	1.002850	5.502258	0.462062
H	1.910294	3.479649	1.565275
H	-1.365377	5.581580	-0.254058
H	-3.688787	2.642635	-0.058689
H	-3.782175	5.476696	1.128127
H	-4.050887	3.981087	2.050145
H	-5.190683	4.445145	0.763650
H	-4.544168	4.201776	-1.692550
H	-2.865643	3.791964	-2.135541
H	-3.246571	5.371736	-1.388154
H	-0.087160	0.337581	2.118702
H	-0.140150	1.765697	4.174315
H	1.536804	2.280788	3.861283
H	1.185911	0.573485	4.233576
H	1.817999	0.479757	0.503345
H	2.275843	-0.246543	2.055224
H	2.745885	1.427741	1.692308
H	-3.241320	2.052475	3.008539
H	-4.787590	-0.209723	2.503676
H	-5.697799	-2.450897	-2.515906
H	-5.504030	-4.683933	-1.474333
H	-4.334663	-4.961094	0.687822
H	-3.910376	0.562801	-1.347907
H	-6.941079	0.133912	-1.087302
H	-6.106914	1.700994	-1.277384
H	-5.876772	0.744107	0.203883
H	-4.144939	-0.576731	-3.571321
H	-4.944053	1.008548	-3.452090
H	-5.919569	-0.473810	-3.405273
H	-2.484877	-2.195514	2.413408
H	-4.825675	-2.239429	3.387199
H	-3.693789	-3.225129	4.344623
H	-4.841058	-4.007828	3.226649
H	-2.814986	-5.243104	2.246860
H	-1.661948	-4.322279	3.230161
H	-1.512705	-4.307212	1.454551
Cl	-1.572838	1.405857	-2.409764
N	0.823978	-0.682421	-2.095020

C	1.281070	-1.930239	-2.306970
C	1.638601	0.356393	-2.347586
C	2.587521	-2.180784	-2.712306
C	2.963792	0.185433	-2.739122
C	3.473327	-1.108141	-2.890705
H	0.586911	-2.744901	-2.097396
H	2.919208	-3.213326	-2.840792
H	1.215944	1.351152	-2.197762
H	3.599385	1.060825	-2.875289
C	4.959936	-1.359032	-3.067223
H	5.134522	-2.186441	-3.768154
H	5.465331	-0.469868	-3.459607
N	5.539864	-1.763711	-1.781091
H	5.425197	-2.756564	-1.573348
C	5.499746	-1.041832	-0.629795
C	5.250189	-1.909401	0.596718
C	5.641840	0.307542	-0.446634
C	5.140152	-1.284597	1.933482
C	5.465734	0.947492	0.865700
C	5.225834	0.063347	2.061034
Cl	6.082053	1.396103	-1.745392
O	5.510708	2.164039	1.001097
O	5.128288	-3.114253	0.430095
C	4.887254	-2.188839	3.105658
H	3.906269	-1.965964	3.559061
H	4.897165	-3.242631	2.802985
H	5.642593	-2.036671	3.893124
C	5.078574	0.740035	3.390133
H	4.097084	0.508636	3.835539
H	5.841312	0.376699	4.098573
H	5.173015	1.827326	3.290934

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**IPrCl2Py6del3** SCF Done: -3468.37390822 A.U.

Pd	0.656563	-0.270432	-0.908410
N	2.713915	-0.575723	1.252243
C	2.970244	-4.765994	0.887892
N	2.436377	1.510997	0.756768
C	1.854721	-4.195295	1.499324
C	1.734564	-2.803278	1.636276
Cl	-0.959125	0.670444	0.562181
C	2.783960	-2.012797	1.129325
C	3.924431	-2.559637	0.498373
C	3.994309	-3.955524	0.395735
C	5.070091	-1.693667	-0.018705

C	6.235369	-1.677970	0.988895
C	5.573600	-2.118842	-1.406328
C	0.534951	-2.204657	2.359108
C	0.702582	-2.351527	3.882309
C	-0.797689	-2.799740	1.883427
C	3.470566	0.157126	2.161895
C	3.305587	1.466154	1.843861
C	2.097784	2.716864	0.038506
C	2.711032	2.928243	-1.220136
C	2.374905	4.102001	-1.908674
C	1.487329	5.030367	-1.361799
C	0.919824	4.806029	-0.109396
C	1.207860	3.642653	0.621746
C	3.753965	1.963981	-1.779913
C	5.137812	2.243500	-1.162404
C	3.834981	1.961658	-3.310511
C	0.611238	3.450550	2.011473
C	1.406236	4.257295	3.056249
C	-0.877747	3.822848	2.080823
C	2.058693	0.254879	0.400993
H	3.044017	-5.852586	0.794934
H	1.064770	-4.842184	1.885389
H	4.861513	-4.416986	-0.080219
H	4.698229	-0.664100	-0.119793
H	6.658116	-2.689394	1.105736
H	5.918685	-1.331860	1.983537
H	7.039287	-1.011274	0.637262
H	6.308972	-1.384965	-1.774028
H	4.744640	-2.166673	-2.124997
H	6.077063	-3.098521	-1.378694
H	0.495879	-1.131201	2.134070
H	1.632325	-1.874036	4.231178
H	0.737721	-3.413766	4.176347
H	-0.143197	-1.880166	4.408988
H	-0.909589	-2.693311	0.794262
H	-1.641870	-2.277904	2.355565
H	-0.885634	-3.869067	2.135254
H	4.056174	-0.322741	2.938880
H	3.733961	2.364205	2.275247
H	2.820106	4.302460	-2.883707
H	1.242950	5.940447	-1.915630
H	0.238030	5.547823	0.309852
H	3.463230	0.945614	-1.494127
H	5.494227	3.249515	-1.439020

H	5.873179	1.506878	-1.524931
H	5.116384	2.181906	-0.064351
H	2.843453	1.814069	-3.764953
H	4.485025	1.137833	-3.642936
H	4.261421	2.897345	-3.707068
H	0.686083	2.382460	2.260569
H	2.473388	3.991340	3.065285
H	1.004157	4.080512	4.066929
H	1.336156	5.337380	2.846592
H	-1.038837	4.905124	1.952071
H	-1.284505	3.549130	3.066502
H	-1.453460	3.284404	1.316030
Cl	2.178952	-1.294304	-2.392029
N	-0.986712	-0.852909	-2.116708
C	-1.828329	0.090784	-2.574629
C	-1.416516	-2.120475	-2.028084
C	-3.159337	-0.184786	-2.854952
C	-2.741626	-2.472450	-2.277605
C	-3.655983	-1.478132	-2.634710
H	-1.429648	1.103392	-2.658637
H	-3.820438	0.629563	-3.157147
H	-0.690677	-2.860074	-1.683745
H	-3.064432	-3.500024	-2.105631
C	-5.156495	-1.720711	-2.623840
H	-5.576240	-1.601698	-3.633401
H	-5.371075	-2.746117	-2.295961
N	-5.825675	-0.735903	-1.768327
H	-6.217683	0.061124	-2.267670
C	-5.355514	-0.346391	-0.548271
C	-5.430106	1.155876	-0.327374
C	-4.804751	-1.117461	0.436441
C	-4.855168	1.759926	0.899092
C	-4.254797	-0.535413	1.669461
C	-4.263256	0.960714	1.822264
Cl	-4.783693	-2.864432	0.362033
O	-3.803073	-1.232112	2.569764
O	-5.938132	1.834599	-1.209501
C	-3.578187	1.458969	3.055477
H	-3.703876	2.536818	3.204862
H	-3.942895	0.919126	3.942095
H	-2.500529	1.240539	2.974803
C	-4.916167	3.260882	1.009219
H	-5.497633	3.687592	0.183329
H	-5.375293	3.574046	1.959425



H	-3.903310	3.694410	0.976424
100			
<b>IPrCl2Py6del5</b> SCF Done: -3468.37217493 A.U.			
Pd	-0.891660	-0.269363	-0.891798
N	-2.164195	1.317922	1.273962
C	0.355610	4.638138	0.632412
N	-3.343306	-0.456851	0.900729
C	0.865011	3.498128	1.251748
C	0.054233	2.375843	1.485345
Cl	-0.222514	-1.999950	0.580648
C	-1.287674	2.447403	1.063452
C	-1.832434	3.587043	0.427784
C	-0.980098	4.681491	0.229489
C	-3.295915	3.668212	0.001727
C	-4.126087	4.432694	1.050665
C	-3.489190	4.297676	-1.386215
C	0.627876	1.164524	2.207547
C	0.810562	1.464922	3.706044
C	1.942135	0.684751	1.575820
C	-3.158605	1.284841	2.246625
C	-3.905582	0.177793	2.005859
C	-3.916225	-1.616103	0.259027
C	-4.605202	-1.421475	-0.962139
C	-5.162793	-2.553999	-1.571524
C	-5.058308	-3.815420	-0.982608
C	-4.396591	-3.970329	0.233681
C	-3.806194	-2.875350	0.884389
C	-4.808266	-0.030897	-1.557845
C	-6.001947	0.675987	-0.886987
C	-4.964394	-0.027846	-3.082658
C	-3.132231	-3.066662	2.238447
C	-4.184485	-3.132611	3.362086
C	-2.230611	-4.310047	2.286028
C	-2.262062	0.234971	0.457881
H	1.003697	5.501734	0.462519
H	1.910731	3.478877	1.565606
H	-1.364499	5.581562	-0.253643
H	-3.688435	2.643016	-0.058608
H	-3.781379	5.476935	1.128600
H	-4.050398	3.981248	2.050401
H	-5.190061	4.445687	0.763930
H	-4.543541	4.202535	-1.692268
H	-2.865075	3.792526	-2.135289
H	-3.245767	5.372248	-1.387674

H	-0.087306	0.337120	2.118685
H	-0.140368	1.765076	4.174424
H	1.536714	2.279920	3.861673
H	1.185490	0.572641	4.233769
H	1.818081	0.479164	0.503603
H	2.275589	-0.247380	2.055464
H	2.745971	1.426863	1.692801
H	-3.241231	2.052510	3.008591
H	-4.787713	-0.209524	2.503601
H	-5.698144	-2.450470	-2.515932
H	-5.504600	-4.683552	-1.474411
H	-4.335173	-4.960898	0.687691
H	-3.910406	0.563051	-1.347770
H	-6.941153	0.134342	-1.087455
H	-6.106869	1.701381	-1.277401
H	-5.876908	0.744411	0.203843
H	-4.144807	-0.576352	-3.571264
H	-4.943831	1.008973	-3.452034
H	-5.919448	-0.473326	-3.405399
H	-2.484989	-2.195568	2.413253
H	-4.825699	-2.239284	3.387236
H	-3.693849	-3.225165	4.344513
H	-4.841295	-4.007675	3.226588
H	-2.815417	-5.243120	2.246648
H	-1.662175	-4.322431	3.229837
H	-1.513125	-4.307355	1.454209
Cl	-1.572792	1.406199	-2.409586
N	0.823846	-0.682249	-2.095114
C	1.280851	-1.930015	-2.307501
C	1.638527	0.356617	-2.347304
C	2.587294	-2.180498	-2.712921
C	2.963708	0.185718	-2.738881
C	3.473164	-1.107841	-2.890911
H	0.586634	-2.744708	-2.098223
H	2.918926	-3.213011	-2.841781
H	1.215926	1.351348	-2.197130
H	3.599355	1.061116	-2.874760
C	4.959774	-1.358741	-3.067420
H	5.134381	-2.186040	-3.768476
H	5.465223	-0.469526	-3.459613
N	5.539599	-1.763638	-1.781307
H	5.424745	-2.756491	-1.573652
C	5.499647	-1.041877	-0.629941
C	5.250056	-1.909593	0.596483

C	5.641886	0.307460	-0.446590
C	5.140208	-1.284974	1.933342
C	5.465897	0.947235	0.865839
C	5.225997	0.062947	2.061066
Cl	6.082100	1.396207	-1.745205
O	5.510942	2.163762	1.001409
O	5.127934	-3.114398	0.429688
C	5.078817	0.739482	3.390251
H	5.841466	0.375920	4.098670
H	5.173438	1.826772	3.291195
H	4.097268	0.508193	3.835590
C	4.887316	-2.189362	3.105408
H	3.906430	-1.966411	3.558986
H	4.897025	-3.243108	2.802565
H	5.642791	-2.037435	3.892792
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<b>IPrCl2Py6isomer</b> SCF Done: -3468.37109623 A.U.			
Pd	1.042381	-0.114325	-0.461106
N	3.715097	-0.683031	0.812207
C	3.076413	-4.845438	0.930518
N	3.458385	1.435455	0.474708
C	2.525639	-4.029770	1.919360
C	2.729303	-2.642063	1.907171
Cl	0.025291	0.655260	1.527944
C	3.498374	-2.109969	0.850073
C	4.083088	-2.910161	-0.155217
C	3.852112	-4.292268	-0.088373
C	4.981214	-2.326622	-1.240724
C	6.461192	-2.401678	-0.817209
C	4.792883	-2.998863	-2.608465
C	2.212584	-1.765087	3.041130
C	3.253291	-1.703475	4.175419
C	0.842763	-2.201047	3.575044
C	4.861581	-0.057973	1.292894
C	4.704989	1.271696	1.070949
C	2.923783	2.711630	0.062701
C	3.051629	3.080260	-1.294518
C	2.521154	4.321055	-1.676438
C	1.907671	5.158326	-0.743921
C	1.820003	4.777330	0.594763
C	2.325863	3.544108	1.032869
C	3.812228	2.213569	-2.291511
C	5.305910	2.591444	-2.287852
C	3.237213	2.266902	-3.711856

C	2.276905	3.170009	2.510201
C	3.475507	3.780487	3.262497
C	0.963840	3.580121	3.192992
C	2.845568	0.233662	0.312674
H	2.905922	-5.924749	0.958753
H	1.935644	-4.481321	2.718311
H	4.284990	-4.947407	-0.845946
H	4.707349	-1.268476	-1.362034
H	6.774025	-3.451363	-0.691408
H	6.650540	-1.881401	0.132352
H	7.104326	-1.944729	-1.586719
H	5.343650	-2.435005	-3.378180
H	3.732735	-3.021796	-2.894417
H	5.185708	-4.028417	-2.617242
H	2.081361	-0.747636	2.651228
H	4.222628	-1.325678	3.815599
H	3.420451	-2.703522	4.608828
H	2.906699	-1.034977	4.980284
H	0.108174	-2.285083	2.760581
H	0.467926	-1.451119	4.288791
H	0.890354	-3.165647	4.105766
H	5.671917	-0.615173	1.750363
H	5.361218	2.111429	1.272173
H	2.596771	4.643348	-2.715908
H	1.501557	6.121784	-1.062673
H	1.349355	5.450941	1.312594
H	3.730024	1.168535	-1.966165
H	5.446729	3.634578	-2.616307
H	5.869760	1.937416	-2.972796
H	5.747659	2.490979	-1.284771
H	2.161423	2.037518	-3.712744
H	3.740593	1.518467	-4.343283
H	3.387160	3.250612	-4.185364
H	2.344802	2.074472	2.575936
H	4.439396	3.465189	2.838044
H	3.458217	3.478237	4.322172
H	3.437017	4.881588	3.221896
H	0.881574	4.673675	3.301346
H	0.921531	3.149504	4.206164
H	0.095275	3.213488	2.629385
Cl	2.000094	-0.893713	-2.475299
N	-0.891197	-0.501538	-1.263525
C	-1.862066	0.424585	-1.196580
C	-1.174853	-1.696935	-1.813700

C	-3.149829	0.190183	-1.671502
C	-2.441489	-2.011807	-2.291489
C	-3.463610	-1.056080	-2.222243
H	-1.596916	1.372993	-0.727275
H	-3.901174	0.976505	-1.592212
H	-0.352896	-2.412222	-1.867959
H	-2.626973	-3.005682	-2.703934
C	-4.851183	-1.387979	-2.738425
H	-4.843552	-1.304234	-3.836521
H	-5.080866	-2.437616	-2.508882
N	-5.900369	-0.513071	-2.259190
H	-6.247885	0.200334	-2.898050
C	-6.405969	-0.370877	-1.016930
C	-7.367747	0.810946	-0.944014
C	-6.183400	-1.084623	0.133268
C	-8.049283	1.156585	0.325042
C	-6.833616	-0.740303	1.400371
C	-7.791660	0.427872	1.440294
Cl	-5.115983	-2.476378	0.219114
O	-6.627999	-1.372785	2.430168
O	-7.553180	1.464344	-1.959981
C	-8.391461	0.667653	2.792071
H	-9.085667	1.514410	2.808768
H	-8.920628	-0.236132	3.133625
H	-7.592694	0.845812	3.529536
C	-8.977112	2.333800	0.223553
H	-8.423271	3.226186	-0.109635
H	-9.746395	2.145505	-0.542336
H	-9.475427	2.564545	1.171011

112

**IPrCl2Py6isomer+DMF** SCF Done: -3716.73477640 A.U.

Pd	-0.958158	-0.450730	-0.391930
N	-1.259876	2.298170	0.596343
C	2.687051	2.982987	-0.711615
N	-3.170236	1.309505	0.819711
C	2.464083	2.474592	0.567008
C	1.160058	2.263861	1.041500
Cl	-0.701464	-1.260180	1.818793
C	0.094761	2.579164	0.172117
C	0.289363	3.141117	-1.110426
C	1.613057	3.326075	-1.533684
C	-0.878883	3.594429	-1.979396
C	-1.274749	5.043512	-1.632769
C	-0.610974	3.471647	-3.485120

C	0.921059	1.782927	2.465775
C	0.877671	2.987047	3.426159
C	1.950835	0.747872	2.934815
C	-2.102121	3.198500	1.238742
C	-3.303319	2.580433	1.375487
C	-4.263945	0.375601	0.690728
C	-4.987959	0.364980	-0.523277
C	-6.055684	-0.537495	-0.624395
C	-6.393738	-1.375456	0.438844
C	-5.676257	-1.322977	1.632511
C	-4.593124	-0.444854	1.789016
C	-4.682159	1.347289	-1.649601
C	-5.471169	2.655208	-1.445924
C	-4.937672	0.780958	-3.051640
C	-3.863687	-0.345823	3.123340
C	-4.646099	0.561231	4.092148
C	-3.592949	-1.713891	3.765259
C	-1.910701	1.127807	0.351792
H	3.708266	3.123646	-1.071653
H	3.312485	2.241130	1.210695
H	1.810599	3.744010	-2.521412
H	-1.732831	2.940908	-1.751904
H	-0.445354	5.734403	-1.856893
H	-1.531955	5.162648	-0.571024
H	-2.148489	5.354271	-2.228241
H	-1.542606	3.658664	-4.042361
H	-0.255987	2.465071	-3.744000
H	0.128865	4.211100	-3.832039
H	-0.060590	1.291663	2.492493
H	0.099861	3.711228	3.138939
H	1.844912	3.516380	3.432437
H	0.665761	2.651416	4.454375
H	2.026183	-0.088321	2.225699
H	1.643551	0.332328	3.907520
H	2.954516	1.179531	3.064595
H	-1.770827	4.187970	1.535441
H	-4.238473	2.923622	1.805079
H	-6.635467	-0.585087	-1.547041
H	-7.228447	-2.073422	0.336201
H	-5.961071	-1.977264	2.458016
H	-3.611293	1.584778	-1.604498
H	-6.556218	2.467292	-1.500368
H	-5.210209	3.385728	-2.228850
H	-5.257227	3.116520	-0.470905

H	-4.401176	-0.165363	-3.204707
H	-4.575750	1.495447	-3.807477
H	-6.010026	0.616225	-3.244206
H	-2.883889	0.113711	2.933922
H	-4.804723	1.567562	3.676366
H	-4.100341	0.669936	5.043396
H	-5.636686	0.131225	4.314639
H	-4.522615	-2.213709	4.081553
H	-2.969661	-1.584901	4.664423
H	-3.051889	-2.373934	3.073556
Cl	-1.438944	0.187003	-2.618339
N	0.525710	-1.856900	-1.071036
C	0.817041	-2.996984	-0.420431
C	1.443949	-1.342948	-1.912603
C	2.062950	-3.609921	-0.520452
C	2.711149	-1.895561	-2.062638
C	3.058095	-3.029187	-1.315791
H	0.040983	-3.405066	0.223558
H	2.260218	-4.514961	0.058215
H	1.151734	-0.442285	-2.454645
H	3.432422	-1.416688	-2.725751
C	4.498448	-3.492231	-1.228767
H	4.549929	-4.572084	-1.036133
H	5.046726	-3.272854	-2.148367
N	5.147184	-2.829932	-0.083762
H	4.925086	-3.280483	0.801303
C	5.356747	-1.490437	0.062197
C	5.793880	-0.668060	-1.132361
C	5.266813	-0.853458	1.276349
C	6.080840	0.782530	-0.952688
C	5.556639	0.567496	1.470365
C	6.001431	1.358988	0.272405
Cl	4.734418	-1.734343	2.692765
O	5.407404	1.120523	2.555430
O	5.923396	-1.200402	-2.224026
O	-1.261558	-5.252152	-0.916665
N	-2.905560	-3.665120	-1.154375
C	-3.642136	-2.788423	-2.045111
H	-4.720000	-3.020124	-2.017788
H	-3.505472	-1.739291	-1.745951
H	-3.277659	-2.903611	-3.075234
C	-3.250199	-3.605694	0.255458
H	-2.646343	-4.339185	0.802453
H	-3.048255	-2.601266	0.656322

H	-4.320489	-3.827032	0.397970
C	-1.934515	-4.490647	-1.603760
H	-1.791781	-4.407603	-2.706380
C	6.489319	1.557388	-2.173342
H	6.525521	0.912673	-3.059134
H	5.782193	2.380845	-2.368092
H	7.480114	2.018703	-2.031025
C	6.344043	2.801265	0.498481
H	7.401578	2.988583	0.247059
H	5.749150	3.461047	-0.153064
H	6.172281	3.086763	1.542682

100

**IPrCl2Py6del2Isomer** SCF Done: -3468.37308043 A.U.

Pd	-0.713067	-0.746677	-0.348345
N	-2.337817	1.798610	-0.275884
C	0.757388	4.439709	-1.382740
N	-3.479607	0.117847	0.464034
C	0.313973	4.396258	-0.060638
C	-0.698537	3.512486	0.336810
Cl	0.578766	0.381798	1.281422
C	-1.253382	2.673244	-0.657106
C	-0.816545	2.685284	-1.995708
C	0.199164	3.591806	-2.336583
C	-1.422508	1.788252	-3.066316
C	-2.326998	2.599743	-4.009730
C	-0.343241	1.017629	-3.841762
C	-1.189194	3.516725	1.782615
C	-2.141098	4.702908	2.030933
C	-0.046702	3.539978	2.810037
C	-3.618499	2.269791	-0.000777
C	-4.329916	1.219343	0.478671
C	-3.839522	-1.177124	0.990780
C	-4.717342	-1.999237	0.253495
C	-5.059581	-3.239271	0.814234
C	-4.544645	-3.641086	2.045681
C	-3.685231	-2.802201	2.756565
C	-3.318874	-1.546108	2.252608
C	-5.324823	-1.567270	-1.076559
C	-6.747662	-1.012401	-0.870732
C	-5.349124	-2.696292	-2.118735
C	-2.464604	-0.592572	3.082102
C	-3.363088	0.324139	3.933811
C	-1.418270	-1.302429	3.948990
C	-2.254641	0.468246	-0.010677



H	1.550768	5.134956	-1.668194
H	0.766804	5.060496	0.677461
H	0.559684	3.629936	-3.366337
H	-2.050848	1.035537	-2.574106
H	-1.751624	3.372993	-4.545192
H	-3.133251	3.103717	-3.453162
H	-2.790486	1.940175	-4.761446
H	-0.811475	0.271339	-4.501575
H	0.328427	0.486386	-3.151842
H	0.269711	1.685141	-4.468523
H	-1.749530	2.585736	1.951889
H	-2.999762	4.701078	1.344312
H	-1.608689	5.658751	1.895943
H	-2.531336	4.673988	3.061092
H	0.657107	2.716054	2.636439
H	-0.460466	3.432009	3.825587
H	0.509868	4.490413	2.784653
H	-3.895593	3.304420	-0.170611
H	-5.350748	1.152784	0.838323
H	-5.738017	-3.902955	0.275528
H	-4.820385	-4.614375	2.459683
H	-3.303628	-3.126484	3.725612
H	-4.691114	-0.766279	-1.484171
H	-7.413813	-1.795993	-0.473658
H	-7.167034	-0.663253	-1.828149
H	-6.770895	-0.169702	-0.164866
H	-4.356524	-3.153672	-2.228094
H	-5.653209	-2.292899	-3.097908
H	-6.073363	-3.483173	-1.853164
H	-1.899854	0.049515	2.395978
H	-4.071463	0.888933	3.308391
H	-2.750100	1.051765	4.490428
H	-3.946528	-0.262972	4.662252
H	-1.875221	-1.871653	4.774546
H	-0.742650	-0.557677	4.396905
H	-0.807208	-1.993945	3.348810
Cl	-1.938839	-1.801757	-2.071486
N	0.967705	-2.010073	-0.744380
C	1.742216	-2.445285	0.266425
C	1.421459	-2.134117	-2.003861
C	3.031571	-2.920020	0.058809
C	2.705574	-2.591127	-2.289731
C	3.560992	-2.937414	-1.239273
H	1.333130	-2.348839	1.272276

H	3.644738	-3.193752	0.919347
H	0.743923	-1.810105	-2.794958
H	3.056523	-2.589821	-3.322776
C	5.049126	-3.147250	-1.453805
H	5.325669	-4.188200	-1.230210
H	5.307123	-2.948135	-2.501899
N	5.839631	-2.299781	-0.547828
H	6.357323	-2.801723	0.167306
C	5.465349	-1.044368	-0.176230
C	4.766637	-0.171988	-1.196318
C	5.743668	-0.477017	1.038380
C	4.003553	1.006801	-0.721633
C	5.175514	0.807886	1.467832
C	4.225379	1.497434	0.523629
Cl	6.647034	-1.379269	2.238037
O	5.404724	1.278181	2.575738
O	4.843196	-0.460046	-2.380185
C	3.025210	1.629983	-1.672763
H	3.224089	2.703111	-1.818142
H	3.045447	1.132427	-2.649920
H	2.006940	1.555896	-1.257877
C	3.516342	2.717837	1.025531
H	3.701137	3.582514	0.367054
H	2.428250	2.542783	1.017514
H	3.833611	2.970049	2.044185
100			
<b>IPrCl2Py6del2Isomer180</b> SCF Done: -3468.37126502 A.U.			
Pd	-1.041395	-0.188632	-0.424485
N	-3.474695	1.316815	0.538654
C	-2.033262	5.072332	-0.716226
N	-3.685575	-0.805577	0.885763
C	-1.962907	4.719251	0.630885
C	-2.429400	3.474689	1.080427
Cl	-0.019517	0.741682	1.493964
C	-2.974281	2.602563	0.113760
C	-3.080344	2.940172	-1.253547
C	-2.588709	4.193364	-1.646733
C	-3.776409	2.024447	-2.253877
C	-5.287141	2.324762	-2.284950
C	-3.173553	2.087939	-3.662253
C	-2.387138	3.127829	2.564854
C	-3.603851	3.726153	3.297621
C	-1.089409	3.579876	3.251625
C	-4.706413	1.131216	1.159045

C	-4.832909	-0.200082	1.389130
C	-3.458828	-2.231274	0.900960
C	-4.105895	-3.027895	-0.068631
C	-3.877285	-4.410953	-0.017954
C	-3.039603	-4.968887	0.947759
C	-2.418919	-4.155850	1.896394
C	-2.618614	-2.767428	1.899677
C	-5.057330	-2.441183	-1.106448
C	-6.517843	-2.539462	-0.624345
C	-4.919524	-3.095465	-2.489489
C	-2.013608	-1.894097	2.991525
C	-2.961065	-1.832610	4.204305
C	-0.604874	-2.333425	3.409147
C	-2.842379	0.126067	0.368706
H	-1.657747	6.045176	-1.043826
H	-1.534788	5.423097	1.346430
H	-2.649316	4.492430	-2.694056
H	-3.650912	0.988651	-1.914693
H	-5.475445	3.355516	-2.628374
H	-5.742799	2.211698	-1.289242
H	-5.802329	1.634588	-2.972814
H	-3.614205	1.298155	-4.289894
H	-2.084908	1.929552	-3.636008
H	-3.372639	3.051906	-4.157846
H	-2.431339	2.032161	2.649391
H	-4.558558	3.385962	2.871848
H	-3.586388	4.826941	3.238740
H	-3.588852	3.442482	4.362444
H	-0.207518	3.228161	2.699600
H	-1.044748	3.165855	4.271653
H	-1.035358	4.676588	3.344256
H	-5.375118	1.958846	1.368535
H	-5.622835	-0.771019	1.864828
H	-4.359695	-5.062802	-0.748067
H	-2.872695	-6.048990	0.964281
H	-1.776511	-4.610056	2.652295
H	-4.800961	-1.378257	-1.226187
H	-6.812476	-3.594613	-0.500567
H	-7.197125	-2.080866	-1.361076
H	-6.675565	-2.034617	0.339103
H	-3.871998	-3.105600	-2.819157
H	-5.507985	-2.528681	-3.228629
H	-5.302433	-4.128733	-2.493823
H	-1.913177	-0.875086	2.597893

H	-3.953541	-1.449502	3.920057
H	-2.550265	-1.167508	4.981338
H	-3.098682	-2.833119	4.646929
H	-0.610679	-3.293579	3.949928
H	-0.163751	-1.579896	4.079452
H	0.054836	-2.433648	2.533803
Cl	-2.000984	-1.129625	-2.367213
N	0.888598	-0.527580	-1.247156
C	1.833979	-1.162134	-0.534775
C	1.195711	-0.081772	-2.479272
C	3.120508	-1.371329	-1.024572
C	2.463804	-0.233858	-3.027586
C	3.460280	-0.889495	-2.292453
H	1.549117	-1.492818	0.465059
H	3.850718	-1.893508	-0.405714
H	0.392543	0.408946	-3.031006
H	2.670859	0.171055	-4.020312
C	4.849135	-1.058915	-2.879128
H	4.823185	-1.890580	-3.600596
H	5.111227	-0.158855	-3.452225
N	5.880852	-1.375792	-1.913914
H	6.203687	-2.341098	-1.871588
C	6.395088	-0.627330	-0.916520
C	7.323333	-1.456735	-0.029930
C	6.203657	0.693220	-0.594131
C	7.992706	-0.830357	1.128770
C	6.846719	1.318300	0.565156
C	7.763407	0.475347	1.417089
Cl	5.182535	1.775593	-1.527451
O	6.662581	2.495739	0.852695
O	7.478590	-2.635993	-0.310962
C	8.904652	-1.691909	1.956248
H	8.554476	-1.742024	3.000489
H	8.957232	-2.711534	1.556250
H	9.922956	-1.270609	1.983716
C	8.410219	1.147377	2.590089
H	8.150929	0.627673	3.527576
H	9.509071	1.106159	2.503873
H	8.098238	2.195253	2.664730
100			
<b>IPrCl2Py6del6Isomer</b> SCF Done: -3468.36980265 A.U.			
Pd	0.639817	-0.060577	-0.827151
N	3.177922	-0.855378	0.605956
C	1.795344	-4.726526	1.537533

N	3.162770	1.255070	0.137184
C	1.438996	-3.643598	2.343671
C	1.900007	-2.350019	2.063285
Cl	-0.520839	0.888029	1.005856
C	2.717587	-2.188681	0.918213
C	3.116877	-3.266727	0.102676
C	2.633640	-4.541144	0.439817
C	4.090192	-3.094082	-1.057087
C	5.523923	-3.434325	-0.606362
C	3.709569	-3.923755	-2.291953
C	1.593607	-1.186770	3.003184
C	2.754416	-0.965744	3.992499
C	0.271072	-1.332576	3.763290
C	4.426199	-0.353452	0.964717
C	4.419418	0.969870	0.662923
C	2.685473	2.594312	-0.116394
C	2.682051	3.086283	-1.435355
C	2.215590	4.395255	-1.634110
C	1.776300	5.172404	-0.563139
C	1.797879	4.659222	0.734868
C	2.250703	3.357867	0.991478
C	3.216267	2.271721	-2.604871
C	4.636435	2.737448	-2.973379
C	2.279497	2.305005	-3.820242
C	2.314492	2.832091	2.422612
C	3.590324	3.331978	3.127339
C	1.075732	3.185387	3.258927
C	2.406573	0.128763	0.073444
H	1.424181	-5.726552	1.776124
H	0.798707	-3.812578	3.210126
H	2.919524	-5.401835	-0.167066
H	4.060468	-2.037814	-1.359360
H	5.594717	-4.491693	-0.302103
H	5.847050	-2.821082	0.247761
H	6.236295	-3.268944	-1.430794
H	4.366204	-3.657775	-3.135703
H	2.671782	-3.726483	-2.593758
H	3.829632	-5.004731	-2.114883
H	1.491169	-0.281276	2.391838
H	3.710088	-0.791988	3.478156
H	2.877215	-1.842091	4.650114
H	2.551256	-0.087248	4.626432
H	-0.562784	-1.541541	3.081620
H	0.043978	-0.392418	4.289166

H	0.312457	-2.131714	4.521140
H	5.190957	-0.978870	1.412509
H	5.181272	1.734021	0.775417
H	2.203839	4.813919	-2.642222
H	1.417615	6.189717	-0.739547
H	1.455744	5.282487	1.562927
H	3.281135	1.222437	-2.290050
H	4.634854	3.789448	-3.303794
H	5.043651	2.123420	-3.793155
H	5.320122	2.655459	-2.113363
H	1.265505	1.982254	-3.539994
H	2.647926	1.617479	-4.597099
H	2.216914	3.309938	-4.267785
H	2.363188	1.735324	2.375980
H	4.502919	3.052555	2.581415
H	3.659082	2.907559	4.142043
H	3.576634	4.430675	3.217040
H	1.019215	4.264560	3.473969
H	1.123225	2.662335	4.227716
H	0.154543	2.875890	2.747671
Cl	1.734958	-1.055821	-2.671568
N	-1.221741	-0.283045	-1.835409
C	-2.114346	0.722682	-1.854045
C	-1.594205	-1.488537	-2.299075
C	-3.430008	0.536235	-2.262358
C	-2.897817	-1.755070	-2.709989
C	-3.859168	-0.741120	-2.649788
H	-1.769726	1.688021	-1.481838
H	-4.130409	1.371229	-2.205740
H	-0.826390	-2.263880	-2.302207
H	-3.170250	-2.770330	-3.002509
C	-5.338282	-1.031086	-2.834384
H	-5.703506	-0.567431	-3.762755
H	-5.495787	-2.114410	-2.917100
N	-6.139174	-0.465689	-1.739528
H	-6.766579	0.287666	-2.004241
C	-5.707918	-0.402932	-0.451235
C	-4.838030	-1.526100	0.068715
C	-6.063415	0.567804	0.446630
C	-4.000726	-1.278585	1.267651
C	-5.417883	0.711444	1.757634
C	-4.288804	-0.234222	2.083678
Cl	-7.176252	1.834009	-0.028953
O	-5.725493	1.605733	2.536391

O	-4.837715	-2.598756	-0.513271
C	-3.490895	0.053198	3.320065
H	-3.462989	-0.822631	3.988944
H	-2.446983	0.275530	3.041722
H	-3.908381	0.906344	3.867658
C	-2.861402	-2.225012	1.511738
H	-2.931303	-3.102030	0.856621
H	-1.911557	-1.703184	1.303498
H	-2.826109	-2.562808	2.558416
79			
<b>IPrCl2PEPPSI</b> SCF Done: -2915.16561906 A.U.			
Pd	0.561645	-0.672184	-0.047840
N	-0.861351	1.879960	0.639445
C	2.629503	4.241149	0.719140
N	-2.282305	0.311963	0.193537
C	2.374102	3.352527	1.762278
C	1.223836	2.547663	1.763907
Cl	-0.067634	-1.797688	1.932859
C	0.344656	2.673311	0.671285
C	0.579078	3.558894	-0.405651
C	1.739301	4.342962	-0.351074
C	-0.392534	3.707448	-1.573324
C	-1.294598	4.941342	-1.378748
C	0.308703	3.779089	-2.938497
C	0.944369	1.620172	2.938673
C	0.479595	2.427380	4.163753
C	2.151619	0.731702	3.273671
C	-2.127424	2.403422	0.883413
C	-3.019655	1.424117	0.590628
C	-2.873199	-0.908238	-0.303532
C	-2.850583	-1.132138	-1.700415
C	-3.433322	-2.317578	-2.170126
C	-4.028419	-3.225493	-1.292711
C	-4.057993	-2.963854	0.075780
C	-3.478929	-1.800227	0.605704
C	-2.293594	-0.096486	-2.672651
C	-3.362277	0.964463	-2.998753
C	-1.717096	-0.703620	-3.956780
C	-3.569332	-1.515144	2.100605
C	-4.950112	-0.931961	2.458378
C	-3.281711	-2.752887	2.964618
C	-0.951829	0.586171	0.235943
H	3.529439	4.861164	0.739239
H	3.075653	3.286749	2.596303

H	1.953764	5.042549	-1.160948
H	-1.034612	2.814935	-1.592831
H	-0.690382	5.863433	-1.375708
H	-1.851782	4.905315	-0.431650
H	-2.025965	5.016459	-2.199643
H	-0.443654	3.746943	-3.743053
H	0.993834	2.931625	-3.072996
H	0.875198	4.716262	-3.060316
H	0.126982	0.943511	2.659496
H	-0.420215	3.019963	3.933423
H	1.264711	3.123556	4.502498
H	0.239615	1.752565	5.001585
H	2.489128	0.179426	2.383684
H	1.874196	-0.006572	4.041603
H	2.999679	1.317919	3.662670
H	-2.269236	3.418980	1.237033
H	-4.103740	1.416439	0.614468
H	-3.433938	-2.531567	-3.239559
H	-4.480170	-4.141536	-1.681957
H	-4.538562	-3.677536	0.747130
H	-1.457901	0.417424	-2.182885
H	-4.223101	0.508778	-3.515555
H	-2.940101	1.743010	-3.655011
H	-3.735803	1.458650	-2.089295
H	-0.995469	-1.503825	-3.732437
H	-1.189209	0.075725	-4.527452
H	-2.501021	-1.118024	-4.611276
H	-2.799159	-0.768652	2.342182
H	-5.178251	-0.017947	1.890960
H	-4.997660	-0.685161	3.531355
H	-5.746322	-1.663253	2.242244
H	-4.084398	-3.503679	2.885726
H	-3.214578	-2.459889	4.024640
H	-2.330755	-3.221583	2.677224
Cl	1.247211	0.433393	-2.019095
N	2.203153	-2.020678	-0.264532
C	2.016789	-3.349824	-0.190620
C	3.437707	-1.531457	-0.451682
C	3.075389	-4.248551	-0.312459
C	4.543585	-2.376285	-0.565504
C	4.369014	-3.760600	-0.500317
H	0.994826	-3.688162	-0.015744
H	2.885190	-5.321352	-0.256228
H	3.542098	-0.448567	-0.524948



H	5.224327	-4.431645	-0.594039
Cl	6.123795	-1.681323	-0.790119
91			
<b>IPrC12PEPPSI+DMF</b> SCF Done: -3163.52886099 A.U.			
Pd	-0.405994	-0.167875	0.389197
N	2.422154	-1.075083	0.029608
C	1.409224	-5.143164	-0.403675
N	2.336382	1.085213	0.031612
C	1.338784	-4.544727	0.853433
C	1.666252	-3.191284	1.031165
Cl	-0.090829	0.732384	2.551798
C	2.061587	-2.466034	-0.109094
C	2.139266	-3.042269	-1.397670
C	1.809062	-4.399151	-1.514839
C	2.600822	-2.256954	-2.622592
C	4.084520	-2.542911	-2.924938
C	1.749897	-2.527395	-3.872931
C	1.640425	-2.575492	2.423670
C	2.862874	-3.038334	3.236202
C	0.327417	-2.866244	3.164824
C	3.736094	-0.621754	-0.025880
C	3.681773	0.733218	-0.039253
C	1.881695	2.452577	-0.066555
C	1.331306	2.881452	-1.296238
C	0.955464	4.227603	-1.396463
C	1.129401	5.106808	-0.327711
C	1.681531	4.656161	0.870173
C	2.069584	3.317344	1.032235
C	1.200780	1.944773	-2.492925
C	2.515774	1.894478	-3.293308
C	0.011050	2.281373	-3.400298
C	2.712603	2.864143	2.338520
C	4.191088	3.293011	2.398741
C	1.963874	3.379963	3.577699
C	1.557345	-0.027064	0.087489
H	1.153268	-6.199482	-0.519525
H	1.033644	-5.140515	1.715896
H	1.860579	-4.882161	-2.492311
H	2.498341	-1.185907	-2.395146
H	4.226567	-3.604794	-3.184954
H	4.735729	-2.320752	-2.067503
H	4.427527	-1.935041	-3.777730
H	2.049608	-1.839538	-4.680054
H	0.683609	-2.370052	-3.663809

H	1.889713	-3.552813	-4.251088
H	1.706062	-1.484979	2.321316
H	3.803419	-2.775580	2.726079
H	2.851837	-4.131197	3.382326
H	2.868315	-2.562219	4.230294
H	-0.538477	-2.550138	2.563798
H	0.299925	-2.309571	4.114181
H	0.214841	-3.936364	3.402040
H	4.577686	-1.305293	-0.054370
H	4.465832	1.479296	-0.106716
H	0.519469	4.596762	-2.325208
H	0.831590	6.153594	-0.429989
H	1.815228	5.357059	1.696205
H	1.010409	0.933777	-2.113755
H	2.753590	2.882720	-3.720941
H	2.431231	1.173064	-4.122543
H	3.364179	1.584556	-2.664310
H	-0.907853	2.403697	-2.808306
H	-0.144724	1.464403	-4.121900
H	0.178201	3.204545	-3.979443
H	2.664335	1.766223	2.368746
H	4.774031	2.903440	1.551460
H	4.660329	2.929447	3.327309
H	4.276717	4.392076	2.383089
H	2.069963	4.470372	3.695931
H	2.377883	2.912541	4.485648
H	0.894924	3.133403	3.521993
Cl	-0.761571	-1.080765	-1.765260
N	-2.488499	-0.417193	0.811426
C	-3.205194	0.581468	1.351990
C	-3.088435	-1.579282	0.512508
C	-4.572089	0.458417	1.595722
C	-4.451054	-1.772963	0.743661
C	-5.217437	-0.739024	1.287877
H	-2.661944	1.498318	1.574951
H	-5.124627	1.299742	2.016259
H	-2.475323	-2.358286	0.059362
H	-6.286447	-0.873006	1.460395
Cl	-5.174608	-3.301660	0.329236
O	-2.217258	2.918045	-0.631486
N	-4.298670	2.253365	-1.343379
C	-5.721089	2.535141	-1.388039
H	-6.073967	2.605169	-2.430840
H	-6.290027	1.734199	-0.885422

H	-5.935287	3.486417	-0.880991
C	-3.846492	1.031205	-1.985966
H	-2.776128	0.886476	-1.804134
H	-4.395379	0.165759	-1.580314
H	-4.029248	1.074872	-3.073242
C	-3.427864	3.087066	-0.730095
H	-3.934861	3.977273	-0.291551

87

**IPrCl2PEPPSI+K3PO4** SCF Done: -5357.39675559 A.U.

Pd	-0.322790	-0.418408	-0.240690
N	-3.164455	0.362609	-0.064128
C	-4.301570	-3.675967	0.340331
N	-1.984354	2.173376	-0.085518
C	-3.884643	-3.196260	-0.900712
C	-3.513802	-1.853434	-1.069959
Cl	0.132621	0.460938	-2.390921
C	-3.565832	-1.019576	0.064847
C	-3.993921	-1.472532	1.333310
C	-4.363932	-2.820059	1.440791
C	-4.102510	-0.546103	2.541334
C	-5.546471	-0.029905	2.699334
C	-3.638914	-1.194331	3.855042
C	-3.144869	-1.326643	-2.451251
C	-4.420763	-1.053389	-3.268541
C	-2.182810	-2.255093	-3.204751
C	-4.062162	1.422664	-0.104244
C	-3.323958	2.559482	-0.102769
C	-0.918686	3.143521	-0.013988
C	-0.246802	3.314757	1.220431
C	0.705160	4.343194	1.295996
C	0.962882	5.172751	0.201391
C	0.287486	4.976649	-1.003699
C	-0.663712	3.951514	-1.144561
C	-0.576974	2.462471	2.442111
C	-1.812482	3.014944	3.178236
C	0.607602	2.290742	3.401302
C	-1.392854	3.772063	-2.472968
C	-2.455705	4.869492	-2.670688
C	-0.431552	3.745659	-3.672970
C	-1.881285	0.818922	-0.071529
H	-4.587433	-4.725154	0.450339
H	-3.857486	-3.873369	-1.756240
H	-4.700357	-3.210039	2.402839
H	-3.445771	0.317952	2.361649

H	-6.232405	-0.867611	2.906532
H	-5.910602	0.481144	1.797060
H	-5.611545	0.679425	3.540112
H	-3.606865	-0.433194	4.651118
H	-2.635599	-1.628218	3.751931
H	-4.331277	-1.983586	4.189237
H	-2.622654	-0.369340	-2.327830
H	-5.081420	-0.339512	-2.751295
H	-4.990569	-1.982884	-3.432680
H	-4.164931	-0.630931	-4.253876
H	-1.285069	-2.460898	-2.603685
H	-1.858379	-1.778106	-4.142271
H	-2.653796	-3.215563	-3.467623
H	-5.135127	1.267082	-0.128549
H	-3.617713	3.603224	-0.098371
H	1.249590	4.506762	2.226167
H	1.700994	5.973951	0.288306
H	0.503886	5.628582	-1.852012
H	-0.831264	1.455410	2.090645
H	-1.613345	4.023392	3.577051
H	-2.075818	2.357355	4.022521
H	-2.689845	3.078515	2.517124
H	1.509274	1.961676	2.861016
H	0.355010	1.536569	4.163602
H	0.847275	3.223483	3.937499
H	-1.898873	2.796235	-2.447647
H	-3.188143	4.893823	-1.850738
H	-3.005877	4.705398	-3.610991
H	-1.982453	5.863679	-2.723811
H	0.062066	4.718679	-3.825182
H	-0.991731	3.515479	-4.593220
H	0.340193	2.974411	-3.545956
Cl	-0.640194	-1.230651	1.967082
N	1.048969	-2.019610	-0.588359
C	2.309878	-1.907695	-1.038735
C	0.489070	-3.238238	-0.459565
C	3.053876	-3.038039	-1.391812
C	1.181533	-4.396755	-0.798517
C	2.492304	-4.306539	-1.279135
H	2.774865	-0.916414	-1.099152
H	4.078272	-2.908657	-1.743222
H	-0.531198	-3.286748	-0.077987
H	3.047142	-5.206992	-1.548288
Cl	0.393023	-5.942109	-0.614844

O	3.258484	1.180832	1.260261
P	4.512902	0.435274	0.642963
O	4.541424	-1.062147	1.167615
K	2.582219	2.238055	-1.059962
O	4.363119	0.408144	-0.941931
O	5.864041	1.136266	1.010501
K	2.466089	-0.914254	2.664135
K	6.860744	-1.061452	-0.285179
136			
<b>DimerIPrCl2</b> SCF Done: -4415.14193584 A.U.			
Pd	1.591911	-0.497786	-0.652498
N	3.904574	1.266588	0.062368
C	2.080100	4.927479	-0.952599
N	4.267219	-0.784288	0.655524
C	3.023511	4.365811	-1.810456
Cl	-0.672608	-1.072553	-1.495289
C	3.634101	3.137378	-1.513964
Cl	2.436907	-0.097866	-2.800578
C	3.250149	2.498132	-0.317110
C	2.295320	3.041565	0.573071
C	1.722203	4.271932	0.225129
C	1.937469	2.370227	1.895079
C	2.900369	2.818725	3.010054
C	0.475030	2.580689	2.304362
C	4.704898	2.573576	-2.440692
C	6.051433	3.287050	-2.214203
C	4.306813	2.650775	-3.922912
C	5.189735	1.219388	0.595306
C	5.422408	-0.068892	0.953319
C	4.048590	-2.157652	1.046288
C	3.761712	-2.420762	2.405919
C	3.559155	-3.759086	2.768943
C	3.632008	-4.782504	1.822615
C	3.915031	-4.489133	0.489468
C	4.130879	-3.167657	0.068878
C	3.713319	-1.321169	3.464362
C	5.056512	-1.231288	4.215158
C	2.567239	-1.491444	4.474311
C	4.491032	-2.872940	-1.381083
C	5.954495	-3.261128	-1.657683
C	3.530224	-3.550257	-2.368733
C	3.343709	0.030953	0.086494
H	1.616370	5.884712	-1.204252
H	3.294913	4.891918	-2.727320

H	0.981054	4.723112	0.883855
H	2.064584	1.288163	1.774505
H	2.808993	3.901868	3.194335
H	3.948917	2.605320	2.751072
H	2.670056	2.289581	3.949099
H	0.233855	1.941006	3.165668
H	-0.214163	2.317600	1.489026
H	0.268575	3.622339	2.595900
H	4.828386	1.508890	-2.195860
H	6.392247	3.212938	-1.171057
H	5.969037	4.358303	-2.461175
H	6.832017	2.849246	-2.857136
H	3.320685	2.196140	-4.089439
H	5.044070	2.108258	-4.536147
H	4.282686	3.690417	-4.287154
H	5.806841	2.107100	0.681162
H	6.292977	-0.544033	1.392065
H	3.337368	-4.006384	3.808411
H	3.468199	-5.818690	2.129192
H	3.977033	-5.300701	-0.238049
H	3.546598	-0.362936	2.949825
H	5.248847	-2.165148	4.768296
H	5.035957	-0.402815	4.941285
H	5.905319	-1.065994	3.536945
H	1.600198	-1.618435	3.970114
H	2.505319	-0.597537	5.115243
H	2.731572	-2.355879	5.137091
H	4.398875	-1.791966	-1.547436
H	6.643501	-2.727842	-0.983376
H	6.229836	-3.012027	-2.695400
H	6.111412	-4.342997	-1.514256
H	3.612121	-4.648501	-2.336983
H	3.759052	-3.228820	-3.396490
H	2.488050	-3.271108	-2.152732
Pd	-1.591910	-0.497839	0.652525
N	-4.267236	-0.784490	-0.655387
C	-3.631675	-4.782522	-1.822949
N	-3.904699	1.266414	-0.062253
C	-3.914588	-4.489326	-0.489742
Cl	0.672647	-1.072405	1.495359
C	-4.130536	-3.167917	-0.068988
Cl	-2.436982	-0.097771	2.800557
C	-4.048488	-2.157799	-1.046304
C	-3.761742	-2.420738	-2.406000

C	-3.559045	-3.758997	-2.769178
C	-3.713623	-1.321036	-3.464342
C	-5.056873	-1.231361	-4.215059
C	-2.567566	-1.490993	-4.474366
C	-4.490456	-2.873405	1.381073
C	-5.953814	-3.261823	1.657911
C	-3.529362	-3.550720	2.368444
C	-5.422534	-0.069192	-0.953014
C	-5.189925	1.219107	-0.595032
C	-3.250307	2.498006	0.317122
C	-2.295527	3.041440	-0.573119
C	-1.722472	4.271860	-0.225263
C	-2.080367	4.927457	0.952437
C	-3.023721	4.365788	1.810353
C	-3.634254	3.137305	1.513948
C	-1.937642	2.370032	-1.895083
C	-2.900636	2.818337	-3.010055
C	-0.475239	2.580600	-2.304428
C	-4.704973	2.573496	2.440762
C	-6.051522	3.286983	2.214413
C	-4.306738	2.650662	3.922944
C	-3.343740	0.030825	-0.086444
H	-3.467763	-5.818654	-2.129654
H	-3.976392	-5.300974	0.237703
H	-3.337341	-4.006163	-3.808695
H	-3.547065	-0.362815	-2.949732
H	-5.249041	-2.165202	-4.768287
H	-5.905677	-1.066318	-3.536782
H	-5.036532	-0.402805	-4.941097
H	-2.505887	-0.597036	-5.115252
H	-1.600468	-1.617789	-3.970228
H	-2.731739	-2.355428	-5.137185
H	-4.398403	-1.792436	1.547531
H	-6.643023	-2.728559	0.983794
H	-6.110612	-4.343697	1.514397
H	-6.228991	-3.012875	2.695707
H	-2.487266	-3.271464	2.152210
H	-3.757966	-3.229378	3.396282
H	-3.611179	-4.648968	2.336628
H	-6.293115	-0.544416	-1.391643
H	-5.807118	2.106768	-0.680793
H	-0.981353	4.723036	-0.884025
H	-1.616678	5.884727	1.204021
H	-3.295124	4.891928	2.727197

H	-2.064627	1.287965	-1.774412
H	-2.809337	3.901463	-3.194474
H	-2.670353	2.289093	-3.949051
H	-3.949154	2.604903	-2.750977
H	0.213999	2.317718	-1.489061
H	-0.234028	1.940801	-3.165639
H	-0.268905	3.622222	-2.596152
H	-4.828489	1.508814	2.195927
H	-6.392421	3.212916	1.171291
H	-6.832056	2.849156	2.857391
H	-5.969105	4.358226	2.461420
H	-4.282554	3.690298	4.287203
H	-5.043942	2.108146	4.536244
H	-3.320601	2.196005	4.089360

BP86/def2SVP  
geometries

32

Py1 SCF Done: -1335.76007416 A.U.

N	-4.462905	-0.119718	-0.778012
C	-5.447021	-0.022058	0.129729
C	-3.230086	-0.449640	-0.345549
C	-5.260781	-0.250464	1.505928
C	-2.937650	-0.702014	1.008537
C	-3.975849	-0.599524	1.949178
H	-6.445279	0.252551	-0.258977
H	-6.104157	-0.156526	2.207456
H	-1.916008	-0.970911	1.315932
H	-3.780286	-0.788583	3.016915
C	-2.175653	-0.514401	-1.449279
H	-2.565932	-1.179694	-2.248885
H	-2.083669	0.492080	-1.900322
N	-0.870685	-1.005544	-1.048179
H	-0.695228	-2.022458	-1.088811
C	0.252187	-0.358024	-0.645030
C	1.386164	-1.356844	-0.437608
C	0.488366	0.990312	-0.398049
C	2.716493	-0.857242	-0.022007
C	1.796576	1.520472	0.025494
C	2.917208	0.526948	0.195169
Cl	-0.760672	2.212394	-0.532523
O	1.988699	2.720446	0.241338
O	1.153535	-2.556088	-0.624296
C	4.185169	0.990203	0.586820
C	5.244415	0.082939	0.759936
C	3.780955	-1.765931	0.155061
C	5.043607	-1.294837	0.544856



H	4.309757	2.071710	0.750007
H	6.236405	0.451957	1.065857
H	5.876504	-2.002238	0.682079
H	3.591980	-2.835978	-0.020471
32			
<b>Py2</b> SCF Done: -1335.75599419 A.U.			
N	-4.095111	0.281584	1.863820
C	-5.052188	-0.643367	1.666583
C	-3.239134	0.516526	0.856767
C	-5.200488	-1.360978	0.466684
C	-3.284721	-0.145981	-0.392100
C	-4.298671	-1.105014	-0.578435
H	-5.744008	-0.820939	2.510680
H	-6.007326	-2.102157	0.354062
H	-2.465692	1.287306	1.036196
H	-4.385614	-1.643041	-1.538076
C	-2.259034	0.157122	-1.476461
H	-2.650599	-0.185666	-2.458683
H	-2.080496	1.244424	-1.549061
N	-0.981253	-0.512672	-1.249379
H	-0.965783	-1.543702	-1.330406
C	0.201125	-0.079569	-0.747615
C	1.149782	-1.265898	-0.568738
C	0.652890	1.191574	-0.406135
C	2.519104	-1.023585	-0.062123
C	2.004517	1.466665	0.111234
C	2.931551	0.289409	0.266802
Cl	-0.340604	2.634072	-0.548581
O	2.383735	2.603357	0.407778
O	0.736710	-2.394095	-0.855188
C	4.233519	0.506638	0.750124
C	3.408367	-2.107809	0.094351
C	4.706184	-1.882115	0.576416
C	5.117325	-0.574947	0.903966
H	3.056849	-3.117052	-0.168849
H	5.402017	-2.726910	0.699163
H	6.136669	-0.398903	1.283076
H	4.524477	1.538912	0.998037
32			
<b>Py2isom</b> SCF Done: -1335.75719007 A.U.			
N	-5.273650	-1.314712	0.402589
C	-5.167412	-0.650244	1.565915
C	-4.342644	-1.073091	-0.534979
C	-4.143272	0.276984	1.837827

C	-3.268424	-0.171723	-0.376293
C	-3.177542	0.518495	0.850471
H	-5.941047	-0.864510	2.326396
H	-4.108158	0.801471	2.805689
H	-4.453640	-1.626232	-1.488707
H	-2.364179	1.244172	1.016844
C	-2.247626	0.030559	-1.487622
H	-2.643358	-0.406244	-2.429696
H	-2.075961	1.107134	-1.665950
N	-0.964816	-0.611313	-1.211448
H	-0.932995	-1.644193	-1.253858
C	0.209457	-0.138172	-0.729888
C	1.184631	-1.297889	-0.516691
C	0.634337	1.152201	-0.427402
C	2.552940	-1.008065	-0.032726
C	1.980972	1.473973	0.073560
C	2.937820	0.323809	0.251137
Cl	-0.399698	2.564711	-0.594414
O	2.333168	2.626627	0.341504
O	0.793021	-2.443565	-0.758552
C	4.239629	0.585675	0.712312
C	5.150489	-0.469873	0.887892
C	3.468944	-2.066197	0.146707
C	4.766610	-1.795751	0.605494
H	4.508987	1.631361	0.926054
H	6.169790	-0.258634	1.248689
H	5.483602	-2.619986	0.745030
H	3.138114	-3.090890	-0.081346

32

**Py3** SCF Done: -1335.75607316 A.U.

N	-5.217706	-0.611844	1.614294
C	-3.988377	-1.130740	1.767835
C	-5.464455	0.036277	0.460498
C	-2.968032	-1.033339	0.802783
C	-4.519951	0.190642	-0.566923
C	-3.230659	-0.355825	-0.400364
H	-3.794286	-1.660024	2.719295
H	-1.978945	-1.478410	0.992281
H	-6.478393	0.462276	0.344799
H	-4.788878	0.736312	-1.486850
C	-2.195134	-0.206727	-1.511357
H	-2.582420	-0.712784	-2.423743
H	-2.090179	0.864642	-1.767646
N	-0.888556	-0.766677	-1.224518

H	-0.745407	-1.779570	-1.370005
C	0.243824	-0.208538	-0.722673
C	1.332266	-1.270930	-0.597103
C	0.530135	1.095640	-0.337139
C	2.669156	-0.876456	-0.100075
C	1.846447	1.520182	0.176506
C	2.919266	0.466455	0.270189
Cl	-0.649544	2.390989	-0.399349
O	2.080471	2.682505	0.517600
O	1.055748	-2.432392	-0.916323
C	4.192972	0.830274	0.740165
C	3.690947	-1.843872	0.001847
C	4.959908	-1.471766	0.470115
C	5.209592	-0.135131	0.838583
H	3.464774	-2.879731	-0.293594
H	5.759628	-2.224830	0.549096
H	6.206455	0.155671	1.206564
H	4.356544	1.881505	1.022758
32			
<b>Py3isom</b> SCF Done: -1335.75607319 A.U.			
N	-5.218943	-0.612839	1.613369
C	-3.989244	-1.130672	1.767532
C	-5.465695	0.034993	0.459411
C	-2.968518	-1.032457	0.802964
C	-4.520833	0.190099	-0.567566
C	-3.231145	-0.355240	-0.400350
H	-3.795161	-1.659744	2.719112
H	-1.979152	-1.476697	0.992948
H	-6.479945	0.460106	0.343190
H	-4.789799	0.735448	-1.487673
C	-2.195166	-0.205137	-1.510775
H	-2.582196	-0.710099	-2.423880
H	-2.089895	0.866495	-1.765833
N	-0.888800	-0.765583	-1.223956
H	-0.746031	-1.778508	-1.369620
C	0.243882	-0.207906	-0.722288
C	1.331975	-1.270714	-0.597109
C	0.530760	1.096110	-0.336614
C	2.669107	-0.876806	-0.100288
C	1.847333	1.520092	0.176818
C	2.919784	0.465957	0.270130
Cl	-0.648459	2.391913	-0.398322
O	2.081853	2.682276	0.518045
O	1.054975	-2.432023	-0.916461

C	4.193715	0.829233	0.739915
C	5.209999	-0.136561	0.837984
C	3.690563	-1.844613	0.001282
C	4.959752	-1.473047	0.469357
H	4.357731	1.880360	1.022639
H	6.207040	0.153816	1.205819
H	5.759211	-2.226418	0.548063
H	3.463950	-2.880343	-0.294274
32			
<b>Py4</b> SCF Done: -1260.78710913 A.U.			
N	-3.611437	-1.118336	-0.489456
C	-4.477012	-1.331900	0.516249
C	-2.845824	-0.008545	-0.443124
C	-4.627424	-0.459188	1.609495
C	-2.912889	0.923022	0.614299
C	-3.825191	0.692374	1.655937
H	-5.089955	-2.249638	0.447455
H	-5.357152	-0.681022	2.403801
H	-2.254817	1.806592	0.612648
H	-3.907979	1.403516	2.493532
C	-1.854233	0.162761	-1.590996
H	-2.323682	-0.243952	-2.509683
H	-1.607895	1.226270	-1.750632
N	-0.623452	-0.587901	-1.357150
H	-0.694704	-1.618252	-1.406631
C	0.534976	-0.227962	-0.752119
C	1.382578	-1.466980	-0.446390
C	1.049193	1.012569	-0.406160
C	2.709053	-1.321924	0.196180
C	2.348659	1.170557	0.256460
C	3.163801	-0.076749	0.539999
Cl	0.222220	2.535395	-0.719919
O	2.795748	2.277061	0.581346
O	0.918126	-2.572592	-0.745958
C	4.489740	0.138373	1.209090
H	4.556479	-0.435952	2.158392
H	5.323279	-0.221917	0.567022
H	4.636850	1.213912	1.419851
C	3.491927	-2.583001	0.453062
H	3.697294	-2.714334	1.537470
H	2.933718	-3.466396	0.091281
H	4.479932	-2.553084	-0.054628
32			
<b>Py5</b> SCF Done: -1260.78199533 A.U.			

N	-3.748012	0.618086	1.739240
C	-4.729786	-0.289662	1.591646
C	-2.860798	0.744585	0.739269
C	-4.873916	-1.096416	0.448969
C	-2.899124	-0.014496	-0.453425
C	-3.940040	-0.953170	-0.589262
H	-5.446561	-0.377411	2.429077
H	-5.702329	-1.818377	0.374684
H	-2.066027	1.502220	0.876670
H	-4.022669	-1.563324	-1.505161
C	-1.834775	0.161884	-1.528730
H	-2.234424	-0.189987	-2.504341
H	-1.567703	1.227717	-1.640271
N	-0.619015	-0.597332	-1.247382
H	-0.684405	-1.628858	-1.279689
C	0.562928	-0.233709	-0.689910
C	1.405744	-1.477197	-0.389944
C	1.100765	1.005632	-0.382346
C	2.757289	-1.338422	0.197521
C	2.435339	1.159622	0.209998
C	3.246573	-0.092088	0.485689
Cl	0.267064	2.528902	-0.663633
O	2.912314	2.266905	0.483061
O	0.915585	-2.582400	-0.651321
C	4.604490	0.119332	1.087713
H	5.399743	-0.313999	0.442857
H	4.794253	1.200197	1.223679
H	4.687861	-0.391505	2.071793
C	3.530094	-2.605098	0.457562
H	3.792835	-2.701124	1.533036
H	2.937789	-3.489632	0.158336
H	4.488866	-2.613347	-0.104345

32

**Py5isom** SCF Done: -1260.78316266 A.U.

N	-5.004796	-1.024152	0.318429
C	-4.895604	-0.306091	1.449202
C	-4.024862	-0.897425	-0.591327
C	-3.820839	0.564095	1.713717
C	-2.896572	-0.063922	-0.435660
C	-2.804326	0.686029	0.755497
H	-5.709593	-0.426407	2.187942
H	-3.785944	1.137601	2.653400
H	-4.138437	-1.493017	-1.518851
H	-1.950010	1.364414	0.916133

C	-1.820686	0.002334	-1.511035
H	-2.211929	-0.454107	-2.445701
H	-1.559212	1.052128	-1.735616
N	-0.602522	-0.715448	-1.146200
H	-0.644358	-1.748269	-1.126104
C	0.579127	-0.292262	-0.635399
C	1.468530	-1.495475	-0.302996
C	1.082735	0.974982	-0.387835
C	2.834970	-1.288368	0.227381
C	2.428018	1.196703	0.154456
C	3.293424	-0.015652	0.441790
Cl	0.178281	2.457300	-0.677771
O	2.871309	2.328782	0.379786
O	1.003904	-2.625296	-0.494323
C	3.657953	-2.517930	0.510196
H	3.976805	-2.552637	1.574039
H	3.079033	-3.432569	0.284235
H	4.587368	-2.528035	-0.099291
C	4.666855	0.264782	0.976582
H	4.805578	-0.192643	1.980746
H	5.448605	-0.178090	0.321936
H	4.828497	1.356049	1.052524
32			
<b>Py6</b> SCF Done: -1260.77982844 A.U.			
N	-4.593878	0.362248	1.630793
C	-3.565553	-0.485267	1.806505
C	-4.714172	0.929033	0.416348
C	-2.631757	-0.804316	0.803815
C	-3.836689	0.682101	-0.652883
C	-2.763083	-0.210557	-0.465439
H	-3.473251	-0.943896	2.808673
H	-1.807255	-1.503433	1.016314
H	-5.558805	1.630673	0.284545
H	-3.984906	1.190851	-1.619595
C	-1.821934	-0.537402	-1.621681
H	-2.301284	-1.313094	-2.258606
H	-1.689412	0.365591	-2.245528
N	-0.524493	-1.073825	-1.232772
H	-0.443029	-2.095432	-1.179074
C	0.553542	-0.436969	-0.686573
C	0.634888	1.074793	-0.680831
C	1.617606	-1.150182	-0.154611
C	1.850747	1.729134	-0.112723
C	2.821926	-0.532944	0.400576

C	2.880374	0.979933	0.392371
Cl	1.544584	-2.904652	-0.123310
O	3.756463	-1.194302	0.866850
O	-0.291384	1.747677	-1.144208
C	4.120510	1.596176	0.971947
H	4.635192	2.239671	0.225714
H	3.874887	2.253173	1.834642
H	4.814902	0.803743	1.308440
C	1.874052	3.234982	-0.127657
H	0.954650	3.631582	-0.596884
H	1.951031	3.644894	0.902494
H	2.754571	3.617708	-0.687132
32			
<b>Py6isom</b> SCF Done: -1260.78192734 A.U.			
N	-4.931150	-0.342611	1.500424
C	-3.730955	-0.896459	1.739067
C	-5.105679	0.235345	0.297185
C	-2.670508	-0.903557	0.813211
C	-4.115974	0.284152	-0.697573
C	-2.857643	-0.298754	-0.441562
H	-3.596204	-1.367259	2.730707
H	-1.708534	-1.372544	1.071699
H	-6.096121	0.690774	0.111251
H	-4.325964	0.776560	-1.661839
C	-1.773043	-0.261396	-1.514606
H	-2.151702	-0.792001	-2.416569
H	-1.600485	0.789459	-1.816775
N	-0.509308	-0.869287	-1.146869
H	-0.406405	-1.892809	-1.237669
C	0.626703	-0.329509	-0.631597
C	1.675208	-1.419858	-0.411125
C	0.955216	0.973106	-0.299450
C	3.014149	-1.071191	0.116107
C	2.275206	1.333879	0.238270
C	3.302490	0.232333	0.422267
Cl	-0.153857	2.324992	-0.455211
O	2.567297	2.495823	0.540010
O	1.360912	-2.584920	-0.685438
C	4.000421	-2.195823	0.292661
H	4.324620	-2.283253	1.352039
H	3.552558	-3.157574	-0.019250
H	4.920032	-2.020718	-0.306132
C	4.636788	0.655832	0.961969
H	4.864300	0.136034	1.918249

H	5.455544	0.387722	0.259209
H	4.647184	1.748202	1.133240
11			
<b>PEPPSIorg</b> SCF Done: -707.611445747 A.U.			
N	1.549112	-1.256182	-0.000020
C	2.231564	-0.097149	-0.000058
C	0.209006	-1.202241	0.000085
C	1.610935	1.165765	0.000038
C	-0.500980	0.017231	-0.000010
C	0.208649	1.230016	0.000018
H	3.333733	-0.176217	-0.000159
H	2.214189	2.087205	0.000113
H	-0.344798	-2.158071	0.000111
H	-0.330113	2.189365	-0.000008
Cl	-2.251285	0.009957	-0.000021
79			
<b>IPrCl2Py</b> SCF Done: -2455.67662676 A.U.			
Pd	-0.000106	1.180104	-0.000038
N	-1.081001	-1.631474	0.149940
C	-5.158093	-0.590342	0.715245
N	1.081358	-1.631266	-0.149822
C	-4.265211	-0.533000	1.793535
C	-2.903639	-0.866247	1.637805
Cl	0.915763	1.178868	2.165506
C	-2.469915	-1.244734	0.336794
C	-3.355640	-1.329407	-0.772934
C	-4.706959	-0.991945	-0.548178
C	-2.919315	-1.814892	-2.157664
C	-3.297804	-3.300469	-2.363518
C	-3.492855	-0.955814	-3.301967
C	-1.975992	-0.889808	2.853064
C	-2.027321	-2.274506	3.540546
C	-2.266976	0.231818	3.866975
C	-0.676284	-2.966943	0.098107
C	0.676903	-2.966813	-0.097925
C	2.470195	-1.244271	-0.336731
C	2.903841	-0.865806	-1.637775
C	4.265361	-0.532352	-1.793544
C	5.158270	-0.589488	-0.715267
C	4.707217	-0.991074	0.548189
C	3.355955	-1.328729	0.772989
C	1.976207	-0.889611	-2.853038
C	2.027797	-2.274347	-3.540426
C	2.266989	0.232012	-3.867009



C	2.919721	-1.814235	2.157741
C	3.298520	-3.299721	2.363688
C	3.493051	-0.954971	3.302009
C	0.000092	-0.794591	0.000028
H	-6.217229	-0.324529	0.862744
H	-4.632176	-0.228958	2.785218
H	-5.418154	-1.040094	-1.386925
H	-1.814909	-1.722561	-2.211644
H	-4.399527	-3.438256	-2.321964
H	-2.852480	-3.962011	-1.592855
H	-2.949881	-3.658021	-3.355766
H	-3.051179	-1.272817	-4.269816
H	-3.250399	0.113981	-3.150325
H	-4.594169	-1.066922	-3.395875
H	-0.939120	-0.717671	2.498338
H	-1.749259	-3.094270	2.846341
H	-3.047110	-2.492365	3.925129
H	-1.324898	-2.308439	4.400118
H	-2.273885	1.226370	3.377969
H	-1.474334	0.248695	4.642386
H	-3.236972	0.089076	4.390321
H	-1.389655	-3.788442	0.207263
H	1.390440	-3.788174	-0.207031
H	4.632266	-0.228327	-2.785254
H	6.217366	-0.323535	-0.862807
H	5.418431	-1.039075	1.386927
H	0.939303	-0.717642	-2.498334
H	3.047630	-2.492060	-3.924970
H	1.325398	-2.308469	-4.400011
H	1.749869	-3.094106	-2.846161
H	2.273666	1.226587	-3.378051
H	1.474360	0.248678	-4.642438
H	3.237026	0.089436	-4.390321
H	1.815298	-1.722124	2.211697
H	2.853402	-3.961391	1.593017
H	2.950594	-3.657316	3.355921
H	4.400275	-3.437276	2.322233
H	4.594381	-1.065864	3.395977
H	3.051388	-1.271988	4.269859
H	3.250394	0.114767	3.150285
Cl	-0.916092	1.178536	-2.165526
N	-0.000375	3.308986	-0.000081
C	1.002646	3.996540	0.596439
C	-1.003567	3.996276	-0.596611

C	1.041272	5.397832	0.608564
C	-1.042525	5.397559	-0.608798
C	-0.000710	6.115239	-0.000136
H	1.768022	3.382244	1.095650
H	-1.768797	3.381767	-1.095786
H	1.882481	5.910703	1.098509
H	-1.883853	5.910209	-1.098768
H	-0.000840	7.216853	-0.000160
91			
<b>IPrCl2Py+DMF</b> SCF Done: -2704.01409449 A.U.			
Pd	0.003643	0.932908	0.061764
N	-2.277006	-1.024342	-0.060686
C	-5.365397	1.827427	0.539221
N	-0.367961	-2.055886	-0.286900
C	-4.661003	1.316606	1.637620
C	-3.626549	0.372596	1.470755
Cl	0.606725	0.476949	2.295855
C	-3.314595	-0.025391	0.140431
C	-4.027223	0.457575	-0.991568
C	-5.054637	1.395402	-0.755944
C	-3.766071	-0.036760	-2.416198
C	-4.779580	-1.137751	-2.807016
C	-3.782541	1.097951	-3.459058
C	-2.941262	-0.240499	2.692935
C	-3.720082	-1.485655	3.178011
C	-2.742037	0.757353	3.847962
C	-2.564837	-2.379855	-0.229622
C	-1.368912	-3.025455	-0.377592
C	1.044652	-2.396028	-0.341883
C	1.741949	-2.248100	-1.572754
C	3.101201	-2.625988	-1.593203
C	3.730570	-3.147338	-0.455243
C	3.009720	-3.308536	0.735269
C	1.651338	-2.938973	0.825117
C	1.059467	-1.768058	-2.853758
C	0.437975	-2.963946	-3.613385
C	1.993777	-0.962608	-3.776309
C	0.881618	-3.192896	2.124261
C	0.455227	-4.676471	2.227249
C	1.668740	-2.777833	3.382474
C	-0.918259	-0.810952	-0.094797
H	-6.168610	2.565385	0.695524
H	-4.923194	1.653293	2.651884
H	-5.618944	1.797301	-1.611076

H	-2.744902	-0.470277	-2.436825
H	-5.817164	-0.740203	-2.805600
H	-4.754997	-2.002062	-2.112533
H	-4.565001	-1.519954	-3.827375
H	-3.469778	0.703553	-4.448304
H	-3.076816	1.903129	-3.176588
H	-4.796244	1.533964	-3.589090
H	-1.924446	-0.562775	2.387858
H	-3.814745	-2.253182	2.382686
H	-4.746805	-1.211273	3.502923
H	-3.204635	-1.957328	4.041369
H	-2.222093	1.673159	3.503249
H	-2.114990	0.296676	4.638361
H	-3.702153	1.054182	4.321801
H	-3.591909	-2.755033	-0.224486
H	-1.132515	-4.080736	-0.539167
H	3.674661	-2.505140	-2.523726
H	4.792837	-3.437013	-0.498982
H	3.510531	-3.730188	1.620307
H	0.238433	-1.079540	-2.565815
H	1.220509	-3.688718	-3.925824
H	-0.082838	-2.610714	-4.528305
H	-0.302725	-3.513915	-2.996654
H	2.531578	-0.164587	-3.224655
H	1.397819	-0.484149	-4.580245
H	2.750065	-1.609717	-4.271907
H	-0.033903	-2.566399	2.098601
H	-0.161049	-5.001170	1.364398
H	-0.139336	-4.848401	3.149366
H	1.343834	-5.342115	2.268982
H	2.569615	-3.408791	3.537994
H	1.030862	-2.895024	4.283385
H	1.977081	-1.716175	3.321097
Cl	-0.526355	1.400952	-2.173949
N	0.912834	2.843335	0.208045
C	0.669536	3.623206	1.287992
C	1.697961	3.319682	-0.787434
C	1.190524	4.918964	1.404023
C	2.269944	4.599065	-0.731827
C	2.007705	5.418655	0.376677
H	0.054813	3.167133	2.078510
H	0.955957	5.518985	2.296003
H	1.865194	2.646346	-1.641025
H	2.436253	6.431453	0.441797

O	4.141836	1.129951	-1.713739
N	4.903755	0.829194	0.449169
C	4.582667	0.462258	1.817821
H	5.138632	-0.448531	2.136170
H	4.844039	1.285821	2.519674
H	3.494236	0.267505	1.906752
C	6.267173	1.221859	0.136940
H	6.310973	1.459737	-0.943368
H	6.571628	2.116525	0.725141
H	6.982981	0.400370	0.364426
C	3.951604	0.810238	-0.538520
H	2.951460	0.472079	-0.151160
H	2.913704	4.934248	-1.558430

91

**IPrCl2Py--DMFnodisp** SCF Done: -2703.99115527 A.U.

Pd	0.047873	0.724427	-0.196482
N	-0.973622	-2.060114	0.232170
C	-5.127144	-1.186862	0.310696
N	1.209782	-1.993097	0.146411
C	-4.342224	-0.959722	1.449428
C	-2.959003	-1.232516	1.453652
Cl	0.678534	1.120899	2.047482
C	-2.387950	-1.727684	0.248152
C	-3.161809	-1.986769	-0.915926
C	-4.542257	-1.701798	-0.852389
C	-2.577287	-2.606165	-2.187875
C	-2.882972	-4.121180	-2.249249
C	-3.065597	-1.907787	-3.472002
C	-2.143714	-1.069273	2.737281
C	-2.122000	-2.392766	3.537956
C	-2.626335	0.088858	3.628232
C	-0.516622	-3.370843	0.386933
C	0.848198	-3.329825	0.326808
C	2.598195	-1.576412	0.035851
C	3.155853	-1.394687	-1.259936
C	4.519377	-1.041748	-1.334943
C	5.298784	-0.891037	-0.180347
C	4.728627	-1.100824	1.081543
C	3.369631	-1.451924	1.224527
C	2.358343	-1.637880	-2.540629
C	2.550449	-3.093639	-3.025680
C	2.690138	-0.634953	-3.660342
C	2.807863	-1.740206	2.618819
C	3.197696	-3.163061	3.082761

C	3.242456	-0.697514	3.667100
C	0.087082	-1.193099	0.080531
H	-6.206258	-0.964853	0.332996
H	-4.814446	-0.566411	2.361864
H	-5.167895	-1.884828	-1.739424
H	-1.476903	-2.469317	-2.150417
H	-3.977791	-4.304766	-2.296869
H	-2.495128	-4.666891	-1.364876
H	-2.424715	-4.575492	-3.153216
H	-2.535272	-2.324480	-4.353763
H	-2.853551	-0.821731	-3.429747
H	-4.152740	-2.059762	-3.644067
H	-1.102066	-0.818703	2.448962
H	-1.703628	-3.232623	2.946243
H	-3.146830	-2.682713	3.855873
H	-1.500179	-2.283607	4.451719
H	-2.704877	1.033509	3.054559
H	-1.900146	0.254445	4.450068
H	-3.612404	-0.119166	4.097067
H	-1.207139	-4.207334	0.525441
H	1.596721	-4.124593	0.389223
H	4.978124	-0.887877	-2.323342
H	6.362127	-0.614223	-0.265334
H	5.351134	-0.989438	1.982725
H	1.284358	-1.487389	-2.308473
H	3.612976	-3.295232	-3.282567
H	1.939106	-3.284957	-3.932910
H	2.247246	-3.831342	-2.253932
H	2.571591	0.408291	-3.306242
H	1.991130	-0.777940	-4.509494
H	3.720833	-0.764648	-4.055940
H	1.702259	-1.683436	2.550481
H	2.847178	-3.946703	2.380754
H	2.759118	-3.382411	4.079215
H	4.300912	-3.264128	3.168592
H	4.332559	-0.745101	3.876870
H	2.718317	-0.885614	4.627468
H	2.981741	0.325127	3.331422
Cl	-0.580903	0.381363	-2.431944
N	-1.799938	2.596759	0.031580
C	-1.980130	3.292169	1.169450
C	-2.581141	2.878338	-1.027136
C	-2.952807	4.299264	1.301520
C	-3.579905	3.868311	-0.991986

C	-3.770242	4.592304	0.196699
H	-1.305482	3.019928	2.002228
H	-3.064409	4.839713	2.254839
H	-2.381804	2.275877	-1.932329
H	-4.544701	5.373948	0.261733
O	1.000141	2.783110	-0.865134
N	2.461017	4.522143	-0.508037
C	3.379620	5.187881	0.399512
H	4.408060	5.223621	-0.024294
H	3.055982	6.232968	0.604068
H	3.415845	4.637768	1.360410
C	2.272538	5.093251	-1.834340
H	1.550982	4.461309	-2.385261
H	1.876908	6.130414	-1.764414
H	3.235176	5.123918	-2.390356
C	1.794163	3.394541	-0.133332
H	2.010445	3.048489	0.908962
H	-4.195391	4.063104	-1.884320
100			
<b>IPrCl2Py1</b> SCF Done: -3543.33334928 A.U.			
Pd	1.172681	0.726556	-0.257906
N	2.125552	-2.057431	0.412021
C	-1.715958	-3.860316	0.538375
N	3.801541	-0.673849	0.219989
C	-1.220724	-3.190329	1.665236
C	0.051125	-2.579849	1.656094
Cl	1.288259	1.471679	1.962938
C	0.800003	-2.653976	0.448344
C	0.335833	-3.349988	-0.702200
C	-0.941081	-3.945032	-0.625614
C	1.184295	-3.530314	-1.963614
C	1.897480	-4.902845	-1.945900
C	0.378224	-3.363907	-3.266005
C	0.605354	-1.940086	2.930021
C	1.355009	-2.993604	3.779381
C	-0.467726	-1.230710	3.776036
C	3.288540	-2.791084	0.653738
C	4.339240	-1.924900	0.528587
C	4.629021	0.503485	0.012599
C	5.009828	0.841980	-1.315982
C	5.831584	1.975900	-1.483368
C	6.270678	2.726273	-0.384321
C	5.906551	2.348453	0.914325
C	5.082256	1.228041	1.149605

C	4.627926	-0.015680	-2.523903
C	5.713574	-1.085499	-2.787278
C	4.357667	0.806996	-3.796824
C	4.769419	0.804511	2.586768
C	5.940852	-0.014268	3.178890
C	4.428526	1.993740	3.505538
C	2.430167	-0.743690	0.143091
H	-2.712946	-4.328412	0.571107
H	-1.831618	-3.140329	2.578708
H	-1.333479	-4.486208	-1.500062
H	1.955502	-2.732516	-1.964587
H	1.159054	-5.733002	-1.950987
H	2.537563	-5.034187	-1.049979
H	2.543350	-5.018421	-2.841820
H	1.062642	-3.403011	-4.138980
H	-0.138686	-2.384908	-3.288202
H	-0.370175	-4.173101	-3.404349
H	1.330251	-1.156277	2.628278
H	2.188096	-3.467229	3.220505
H	0.667957	-3.802719	4.108340
H	1.785538	-2.523216	4.688544
H	-1.051651	-0.507955	3.173180
H	0.018073	-0.663240	4.595905
H	-1.174948	-1.946058	4.248311
H	3.257344	-3.857642	0.893081
H	5.417338	-2.079957	0.625669
H	6.137121	2.271302	-2.498222
H	6.910629	3.609464	-0.541351
H	6.268333	2.936088	1.771750
H	3.677285	-0.535078	-2.283967
H	6.688270	-0.612561	-3.034625
H	5.423001	-1.732894	-3.641549
H	5.873513	-1.742010	-1.907556
H	3.597288	1.591981	-3.615141
H	3.965217	0.143864	-4.594742
H	5.278324	1.286605	-4.193277
H	3.868803	0.157227	2.555992
H	6.173649	-0.916078	2.576543
H	5.698512	-0.351175	4.208955
H	6.866918	0.597499	3.232032
H	5.304349	2.655549	3.675987
H	4.105247	1.620592	4.499579
H	3.598313	2.593115	3.083609
Cl	1.025815	0.053698	-2.517368

N	-0.126751	2.355203	-0.675789
C	0.423648	3.589805	-0.631222
C	-1.438990	2.215587	-0.991808
C	-0.306044	4.748327	-0.923432
C	-2.230481	3.337127	-1.295729
C	-1.660682	4.617225	-1.265701
H	1.484413	3.630919	-0.341874
H	0.187278	5.730119	-0.876324
H	-3.289749	3.186567	-1.547715
H	-2.270599	5.503657	-1.500963
C	-1.983875	0.796647	-1.002905
H	-1.378300	0.222833	-1.740284
H	-1.779589	0.332236	-0.017676
N	-3.384884	0.673295	-1.362054
H	-3.611404	0.423975	-2.337886
C	-4.499366	0.583926	-0.589435
C	-5.693611	0.149702	-1.430242
C	-4.682788	0.841918	0.764298
C	-7.009272	-0.023055	-0.771598
C	-5.975724	0.676082	1.452771
C	-7.143915	0.219734	0.616330
Cl	-3.396367	1.436340	1.793202
O	-6.121201	0.902095	2.657364
O	-5.522321	-0.046352	-2.638093
C	-8.395206	0.043678	1.232244
C	-9.502789	-0.370283	0.472718
C	-8.123112	-0.436840	-1.531806
C	-9.368234	-0.610429	-0.908942
H	-8.469202	0.242000	2.312543
H	-10.480971	-0.506797	0.960946
H	-10.238761	-0.934966	-1.500474
H	-7.984776	-0.617586	-2.608748
100			
<b>IPrCl2Py1isomer</b> SCF Done: -3543.33077971 A.U.			
Pd	-1.145998	-0.613218	-0.490608
N	-2.123559	1.785195	1.040146
C	1.676199	3.652523	1.343802
N	-3.773597	0.435901	0.572808
C	1.341711	2.602740	2.210369
C	0.086230	1.963205	2.138820
Cl	-1.205996	-2.079189	1.339159
C	-0.816450	2.412956	1.134876
C	-0.515060	3.490769	0.257314
C	0.753278	4.094753	0.387519



C	-1.517767	4.046654	-0.756856
C	-2.208344	5.313809	-0.199592
C	-0.885679	4.340709	-2.131216
C	-0.295852	0.896234	3.165734
C	-0.955039	1.555512	4.400283
C	0.882969	0.002944	3.591733
C	-3.278676	2.353579	1.580018
C	-4.313798	1.511387	1.281294
C	-4.590415	-0.662481	0.082555
C	-5.030507	-0.632589	-1.270136
C	-5.855669	-1.690838	-1.704692
C	-6.239774	-2.720428	-0.835358
C	-5.810312	-2.709587	0.497566
C	-4.978846	-1.683543	0.993676
C	-4.708342	0.524439	-2.217102
C	-5.821700	1.596202	-2.153268
C	-4.465153	0.073908	-3.669155
C	-4.584575	-1.679567	2.472801
C	-5.730241	-1.113240	3.344116
C	-4.161172	-3.070744	2.983728
C	-2.417074	0.595318	0.415768
H	2.662995	4.136730	1.421054
H	2.067889	2.275200	2.969350
H	1.021098	4.927324	-0.280778
H	-2.293339	3.270031	-0.920672
H	-1.470190	6.126690	-0.030394
H	-2.718720	5.125857	0.767036
H	-2.968897	5.691222	-0.915401
H	-1.673162	4.645089	-2.851900
H	-0.386915	3.437782	-2.534256
H	-0.149388	5.171323	-2.084388
H	-1.038670	0.219266	2.695839
H	-1.857807	2.140765	4.129049
H	-0.248165	2.245459	4.909514
H	-1.263478	0.781171	5.134067
H	1.391445	-0.447689	2.716294
H	0.508802	-0.830464	4.220513
H	1.636174	0.555830	4.193512
H	-3.253347	3.300583	2.126134
H	-5.383130	1.576604	1.500485
H	-6.209051	-1.701614	-2.746718
H	-6.885068	-3.536133	-1.199247
H	-6.123052	-3.518928	1.174604
H	-3.760126	0.990595	-1.880075

H	-6.797715	1.179549	-2.483012
H	-5.576138	2.452873	-2.815976
H	-5.957593	1.992940	-1.125972
H	-3.688923	-0.715267	-3.719824
H	-4.103808	0.932490	-4.271082
H	-5.389285	-0.304007	-4.156919
H	-3.699584	-1.019073	2.580637
H	-6.022534	-0.086182	3.044595
H	-5.426929	-1.078952	4.411876
H	-6.637252	-1.750646	3.270475
H	-5.011988	-3.784734	3.009728
H	-3.773932	-2.989635	4.020810
H	-3.354990	-3.492392	2.352221
Cl	-1.097111	0.786331	-2.395497
N	0.197472	-1.951480	-1.448085
C	-0.301566	-3.159548	-1.795985
C	1.491778	-1.652416	-1.726400
C	0.462873	-4.124855	-2.461798
C	2.315241	-2.576350	-2.394115
C	1.798688	-3.823961	-2.768974
H	-1.349459	-3.343037	-1.515299
H	0.010740	-5.091756	-2.726629
H	3.357578	-2.301840	-2.610154
H	2.435176	-4.555489	-3.291402
C	1.979889	-0.279279	-1.292493
H	1.321674	0.472116	-1.783513
H	1.813415	-0.179028	-0.202573
N	3.358784	0.024516	-1.646711
H	3.497447	0.555817	-2.514197
C	4.508982	-0.127929	-0.931794
C	4.502306	-0.917828	0.357139
C	5.719629	0.388920	-1.393859
C	5.777611	-1.000959	1.127365
C	7.000964	0.302364	-0.686863
C	6.972583	-0.427014	0.629853
Cl	5.741918	1.252685	-2.920785
O	8.046027	0.795830	-1.122406
O	3.475557	-1.479446	0.745440
C	8.161619	-0.539547	1.371695
C	8.162252	-1.215165	2.603568
C	5.784700	-1.682808	2.361973
C	6.974067	-1.786615	3.099344
H	9.073002	-0.084784	0.953805
H	9.095986	-1.298975	3.182322

H	6.977434	-2.316875	4.064719
H	4.842167	-2.124622	2.719904
100			
<b>IPrCl2Py2</b> SCF Done: -3543.32925988 A.U.			
Pd	-1.220205	-0.832351	-0.087620
N	-2.066873	2.027915	0.195818
C	1.894945	3.458965	-0.343468
N	-3.797668	0.707265	0.359580
C	1.481109	2.996688	0.913336
C	0.166537	2.536129	1.132845
Cl	-1.309514	-1.320343	2.211494
C	-0.717226	2.539401	0.017989
C	-0.343496	3.048073	-1.256223
C	0.983217	3.502087	-1.405520
C	-1.323611	3.168727	-2.425641
C	-1.908873	4.599137	-2.497374
C	-0.700865	2.779982	-3.780381
C	-0.287703	2.129261	2.535927
C	-0.875270	3.349802	3.282896
C	0.819612	1.465463	3.373707
C	-3.179594	2.841899	0.409521
C	-4.265459	2.015529	0.506000
C	-4.684084	-0.444668	0.399296
C	-5.153154	-0.985957	-0.829912
C	-6.051047	-2.071137	-0.757321
C	-6.478883	-2.582370	0.475192
C	-6.016597	-2.014270	1.668918
C	-5.110548	-0.932974	1.664825
C	-4.777350	-0.389220	-2.186928
C	-5.805231	0.688177	-2.605547
C	-4.614822	-1.446561	-3.293845
C	-4.670912	-0.306241	2.989838
C	-5.748692	0.665901	3.522832
C	-4.318132	-1.357587	4.059976
C	-2.437176	0.703925	0.164786
H	2.938387	3.772719	-0.498913
H	2.199754	2.986766	1.746337
H	1.313770	3.880310	-2.384611
H	-2.155976	2.458485	-2.240598
H	-1.107405	5.343821	-2.691186
H	-2.415218	4.897549	-1.556772
H	-2.650496	4.677797	-3.320444
H	-1.483976	2.769199	-4.567188
H	-0.252706	1.768695	-3.729171

H	0.076380	3.503970	-4.105730
H	-1.089158	1.369216	2.429473
H	-1.727230	3.802833	2.735296
H	-0.106952	4.140990	3.420170
H	-1.241542	3.052191	4.288347
H	1.271756	0.607787	2.837319
H	0.390986	1.076986	4.320211
H	1.626541	2.178994	3.646816
H	-3.093887	3.929929	0.476350
H	-5.326107	2.232408	0.660748
H	-6.425741	-2.519279	-1.689775
H	-7.181838	-3.430440	0.505126
H	-6.361810	-2.420207	2.632010
H	-3.786488	0.098247	-2.082426
H	-6.818241	0.247981	-2.729149
H	-5.513701	1.147984	-3.573470
H	-5.882876	1.502960	-1.856423
H	-3.902821	-2.239577	-2.990412
H	-4.209771	-0.969319	-4.209481
H	-5.580443	-1.922305	-3.570136
H	-3.741971	0.267739	2.792699
H	-5.982140	1.473115	2.799123
H	-5.409361	1.145547	4.465188
H	-6.696818	0.128190	3.738787
H	-5.209511	-1.927818	4.398913
H	-3.893389	-0.856798	4.954938
H	-3.559637	-2.067459	3.676441
Cl	-1.170319	-0.455942	-2.407823
N	0.155978	-2.417920	-0.348864
C	-0.028834	-3.613394	0.255851
C	1.249270	-2.226672	-1.121769
C	0.869386	-4.675427	0.080076
C	2.216606	-3.227492	-1.326731
C	2.005652	-4.481002	-0.718365
H	-0.913692	-3.689369	0.906005
H	0.672298	-5.640561	0.570080
H	1.329777	-1.239848	-1.604640
H	2.725670	-5.302930	-0.870383
C	3.466059	-2.935312	-2.150673
H	3.732383	-3.833666	-2.746940
H	3.276559	-2.108215	-2.856773
N	4.625920	-2.608177	-1.322983
H	5.054283	-3.383353	-0.787864
C	5.080038	-1.427008	-0.830102

C	6.093199	-1.686584	0.283289
C	4.799103	-0.112530	-1.187890
C	6.732077	-0.535022	0.958243
C	5.398466	1.056278	-0.519889
C	6.392819	0.785455	0.578720
Cl	3.709381	0.305617	-2.495661
O	5.118930	2.218056	-0.833969
O	6.343590	-2.857921	0.585865
C	6.999498	1.871540	1.233222
C	7.671886	-0.760104	1.985850
C	8.272203	0.329613	2.633961
C	7.935168	1.644455	2.256892
H	7.912256	-1.798949	2.258624
H	9.005121	0.156052	3.437436
H	8.406922	2.499758	2.766407
H	6.717750	2.886989	0.915512
100			
<b>IPrCl2Py2isomer</b> SCF Done: -3543.32736032 A.U.			
Pd	1.238604	-0.526152	0.006537
N	3.207969	1.749501	0.231833
C	0.387413	4.795434	1.123188
N	4.216703	-0.126123	-0.245101
C	0.584347	4.390480	-0.203493
C	1.509195	3.377715	-0.532127
Cl	1.232513	-0.515982	-2.344958
C	2.219420	2.770026	0.540077
C	2.057906	3.175234	1.893667
C	1.123022	4.198683	2.154790
C	2.888326	2.599133	3.043294
C	4.063531	3.542080	3.393200
C	2.046502	2.301845	4.299624
C	1.773121	3.027724	-1.997257
C	2.852737	3.965308	-2.586728
C	0.501453	3.044180	-2.865152
C	4.570695	2.034995	0.126040
C	5.203375	0.858480	-0.165646
C	4.522161	-1.514593	-0.549956
C	4.636676	-2.438870	0.525584
C	4.964872	-3.771486	0.201171
C	5.190348	-4.164581	-1.124749
C	5.101698	-3.225002	-2.159404
C	4.768550	-1.878350	-1.902736
C	4.500227	-2.015899	1.988698
C	5.878636	-1.607920	2.559820

C	3.839019	-3.086608	2.875331
C	4.746914	-0.872575	-3.056252
C	6.181954	-0.419501	-3.413732
C	4.028724	-1.411098	-4.309284
C	2.975883	0.413802	0.001289
H	-0.341617	5.588574	1.354680
H	0.012360	4.873749	-1.009673
H	0.969189	4.530871	3.192801
H	3.306270	1.629847	2.701692
H	3.690606	4.525017	3.752816
H	4.722043	3.736569	2.522051
H	4.689965	3.102942	4.198204
H	2.670526	1.786585	5.059478
H	1.194377	1.639004	4.052925
H	1.658219	3.229303	4.772130
H	2.157679	1.988190	-2.037645
H	3.804552	3.911955	-2.018829
H	2.513730	5.023663	-2.573826
H	3.073003	3.691249	-3.640170
H	-0.290013	2.402907	-2.429034
H	0.732342	2.647058	-3.874708
H	0.094276	4.069526	-2.999642
H	4.958470	3.047945	0.264966
H	6.260595	0.626315	-0.320432
H	5.051584	-4.513347	1.009065
H	5.445273	-5.212076	-1.352745
H	5.291655	-3.541433	-3.196381
H	3.832782	-1.130652	2.026857
H	6.585694	-2.465381	2.549677
H	5.777446	-1.262770	3.610531
H	6.342894	-0.784678	1.978581
H	2.865849	-3.410907	2.456245
H	3.643712	-2.668574	3.883942
H	4.483837	-3.981729	3.009653
H	4.171935	0.013310	-2.716432
H	6.715159	0.021753	-2.547032
H	6.160227	0.343251	-4.220628
H	6.790001	-1.276455	-3.774985
H	4.586430	-2.245654	-4.785501
H	3.939593	-0.606138	-5.068473
H	3.006994	-1.756771	-4.058470
Cl	1.239554	-0.541040	2.359367
N	-0.631541	-1.542903	0.005152
C	-0.898962	-2.484623	-0.930551

C	-1.567003	-1.255217	0.937449
C	-2.117479	-3.175309	-0.952624
C	-2.817555	-1.896960	0.983539
C	-3.090766	-2.878035	0.012804
H	-0.113864	-2.644042	-1.685442
H	-2.296521	-3.935161	-1.727963
H	-1.278770	-0.494867	1.680737
H	-4.063701	-3.395933	0.007361
C	-3.805425	-1.541851	2.089848
H	-3.635721	-2.218821	2.955368
H	-3.607781	-0.510950	2.436853
N	-5.210058	-1.700604	1.726227
H	-5.669272	-2.571336	2.014991
C	-5.981893	-0.954455	0.883642
C	-5.485491	0.381112	0.379596
C	-7.247852	-1.389228	0.496748
C	-6.387803	1.164143	-0.513943
C	-8.169737	-0.649135	-0.372877
C	-7.668785	0.678685	-0.873249
Cl	-7.816081	-2.947957	1.069286
O	-9.283696	-1.076854	-0.688791
O	-4.373015	0.802419	0.704194
C	-8.493471	1.444279	-1.716181
C	-5.945898	2.411316	-1.001861
C	-6.774538	3.170054	-1.842325
C	-8.048065	2.686035	-2.199522
H	-4.945617	2.762829	-0.706067
H	-6.427391	4.143737	-2.222396
H	-8.697754	3.281882	-2.860263
H	-9.482506	1.037003	-1.976866

112

**IPrCl2Py2isomer--DMF250llqst3nodisp** SCF Done: -3791.64127281 A.U.

Pd	-1.997803	-0.641217	0.230615
N	-2.166390	2.278513	-0.333659
C	2.011030	2.916567	-0.759158
N	-4.155458	1.410068	-0.071503
C	1.441865	2.829788	0.518986
C	0.058221	2.619846	0.695549
Cl	-2.462726	-0.435017	2.521763
C	-0.733851	2.475990	-0.477094
C	-0.190824	2.584911	-1.787393
C	1.198475	2.806329	-1.895342
C	-1.049477	2.531762	-3.053545
C	-1.370395	3.958576	-3.557726

C	-0.409740	1.699859	-4.182135
C	-0.551684	2.627518	2.097466
C	-0.961765	4.064159	2.498459
C	0.365534	2.007858	3.166523
C	-3.087646	3.319596	-0.463882
C	-4.331880	2.775677	-0.305367
C	-5.270278	0.496506	0.111478
C	-5.698268	-0.285904	-0.998274
C	-6.794017	-1.149669	-0.797212
C	-7.452126	-1.217740	0.438665
C	-7.031158	-0.409974	1.501410
C	-5.933101	0.466528	1.368483
C	-5.067790	-0.151124	-2.385038
C	-5.742541	0.995152	-3.175610
C	-5.096848	-1.450370	-3.209708
C	-5.544730	1.371410	2.539540
C	-6.486081	2.595952	2.620846
C	-5.517584	0.625392	3.888084
C	-2.815041	1.088102	-0.082021
H	3.095869	3.073187	-0.868713
H	2.087686	2.930529	1.403922
H	1.652298	2.889358	-2.894939
H	-2.003138	2.030952	-2.787640
H	-0.440326	4.499260	-3.835367
H	-1.892354	4.569275	-2.793449
H	-2.019781	3.918130	-4.457809
H	-1.124527	1.594070	-5.024948
H	-0.153925	0.683701	-3.824113
H	0.504297	2.181431	-4.590746
H	-1.465257	1.997990	2.077126
H	-1.685462	4.507356	1.783616
H	-0.076944	4.735582	2.540104
H	-1.437904	4.065645	3.501810
H	0.707588	0.997822	2.865085
H	-0.190438	1.902248	4.120364
H	1.259817	2.634646	3.373351
H	-2.770153	4.348299	-0.655090
H	-5.325891	3.230056	-0.340501
H	-7.139229	-1.780124	-1.629919
H	-8.306331	-1.901219	0.571048
H	-7.560390	-0.462540	2.465148
H	-3.995656	0.100441	-2.249583
H	-6.819955	0.781253	-3.344997
H	-5.259748	1.120527	-4.167938



H	-5.673016	1.966160	-2.644269
H	-4.664422	-2.303790	-2.648967
H	-4.494078	-1.319697	-4.131510
H	-6.125591	-1.728437	-3.525851
H	-4.512301	1.731404	2.352549
H	-6.482676	3.196601	1.688113
H	-6.183161	3.265002	3.453905
H	-7.535117	2.279671	2.805928
H	-6.533513	0.316661	4.215311
H	-5.109533	1.289524	4.678493
H	-4.869214	-0.270332	3.825890
Cl	-1.554622	-0.912933	-2.074771
N	0.376234	-1.397226	0.799475
C	0.733513	-1.789136	2.037815
C	1.334145	-1.187007	-0.115958
C	2.074302	-1.997875	2.397956
C	2.712512	-1.335137	0.154243
C	3.078862	-1.761036	1.443884
H	-0.093919	-1.915521	2.757223
H	2.328815	-2.330542	3.416387
H	0.972628	-0.879849	-1.115564
H	4.141193	-1.903057	1.700503
C	3.721752	-0.976846	-0.927653
H	3.343217	-1.333872	-1.911740
H	3.818780	0.122342	-0.994387
N	5.048150	-1.537674	-0.706204
H	5.113176	-2.563780	-0.727202
C	6.238705	-0.946802	-0.410227
C	6.371408	0.558687	-0.306204
C	7.378460	-1.725918	-0.186531
C	7.718343	1.119361	0.011341
C	8.716931	-1.217090	0.119490
C	8.839706	0.279284	0.212015
Cl	7.233167	-3.473002	-0.272177
O	9.694105	-1.951466	0.298567
O	5.400870	1.303648	-0.472781
C	10.092038	0.844765	0.508039
C	10.230352	2.239636	0.605430
C	7.862754	2.518963	0.112160
C	9.115424	3.077349	0.408009
H	10.941726	0.161075	0.658397
H	11.213842	2.678342	0.837870
H	9.225047	4.170497	0.486054
H	6.971913	3.145872	-0.044884

O	-2.095862	-3.036810	0.488983
N	-2.806911	-5.049710	-0.370335
C	-3.269148	-5.792037	-1.530377
H	-2.529869	-6.563391	-1.844505
H	-4.229644	-6.309700	-1.313237
H	-3.431201	-5.093062	-2.374371
C	-2.651685	-5.765998	0.887713
H	-2.292102	-5.050885	1.651087
H	-3.622232	-6.197540	1.216926
H	-1.917935	-6.595473	0.783128
C	-2.503557	-3.723203	-0.458719
H	-2.641943	-3.286644	-1.480290
100			
<b>IPrCl2Py3</b> SCF Done: -3543.32987828 A.U.			
Pd	1.355399	-0.007479	-0.446746
N	3.898731	-0.928545	0.874064
C	2.906812	-5.055431	1.006402
N	3.931533	1.229239	0.546287
C	2.418526	-4.187105	1.991393
C	2.724833	-2.810332	1.973538
Cl	0.409761	0.751013	1.569676
C	3.533048	-2.335987	0.903780
C	4.061610	-3.196516	-0.098187
C	3.724324	-4.563913	-0.019212
C	5.007016	-2.711247	-1.199807
C	6.481543	-2.968143	-0.809343
C	4.702061	-3.339044	-2.573686
C	2.257829	-1.906797	3.115167
C	3.270496	-1.952715	4.283440
C	0.837365	-2.235230	3.609771
C	5.113040	-0.458744	1.377968
C	5.136785	0.891970	1.166281
C	3.609521	2.595379	0.165534
C	3.869229	3.008622	-1.170878
C	3.586642	4.351041	-1.498428
C	3.088609	5.245627	-0.542045
C	2.868065	4.816488	0.772610
C	3.123543	3.484837	1.163097
C	4.501274	2.082341	-2.210801
C	6.042531	2.209172	-2.181726
C	3.964009	2.309606	-3.635570
C	2.930342	3.073271	2.624365
C	4.146611	3.501468	3.478329
C	1.626482	3.622541	3.234481

C	3.156270	0.108616	0.359843
H	2.651834	-6.126839	1.041615
H	1.786897	-4.584485	2.800015
H	4.109266	-5.255756	-0.783699
H	4.855334	-1.617531	-1.310001
H	6.675827	-4.055218	-0.686513
H	6.759010	-2.472087	0.142768
H	7.165393	-2.588905	-1.597955
H	5.334049	-2.864583	-3.353168
H	3.642406	-3.180262	-2.853394
H	4.923340	-4.427602	-2.594852
H	2.215095	-0.866725	2.731991
H	4.289879	-1.653390	3.963018
H	3.341294	-2.976108	4.711074
H	2.957186	-1.264958	5.097153
H	0.109899	-2.227248	2.774041
H	0.509654	-1.469036	4.341804
H	0.783577	-3.221139	4.119622
H	5.842148	-1.130176	1.839897
H	5.895943	1.644834	1.395909
H	3.767600	4.702132	-2.525421
H	2.875524	6.289507	-0.823415
H	2.485065	5.529993	1.518170
H	4.232501	1.039267	-1.945473
H	6.364118	3.241497	-2.438607
H	6.503271	1.516382	-2.917365
H	6.462325	1.966130	-1.183922
H	2.857743	2.253724	-3.662198
H	4.352574	1.520990	-4.311866
H	4.281121	3.288284	-4.055900
H	2.851411	1.966881	2.650438
H	5.097558	3.069896	3.104895
H	4.018712	3.173107	4.531468
H	4.261561	4.606639	3.479620
H	1.646861	4.728146	3.341480
H	1.478165	3.200430	4.250303
H	0.752460	3.335434	2.618238
Cl	2.297212	-0.746061	-2.471595
N	-0.589916	-0.161939	-1.296600
C	-1.564302	0.717738	-0.969316
C	-0.884433	-1.161884	-2.162438
C	-2.858553	0.633932	-1.499541
C	-2.159227	-1.318145	-2.716263
C	-3.181544	-0.405371	-2.389558

H	-1.282918	1.486696	-0.233134
H	-3.613371	1.376431	-1.200488
H	-0.048198	-1.830927	-2.418613
H	-2.346341	-2.161423	-3.399820
C	-4.563926	-0.547218	-3.017922
H	-4.507393	-0.190130	-4.070141
H	-4.831803	-1.620371	-3.065922
N	-5.622895	0.205249	-2.373477
H	-5.838739	1.155365	-2.715573
C	-6.362568	-0.065674	-1.264531
C	-7.265765	1.119027	-0.940515
C	-6.404369	-1.189584	-0.450451
C	-8.173476	1.032331	0.224995
C	-7.292945	-1.308136	0.722790
C	-8.186073	-0.133645	1.027577
Cl	-5.400319	-2.599509	-0.722610
O	-7.319906	-2.316448	1.432230
O	-7.201694	2.118128	-1.665622
C	-9.047862	-0.202794	2.135771
C	-9.019562	2.117692	0.535196
C	-9.876981	2.039928	1.642834
C	-9.889908	0.879926	2.442058
H	-8.984737	3.010809	-0.107136
H	-10.538148	2.886119	1.887126
H	-10.562646	0.820324	3.312443
H	-9.034676	-1.121495	2.742025
100			
<b>IPrCl2Py3del2</b> SCF Done: -3543.33018407 A.U.			
Pd	-1.429402	-0.388207	-0.051678
N	-3.470017	1.820895	0.138140
C	-0.688104	5.027620	0.052971
N	-4.433896	-0.137261	0.119798
C	-0.911610	4.327119	1.245875
C	-1.828275	3.256979	1.307864
Cl	-1.548560	-0.958171	2.226635
C	-2.501247	2.904574	0.105411
C	-2.312850	3.611553	-1.114183
C	-1.389066	4.677598	-1.107794
C	-3.101241	3.303407	-2.389386
C	-4.282705	4.288443	-2.552842
C	-2.220249	3.308851	-3.653898
C	-2.128521	2.578990	2.645115
C	-3.256129	3.333906	3.387379
C	-0.888059	2.429317	3.544238

C	-4.845563	2.043147	0.224201
C	-5.449875	0.816535	0.206169
C	-4.701497	-1.565600	0.077696
C	-4.728808	-2.215746	-1.187245
C	-5.019307	-3.595953	-1.198457
C	-5.290500	-4.293626	-0.014136
C	-5.287287	-3.619514	1.213514
C	-4.996840	-2.241365	1.293956
C	-4.540938	-1.462804	-2.505057
C	-5.911115	-1.006679	-3.059359
C	-3.765493	-2.269886	-3.562313
C	-5.070955	-1.530543	2.647347
C	-6.537460	-1.199164	3.010461
C	-4.404589	-2.329576	3.784100
C	-3.202796	0.473629	0.073776
H	0.034138	5.859475	0.030069
H	-0.367385	4.619693	2.156432
H	-1.214213	5.240102	-2.037630
H	-3.511846	2.277843	-2.287426
H	-3.916808	5.331362	-2.666115
H	-4.970887	4.273455	-1.683070
H	-4.877097	4.038879	-3.457257
H	-2.809133	2.958837	-4.527295
H	-1.354761	2.629026	-3.531385
H	-1.848712	4.326804	-3.898834
H	-2.481779	1.549030	2.434311
H	-4.186390	3.389468	2.784989
H	-2.949501	4.374966	3.626850
H	-3.503264	2.823403	4.342222
H	-0.058375	1.931172	3.004406
H	-1.136130	1.801224	4.423962
H	-0.524295	3.406556	3.928882
H	-5.261730	3.051974	0.291371
H	-6.504858	0.531511	0.244520
H	-5.039411	-4.131559	-2.159420
H	-5.514196	-5.372021	-0.049423
H	-5.512310	-4.174526	2.137082
H	-3.929993	-0.559579	-2.301141
H	-6.560150	-1.879510	-3.287282
H	-5.778032	-0.426956	-3.997178
H	-6.458088	-0.362798	-2.339904
H	-2.795322	-2.625354	-3.162230
H	-3.547055	-1.626258	-4.438763
H	-4.341490	-3.145367	-3.931933

H	-4.508172	-0.578871	2.555471
H	-7.033060	-0.575978	2.238406
H	-6.585831	-0.646168	3.972348
H	-7.138491	-2.126877	3.122779
H	-4.958995	-3.262503	4.021985
H	-4.382825	-1.719871	4.711476
H	-3.360041	-2.587575	3.521815
Cl	-1.324888	0.143356	-2.340733
N	0.491109	-1.294402	-0.178159
C	0.779495	-2.408773	0.532554
C	1.452544	-0.759180	-0.969736
C	2.036211	-3.026124	0.472150
C	2.735743	-1.309939	-1.064219
C	3.049935	-2.474038	-0.333466
H	-0.026622	-2.781307	1.183647
H	2.213423	-3.939294	1.062453
H	1.147363	0.120220	-1.557946
H	3.482971	-0.838400	-1.721347
C	4.442799	-3.091683	-0.391693
H	4.403168	-4.127295	0.007445
H	4.794627	-3.146036	-1.437499
N	5.416204	-2.347759	0.400056
H	5.338157	-2.407867	1.429880
C	6.342922	-1.414932	0.067882
C	6.986323	-0.855907	1.338084
C	6.771833	-0.932820	-1.163809
C	8.050901	0.164554	1.216346
C	7.821472	0.090442	-1.320842
C	8.453394	0.621741	-0.061132
Cl	6.102935	-1.481042	-2.693633
O	8.181025	0.506703	-2.425455
O	6.590457	-1.279140	2.428364
C	9.463506	1.594040	-0.163044
C	8.658831	0.681148	2.380075
C	9.666154	1.651016	2.269262
C	10.067478	2.106327	0.997778
H	8.322843	0.305854	3.358676
H	10.142002	2.055884	3.176180
H	10.858480	2.868371	0.912166
H	9.754839	1.930619	-1.169789
100			
<b>IPrCl2Py3isomer</b> SCF Done: -3543.32818264 A.U.			
Pd	1.289544	0.121059	-0.433513
N	3.830271	-1.238177	0.470590

C	2.647677	-5.222806	-0.399762
N	3.943452	0.922914	0.751646
C	2.282023	-4.634040	0.817934
C	2.653737	-3.310972	1.134617
Cl	0.395889	0.193907	1.740295
C	3.398044	-2.591386	0.158435
C	3.806846	-3.170901	-1.074102
C	3.407377	-4.500019	-1.327983
C	4.702572	-2.444242	-2.079651
C	6.179099	-2.867417	-1.897480
C	4.259401	-2.653309	-3.540320
C	2.323755	-2.730449	2.510763
C	3.430881	-3.093418	3.528377
C	0.942234	-3.158421	3.038650
C	5.089218	-0.962487	1.008189
C	5.161929	0.392094	1.179776
C	3.654090	2.347348	0.801756
C	3.918025	3.139035	-0.350217
C	3.662143	4.522951	-0.256060
C	3.184095	5.097035	0.929152
C	2.961380	4.296132	2.056541
C	3.193701	2.905059	2.026700
C	4.526682	2.558230	-1.627034
C	6.068202	2.681336	-1.593327
C	3.959365	3.187734	-2.912704
C	3.010401	2.077018	3.300574
C	4.262598	2.181613	4.202700
C	1.745174	2.460088	4.091657
C	3.111071	-0.077495	0.305738
H	2.343145	-6.257775	-0.624018
H	1.696668	-5.214444	1.546751
H	3.700493	-4.975076	-2.276547
H	4.619179	-1.356842	-1.876377
H	6.308779	-3.952421	-2.098801
H	6.549135	-2.674592	-0.869854
H	6.834086	-2.311680	-2.601403
H	4.867291	-2.013950	-4.213827
H	3.197549	-2.368729	-3.673127
H	4.398928	-3.703494	-3.875017
H	2.287619	-1.626067	2.412394
H	4.428467	-2.727306	3.209853
H	3.505129	-4.194194	3.661984
H	3.209105	-2.645143	4.519989
H	0.142582	-2.928999	2.307063

H	0.709453	-2.602720	3.970152
H	0.901307	-4.241241	3.285271
H	5.810955	-1.756895	1.217522
H	5.962997	1.028754	1.565526
H	3.846702	5.162369	-1.132356
H	2.989896	6.180656	0.976705
H	2.597631	4.758540	2.986648
H	4.262784	1.481734	-1.668834
H	6.383265	3.746491	-1.556265
H	6.514971	2.226424	-2.502652
H	6.508697	2.171935	-0.711616
H	2.853516	3.125644	-2.935353
H	4.341183	2.638945	-3.797955
H	4.259902	4.251032	-3.031021
H	2.883156	1.018161	2.994467
H	5.184651	1.847808	3.684609
H	4.141069	1.554613	5.111181
H	4.427575	3.229437	4.533575
H	1.812937	3.481041	4.524454
H	1.604692	1.756949	4.938795
H	0.845276	2.398134	3.449251
Cl	2.168338	0.036495	-2.614428
N	-0.668250	0.354810	-1.237914
C	-1.576018	1.149312	-0.624614
C	-1.032269	-0.283295	-2.376298
C	-2.866490	1.344777	-1.133818
C	-2.310140	-0.152276	-2.930147
C	-3.259663	0.683648	-2.311367
H	-1.244246	1.612527	0.317410
H	-3.563066	2.006009	-0.596319
H	-0.249677	-0.894544	-2.851264
H	-2.558150	-0.712465	-3.845283
C	-4.633337	0.882507	-2.940418
H	-4.538606	1.639187	-3.750359
H	-4.950336	-0.064969	-3.415412
N	-5.667721	1.376352	-2.041967
H	-5.869698	2.381789	-2.067799
C	-6.363345	0.722030	-1.066317
C	-6.192875	-0.767772	-0.880043
C	-7.249167	1.406016	-0.236843
C	-6.991298	-1.428555	0.192139
C	-8.063122	0.794063	0.820506
C	-7.887102	-0.689183	1.002560
Cl	-7.433901	3.138167	-0.443276



O	-8.842586	1.440461	1.525926
O	-5.418819	-1.406854	-1.597196
C	-8.626678	-1.345373	2.001918
C	-6.843717	-2.816739	0.391989
C	-7.584686	-3.464870	1.391654
C	-8.476560	-2.728823	2.195846
H	-6.138153	-3.363789	-0.251735
H	-7.467266	-4.548866	1.546948
H	-9.057810	-3.238205	2.980920
H	-9.312888	-0.741002	2.614958
100			
<b>IPrCl2Py3del2Isomer</b> SCF Done: -3543.32818252 A.U.			
Pd	-1.289548	-0.121208	-0.433834
N	-3.829987	1.238202	0.470836
C	-2.647439	5.222819	-0.399652
N	-3.943215	-0.922881	0.751932
C	-2.281611	4.634026	0.817976
C	-2.653276	3.310948	1.134682
Cl	-0.395537	-0.194130	1.739808
C	-3.397753	2.591390	0.158614
C	-3.806748	3.170945	-1.073846
C	-3.407289	4.500054	-1.327769
C	-4.702735	2.444349	-2.079213
C	-6.179201	2.867572	-1.896661
C	-4.259906	2.653439	-3.539981
C	-2.323058	2.730420	2.510773
C	-3.429827	3.093771	3.528640
C	-0.941257	3.158034	3.038217
C	-5.088808	0.962585	1.008743
C	-5.161572	-0.391997	1.180324
C	-3.653881	-2.347324	0.801994
C	-3.918049	-3.139017	-0.349916
C	-3.662128	-4.522933	-0.255810
C	-3.183816	-5.097005	0.929296
C	-2.960896	-4.296097	2.056645
C	-3.193255	-2.905032	2.026856
C	-4.526981	-2.558236	-1.626607
C	-6.068491	-2.681403	-1.592557
C	-3.959908	-3.187720	-2.912392
C	-3.009800	-2.077007	3.300722
C	-4.261861	-2.181683	4.203023
C	-1.744442	-2.460031	4.091621
C	-3.110886	0.077473	0.305822
H	-2.342936	6.257792	-0.623934

H	-1.696146	5.214409	1.546723
H	-3.700554	4.975129	-2.276278
H	-4.619332	1.356939	-1.876004
H	-6.308896	3.952587	-2.097903
H	-6.548993	2.674710	-0.868953
H	-6.834381	2.311882	-2.600443
H	-4.867975	2.014106	-4.213353
H	-3.198095	2.368814	-3.673038
H	-4.399481	3.703630	-3.874634
H	-2.287278	1.626021	2.412486
H	-4.427594	2.727965	3.210324
H	-3.503717	4.194573	3.662226
H	-3.207975	2.645461	4.520219
H	-0.141899	2.928152	2.306456
H	-0.708423	2.602450	3.969779
H	-0.899895	4.240886	3.284610
H	-5.810445	1.757026	1.218303
H	-5.962585	-1.028613	1.566258
H	-3.846852	-5.162341	-1.132080
H	-2.989567	-6.180619	0.976809
H	-2.596964	-4.758504	2.986680
H	-4.263143	-1.481728	-1.668460
H	-6.383508	-3.746568	-1.555411
H	-6.515481	-2.226515	-2.501786
H	-6.508800	-2.172009	-0.710749
H	-2.854068	-3.125549	-2.935278
H	-4.341955	-2.638968	-3.797569
H	-4.260403	-4.251039	-3.030632
H	-2.882652	-1.018137	2.994622
H	-5.184008	-1.847917	3.685074
H	-4.140237	-1.554688	5.111496
H	-4.426737	-3.229520	4.533908
H	-1.812134	-3.480959	4.524484
H	-1.603825	-1.756846	4.938699
H	-0.844654	-2.398106	3.449060
Cl	-2.168877	-0.036431	-2.614523
N	0.668133	-0.354962	-1.238604
C	1.576218	-1.149070	-0.625271
C	1.031835	0.283046	-2.377154
C	2.866728	-1.344152	-1.134531
C	2.309707	0.152381	-2.931077
C	3.259601	-0.683054	-2.312195
H	1.244681	-1.612271	0.316844
H	3.563562	-2.005055	-0.596963

H	0.248975	0.893921	-2.852165
H	2.557424	0.712483	-3.846347
C	4.633396	-0.881303	-2.941191
H	4.538933	-1.637439	-3.751669
H	4.950316	0.066554	-3.415464
N	5.667738	-1.375500	-2.042897
H	5.869357	-2.381011	-2.068773
C	6.363147	-0.721592	-1.066810
C	6.192946	0.768198	-0.880144
C	7.248510	-1.406016	-0.237203
C	6.991198	1.428483	0.192478
C	8.062243	-0.794567	0.820611
C	7.886536	0.688671	1.003010
Cl	7.432834	-3.138170	-0.443991
O	8.841288	-1.441363	1.526127
O	5.419242	1.407683	-1.597315
C	8.625917	1.344401	2.002817
C	6.843891	2.816649	0.392659
C	7.584669	3.464323	1.392762
C	8.476073	2.727835	2.197072
H	6.138680	3.364049	-0.251156
H	7.467465	4.548305	1.548309
H	9.057165	3.236856	2.982496
H	9.311750	0.739686	2.615939
112			
<b>IPrCl2Py3isomer--DMFnodisp</b> SCF Done: -3791.64296324 A.U.			
Pd	1.952079	0.466988	-0.163962
N	3.405538	-2.110671	0.259044
C	0.418873	-4.728219	-1.236737
N	4.601550	-0.396722	0.897915
C	0.306544	-4.206597	0.059328
C	1.277571	-3.329124	0.584329
Cl	1.377656	0.747401	2.093880
C	2.363117	-2.975853	-0.264702
C	2.512909	-3.501313	-1.577502
C	1.513596	-4.383944	-2.039249
C	3.721653	-3.197598	-2.466246
C	4.743669	-4.357529	-2.416985
C	3.330406	-2.892503	-3.925566
C	1.186539	-2.852369	2.034365
C	1.941723	-3.823422	2.972282
C	-0.258330	-2.646009	2.522389
C	4.615683	-2.613203	0.742227
C	5.366090	-1.540708	1.135853

C	5.096595	0.939340	1.183525
C	5.650318	1.702362	0.117942
C	6.161270	2.978319	0.432406
C	6.140864	3.468741	1.745056
C	5.614469	2.683598	2.777756
C	5.082096	1.401158	2.527990
C	5.774770	1.156105	-1.305107
C	7.135308	0.445147	-1.494025
C	5.567881	2.229813	-2.388659
C	4.575111	0.555448	3.698532
C	5.756665	-0.095148	4.455421
C	3.686855	1.355231	4.671533
C	3.381580	-0.735332	0.350647
H	-0.352165	-5.414862	-1.622010
H	-0.551917	-4.492702	0.685140
H	1.597733	-4.806164	-3.052493
H	4.208084	-2.284169	-2.065924
H	4.298343	-5.295463	-2.812650
H	5.095140	-4.568028	-1.386392
H	5.634949	-4.119383	-3.035373
H	4.226235	-2.572612	-4.497989
H	2.587593	-2.072394	-3.968705
H	2.916290	-3.784708	-4.442125
H	1.674026	-1.857308	2.098452
H	3.010988	-3.925584	2.694612
H	1.489036	-4.838229	2.946959
H	1.901572	-3.458941	4.020579
H	-0.829008	-1.995878	1.829764
H	-0.249025	-2.150006	3.514333
H	-0.809164	-3.604398	2.638772
H	4.824943	-3.686259	0.761563
H	6.372507	-1.482417	1.559666
H	6.590890	3.596901	-0.369961
H	6.544799	4.470018	1.965493
H	5.609900	3.073732	3.807090
H	4.968864	0.409328	-1.457288
H	7.979821	1.153524	-1.352149
H	7.214517	0.020991	-2.517470
H	7.272539	-0.387810	-0.774054
H	4.613013	2.771262	-2.236068
H	5.524948	1.750725	-3.388099
H	6.394717	2.971931	-2.412819
H	3.940717	-0.250872	3.277126
H	6.383909	-0.728798	3.795321

H	5.384667	-0.735708	5.282879
H	6.419636	0.678594	4.898507
H	4.260948	2.131878	5.220835
H	3.252017	0.673890	5.432613
H	2.851187	1.838536	4.128723
Cl	2.473847	0.218038	-2.456579
N	-0.574206	0.175357	-0.733564
C	-1.518807	0.481241	0.174609
C	-0.965125	-0.344170	-1.911152
C	-2.890342	0.282120	-0.055344
C	-2.312938	-0.579819	-2.229418
C	-3.311205	-0.266656	-1.284566
H	-1.141314	0.892235	1.128620
H	-3.622993	0.553332	0.721183
H	-0.150616	-0.564773	-2.624903
H	-2.580055	-1.002298	-3.212115
C	-4.771931	-0.556071	-1.576396
H	-4.920626	-0.630051	-2.679409
H	-5.069388	-1.539070	-1.162921
N	-5.649973	0.463205	-1.011330
H	-5.330321	1.434792	-1.118975
C	-6.887868	0.374054	-0.451916
C	-7.561234	-0.966568	-0.251384
C	-7.565756	1.525281	-0.041695
C	-8.907508	-0.980061	0.393318
C	-8.889745	1.557277	0.584104
C	-9.546492	0.219302	0.789663
Cl	-6.793011	3.084020	-0.265758
O	-9.447825	2.603803	0.929129
O	-7.018210	-2.016349	-0.608403
C	-10.817257	0.168530	1.388376
C	-11.450345	-1.068737	1.594436
C	-9.548086	-2.219479	0.601731
C	-10.815695	-2.263203	1.201816
H	-11.284636	1.120708	1.683169
H	-12.445977	-1.103679	2.064806
H	-11.313121	-3.232285	1.364739
H	-9.027998	-3.135540	0.282672
O	1.066935	2.639351	-0.574918
N	0.842391	4.511783	-1.891000
C	1.011530	5.120493	-3.199393
H	0.038294	5.474243	-3.607269
H	1.700409	5.993208	-3.151080
H	1.436544	4.376954	-3.902163

C	0.295657	5.331551	-0.818410
H	0.255591	4.718717	0.101565
H	0.936970	6.222195	-0.639585
H	-0.728143	5.684249	-1.072564
C	1.190675	3.213225	-1.667104
H	1.611694	2.682891	-2.558984
112			
<b>IPrCl2Py3isomer--DMFisomernodisp</b> SCF Done: -3791.63861467 A.U.			
Pd	-1.880840	-0.389305	-0.262160
N	-3.424494	2.058761	0.453405
C	-0.279972	4.866010	-0.038933
N	-4.672162	0.268464	0.575602
C	-0.371481	4.117523	1.142347
C	-1.400532	3.172872	1.334211
Cl	-1.557186	-1.121610	1.956424
C	-2.328921	2.996131	0.271185
C	-2.278087	3.758939	-0.927858
C	-1.228913	4.693691	-1.054366
C	-3.337648	3.659337	-2.028231
C	-4.365000	4.808361	-1.898764
C	-2.733842	3.637631	-3.445908
C	-1.540351	2.444372	2.671564
C	-2.423570	3.264203	3.641723
C	-0.190541	2.104519	3.328005
C	-4.697536	2.473359	0.849005
C	-5.479925	1.355384	0.919635
C	-5.194440	-1.086497	0.537047
C	-5.637920	-1.610371	-0.709493
C	-6.214252	-2.898103	-0.702250
C	-6.359881	-3.626157	0.487027
C	-5.931515	-3.076312	1.702038
C	-5.343313	-1.794886	1.761907
C	-5.588371	-0.801538	-2.006014
C	-6.918161	-0.039762	-2.214626
C	-5.247810	-1.653005	-3.242507
C	-4.959597	-1.203244	3.120044
C	-6.207007	-0.649233	3.847463
C	-4.212448	-2.205443	4.021327
C	-3.393236	0.691552	0.280459
H	0.534591	5.597336	-0.165023
H	0.369955	4.273136	1.940273
H	-1.156993	5.297846	-1.971801
H	-3.869018	2.694707	-1.894307
H	-3.875050	5.796576	-2.032534

H	-4.863976	4.818947	-0.908186
H	-5.154880	4.714634	-2.673793
H	-3.535174	3.464509	-4.194463
H	-1.995518	2.818078	-3.544393
H	-2.246294	4.600528	-3.708991
H	-2.042210	1.473559	2.480123
H	-3.434893	3.454077	3.227083
H	-1.961935	4.250173	3.865124
H	-2.550703	2.722522	4.602884
H	0.472675	1.562407	2.625690
H	-0.357039	1.447757	4.206145
H	0.343491	3.009277	3.690351
H	-4.923831	3.525397	1.043258
H	-6.535069	1.228049	1.176794
H	-6.568871	-3.331140	-1.649873
H	-6.819440	-4.627630	0.467477
H	-6.057705	-3.651446	2.632205
H	-4.770474	-0.057610	-1.915483
H	-7.772180	-0.743439	-2.318996
H	-6.871056	0.577461	-3.136563
H	-7.144571	0.639321	-1.366941
H	-4.303016	-2.212867	-3.094087
H	-5.104522	-0.993445	-4.122525
H	-6.054346	-2.373603	-3.498477
H	-4.260102	-0.363318	2.931253
H	-6.739497	0.117166	3.248211
H	-5.918115	-0.181193	4.812120
H	-6.933339	-1.460215	4.069906
H	-4.858669	-3.054051	4.332229
H	-3.874941	-1.697955	4.948996
H	-3.314738	-2.600982	3.507284
Cl	-2.204884	0.279634	-2.494472
N	0.696121	0.274212	-0.400733
C	1.578007	-0.213355	0.488769
C	1.166964	0.956841	-1.457546
C	2.966316	-0.036266	0.364497
C	2.537705	1.184747	-1.668068
C	3.471313	0.682557	-0.739772
H	1.138700	-0.771706	1.335509
H	3.643872	-0.457160	1.124821
H	0.403843	1.310553	-2.173915
H	2.873660	1.743251	-2.557017
C	4.955178	0.944384	-0.913706
H	5.159944	1.277525	-1.956882

H	5.276644	1.786701	-0.268602
N	5.737165	-0.243981	-0.577800
H	5.246248	-1.142773	-0.668557
C	7.060376	-0.379814	-0.292524
C	7.956606	0.835397	-0.235198
C	7.619763	-1.637855	-0.056124
C	9.391870	0.624550	0.113569
C	9.024632	-1.891454	0.269751
C	9.906456	-0.673405	0.348494
Cl	6.581654	-3.048758	-0.132909
O	9.478361	-3.022392	0.473625
O	7.511947	1.961355	-0.475483
C	11.266991	-0.837217	0.662499
C	12.111197	0.282697	0.745824
C	10.243933	1.745440	0.197465
C	11.600006	1.574720	0.514396
H	11.633725	-1.860438	0.837377
H	13.176431	0.148965	0.993324
H	12.263615	2.451271	0.580919
H	9.815237	2.741271	0.007194
O	-0.638465	-2.195350	-1.103718
N	-1.820375	-4.176466	-1.355045
C	-2.143428	-5.290543	-2.231692
H	-1.851143	-6.259088	-1.768663
H	-3.234484	-5.325961	-2.443923
H	-1.603155	-5.181347	-3.193060
C	-2.427563	-4.163391	-0.028196
H	-2.030084	-3.308541	0.553208
H	-3.531391	-4.062002	-0.102074
H	-2.193797	-5.113131	0.500702
C	-0.974861	-3.191413	-1.758551
H	-0.566390	-3.372978	-2.788633

100

**IPrCl<sub>2</sub>Py<sub>4</sub>** SCF Done: -3468.35900930 A.U.

Pd	0.929838	0.706756	-0.270351
N	1.969756	-2.035911	0.445707
C	-1.798513	-3.985780	0.581989
N	3.597434	-0.597487	0.243397
C	-1.346861	-3.259594	1.692246
C	-0.100925	-2.598161	1.678971
Cl	1.041357	1.509849	1.930481
C	0.666870	-2.679968	0.483592
C	0.246010	-3.428613	-0.650195
C	-1.005996	-4.073839	-0.569743



C	1.114149	-3.608180	-1.898126
C	1.871283	-4.955972	-1.844800
C	0.316208	-3.494230	-3.211256
C	0.410510	-1.896643	2.938137
C	1.199588	-2.888812	3.824858
C	-0.702016	-1.212206	3.753210
C	3.156294	-2.724835	0.704900
C	4.176807	-1.824367	0.572877
C	4.384697	0.604044	0.018797
C	4.748883	0.938599	-1.315608
C	5.532080	2.096765	-1.500659
C	5.950822	2.874647	-0.412903
C	5.604107	2.501370	0.891748
C	4.818005	1.357544	1.144768
C	4.391076	0.054186	-2.511566
C	5.507465	-0.986512	-2.762913
C	4.094752	0.851027	-3.795073
C	4.524504	0.943980	2.588952
C	5.722309	0.167536	3.185625
C	4.154321	2.134734	3.494318
C	2.229866	-0.716620	0.159492
H	-2.775097	-4.494898	0.618081
H	-1.970870	-3.205621	2.596559
H	-1.364991	-4.656913	-1.431551
H	1.859401	-2.786290	-1.907689
H	1.160635	-5.810048	-1.841793
H	2.504332	-5.048654	-0.938991
H	2.531453	-5.068021	-2.730704
H	1.010140	-3.525112	-4.077048
H	-0.234685	-2.534724	-3.255300
H	-0.402121	-4.331597	-3.340986
H	1.101721	-1.089330	2.619930
H	2.059456	-3.338669	3.287302
H	0.547965	-3.719495	4.171956
H	1.598306	-2.372107	4.723263
H	-1.313634	-0.536247	3.123869
H	-0.249797	-0.598125	4.558490
H	-1.379904	-1.944649	4.242087
H	3.160550	-3.788449	0.958997
H	5.259084	-1.939727	0.677831
H	5.823435	2.389281	-2.520482
H	6.561086	3.776152	-0.583482
H	5.949444	3.111519	1.740197
H	3.456561	-0.490107	-2.263906

H	6.467670	-0.488390	-3.017499
H	5.234752	-1.652385	-3.608774
H	5.687245	-1.627158	-1.875377
H	3.312798	1.616809	-3.622942
H	3.719933	0.165580	-4.582499
H	5.000570	1.351106	-4.200393
H	3.642322	0.271467	2.571575
H	5.977878	-0.735799	2.594971
H	5.495717	-0.161381	4.221844
H	6.630606	0.806500	3.224210
H	5.012458	2.821861	3.654216
H	3.844187	1.765079	4.493846
H	3.307299	2.706612	3.067597
Cl	0.788178	-0.034654	-2.508819
N	-0.408522	2.295591	-0.719655
C	0.116064	3.542060	-0.692681
C	-1.716437	2.123935	-1.037704
C	-0.635859	4.680556	-1.005875
C	-2.529230	3.224326	-1.362658
C	-1.986092	4.516210	-1.351125
H	1.174392	3.609746	-0.399560
H	-0.162888	5.672866	-0.972168
H	-3.584263	3.047799	-1.615161
H	-2.613180	5.386093	-1.602519
C	-2.235007	0.694718	-1.025521
H	-1.616467	0.118132	-1.749746
H	-2.026061	0.253218	-0.030486
N	-3.631979	0.540002	-1.385371
H	-3.855282	0.260177	-2.353160
C	-4.746053	0.472967	-0.608797
C	-5.947424	0.013368	-1.431187
C	-4.935562	0.761979	0.731597
C	-7.274687	-0.134877	-0.789084
C	-6.244301	0.618017	1.383913
C	-7.415841	0.140368	0.545143
Cl	-3.662342	1.372226	1.771908
O	-6.418253	0.878585	2.579576
O	-5.769401	-0.225450	-2.632084
C	-8.728008	0.003349	1.260151
H	-9.502185	0.657705	0.803110
H	-9.116427	-1.035956	1.188472
H	-8.608726	0.275070	2.325456
C	-8.414172	-0.595242	-1.660122
H	-9.243994	0.143842	-1.660998

H	-8.070554	-0.743862	-2.700741
H	-8.842772	-1.551263	-1.289080
100			
<b>IPrCl2Py4isomer</b> SCF Done: -3468.35632628 A.U.			
Pd	0.945412	0.675431	-0.367063
N	1.979981	-1.950599	0.691464
C	-1.802642	-3.868780	0.887745
N	3.610454	-0.534392	0.381529
C	-1.413287	-2.984642	1.903392
C	-0.164003	-2.330294	1.868540
Cl	1.079323	1.801037	1.685813
C	0.676342	-2.590947	0.749872
C	0.318672	-3.499840	-0.284012
C	-0.941523	-4.126839	-0.186299
C	1.256704	-3.859981	-1.438418
C	1.977858	-5.199060	-1.156500
C	0.540994	-3.913947	-2.802195
C	0.276503	-1.446601	3.035636
C	1.028470	-2.289194	4.092878
C	-0.879993	-0.666910	3.686826
C	3.158096	-2.597706	1.069651
C	4.180585	-1.712355	0.868352
C	4.401490	0.642566	0.060313
C	4.772735	0.865823	-1.294800
C	5.562519	2.001651	-1.570102
C	5.980425	2.863771	-0.547576
C	5.622909	2.601707	0.780891
C	4.827657	1.487490	1.122004
C	4.413182	-0.110205	-2.415777
C	5.525083	-1.172955	-2.581274
C	4.120624	0.581069	-3.759841
C	4.512039	1.204734	2.592609
C	5.702271	0.494617	3.279603
C	4.120597	2.471995	3.377313
C	2.247483	-0.671225	0.264557
H	-2.783954	-4.367452	0.938128
H	-2.089944	-2.799921	2.750942
H	-1.252178	-4.831334	-0.972974
H	2.021127	-3.059029	-1.508758
H	1.249698	-6.035622	-1.091870
H	2.545550	-5.181024	-0.203894
H	2.693566	-5.435947	-1.971869
H	1.282832	-4.075518	-3.611927
H	0.016411	-2.960683	-3.008298

H	-0.188856	-4.749500	-2.858813
H	0.974951	-0.681733	2.637963
H	1.913975	-2.802925	3.665156
H	0.365721	-3.068510	4.527093
H	1.383978	-1.642998	4.923122
H	-1.458214	-0.091078	2.936846
H	-0.473405	0.061392	4.417712
H	-1.579159	-1.331383	4.239582
H	3.156819	-3.624095	1.446756
H	5.258759	-1.807669	1.023792
H	5.860294	2.208440	-2.608959
H	6.596978	3.744868	-0.787929
H	5.964473	3.280291	1.577287
H	3.476056	-0.629162	-2.127165
H	6.486489	-0.701338	-2.878474
H	5.247530	-1.905166	-3.368647
H	5.705149	-1.738752	-1.644022
H	3.344638	1.364629	-3.651054
H	3.738994	-0.163975	-4.487420
H	5.029076	1.040468	-4.205583
H	3.632974	0.528366	2.619612
H	5.973899	-0.456737	2.778536
H	5.458958	0.260844	4.337609
H	6.605901	1.141112	3.274686
H	4.975414	3.171992	3.492895
H	3.787341	2.195253	4.399278
H	3.285316	3.001356	2.878903
Cl	0.813366	-0.374783	-2.480520
N	-0.416089	2.157544	-1.045630
C	0.088039	3.396823	-1.244838
C	-1.721914	1.910601	-1.318395
C	-0.683783	4.449045	-1.751332
C	-2.552878	2.921359	-1.832918
C	-2.031625	4.202811	-2.055548
H	1.146940	3.532282	-0.978524
H	-0.227527	5.438748	-1.899096
H	-3.604243	2.685565	-2.051061
H	-2.673325	5.002538	-2.457919
C	-2.211349	0.495519	-1.055771
H	-1.599424	-0.182278	-1.691654
H	-1.972827	0.238392	-0.004453
N	-3.613220	0.254861	-1.360859
H	-3.810260	-0.204253	-2.257513
C	-4.719779	0.356177	-0.568990

C	-4.633104	1.040825	0.777879
C	-5.959291	-0.106366	-0.988568
C	-5.848008	1.087141	1.643545
C	-7.171129	-0.043713	-0.173582
C	-7.044658	0.593942	1.194758
Cl	-6.107734	-0.858760	-2.568077
O	-8.259125	-0.488967	-0.557912
O	-3.571840	1.560166	1.136796
C	-8.300274	0.648356	2.016010
H	-8.171994	0.111371	2.981059
H	-8.564674	1.696823	2.274797
H	-9.137918	0.191820	1.456143
C	-5.688825	1.731684	2.995535
H	-5.967229	1.028908	3.810072
H	-4.643487	2.058845	3.147975
H	-6.353819	2.616185	3.100489
100			
<b>IPrCl2Py5</b> SCF Done: -3468.35505887 A.U.			
Pd	-1.016016	-0.826913	-0.089716
N	-1.920299	1.999107	0.333856
C	2.036298	3.533915	0.172725
N	-3.640637	0.656613	0.258566
C	1.551557	2.969623	1.360443
C	0.237969	2.465295	1.453572
Cl	-1.278378	-1.480451	2.155252
C	-0.570568	2.538468	0.285537
C	-0.125125	3.149372	-0.919184
C	1.197405	3.637948	-0.943737
C	-1.027338	3.339980	-2.141130
C	-1.638143	4.761531	-2.148792
C	-0.306157	3.064830	-3.474862
C	-0.295335	1.937384	2.786342
C	-0.949387	3.082693	3.594676
C	0.769274	1.216723	3.632726
C	-3.057459	2.785252	0.521645
C	-4.136301	1.946093	0.467331
C	-4.509727	-0.502268	0.134135
C	-4.865509	-0.949848	-1.168791
C	-5.746472	-2.047831	-1.256023
C	-6.263283	-2.661256	-0.107023
C	-5.911650	-2.184239	1.161906
C	-5.029648	-1.094298	1.317716
C	-4.390990	-0.241849	-2.438512
C	-5.396516	0.859370	-2.850342

C	-4.127548	-1.201998	-3.612578
C	-4.715409	-0.566602	2.719580
C	-5.853277	0.347845	3.229903
C	-4.436924	-1.692792	3.734207
C	-2.268962	0.678292	0.174744
H	3.078243	3.883505	0.111445
H	2.210703	2.912930	2.239495
H	1.584437	4.094651	-1.866992
H	-1.854316	2.603840	-2.065118
H	-0.841741	5.532545	-2.223590
H	-2.220730	4.978065	-1.230174
H	-2.317621	4.890662	-3.017852
H	-1.035948	3.090298	-4.311041
H	0.169136	2.064816	-3.464959
H	0.467595	3.830433	-3.695943
H	-1.075025	1.179826	2.566132
H	-1.775908	3.567659	3.035437
H	-0.205982	3.870404	3.843341
H	-1.369340	2.696859	4.547804
H	1.275003	0.420636	3.050939
H	0.288304	0.733618	4.507765
H	1.540569	1.913998	4.025307
H	-2.991716	3.865648	0.676897
H	-5.208531	2.142959	0.554230
H	-6.037064	-2.424654	-2.248137
H	-6.949896	-3.517855	-0.202239
H	-6.327412	-2.669737	2.058030
H	-3.417631	0.241912	-2.216051
H	-6.391034	0.424034	-3.088216
H	-5.035462	1.396088	-3.752981
H	-5.543579	1.611977	-2.048466
H	-3.431630	-2.013609	-3.321417
H	-3.658148	-0.646500	-4.450022
H	-5.061724	-1.658736	-4.004644
H	-3.784608	0.032947	2.647421
H	-6.040635	1.206102	2.553006
H	-5.605067	0.757004	4.232047
H	-6.805595	-0.217159	3.321290
H	-5.343375	-2.299185	3.946299
H	-4.103929	-1.256786	4.699207
H	-3.632868	-2.360840	3.368909
Cl	-0.771216	-0.254225	-2.355248
N	0.394368	-2.383918	-0.357427
C	0.186999	-3.612113	0.170454

C	1.526366	-2.145444	-1.058307
C	1.101775	-4.658245	-0.013795
C	2.509559	-3.130015	-1.267594
C	2.276561	-4.415721	-0.740421
H	-0.730431	-3.726893	0.767827
H	0.886586	-5.649350	0.412686
H	1.625904	-1.133027	-1.481720
H	3.009462	-5.224795	-0.899814
C	3.795022	-2.787700	-2.013182
H	4.110006	-3.662013	-2.621701
H	3.624878	-1.942267	-2.702745
N	4.901676	-2.461092	-1.116972
H	5.317236	-3.237219	-0.574136
C	5.318026	-1.277406	-0.596548
C	6.300517	-1.525693	0.550379
C	5.029361	0.033652	-0.937431
C	6.917336	-0.385174	1.264642
C	5.605130	1.175050	-0.214219
C	6.583575	0.895015	0.910483
Cl	3.965156	0.480000	-2.259893
O	5.324091	2.346169	-0.497321
O	6.551221	-2.699285	0.850852
C	7.162389	2.095101	1.600768
H	8.270506	2.110707	1.509813
H	6.751033	3.022105	1.160440
H	6.939074	2.076525	2.689681
C	7.889070	-0.706752	2.369531
H	7.545287	-0.289669	3.340529
H	8.005071	-1.801042	2.478068
H	8.887053	-0.261065	2.168740
100			
<b>IPrCl2Py5isomer</b> SCF Done: -3468.35286563 A.U.			
Pd	-1.055346	-0.462408	0.026453
N	-3.164526	1.695511	-0.090812
C	-0.542798	5.008193	-0.520985
N	-4.063246	-0.281760	0.122162
C	-0.785278	4.468500	0.748821
C	-1.644474	3.364085	0.925543
Cl	-1.140118	-0.622689	2.372583
C	-2.238363	2.806851	-0.240932
C	-2.029296	3.346879	-1.540012
C	-1.164467	4.456052	-1.647810
C	-2.737603	2.816790	-2.788886
C	-3.971189	3.685105	-3.129620

C	-1.802337	2.712154	-4.009306
C	-1.965579	2.861745	2.333495
C	-3.150745	3.656424	2.930215
C	-0.753681	2.893308	3.282392
C	-4.548373	1.878841	-0.048615
C	-5.111650	0.639409	0.078437
C	-4.284236	-1.712071	0.259964
C	-4.302522	-2.515920	-0.914007
C	-4.545940	-3.895311	-0.748957
C	-4.780443	-4.447906	0.517056
C	-4.789138	-3.625729	1.650579
C	-4.545519	-2.239373	1.554578
C	-4.151004	-1.925751	-2.316665
C	-5.535667	-1.547377	-2.893214
C	-3.391094	-2.845768	-3.289455
C	-4.631921	-1.368263	2.810047
C	-6.105233	-1.038111	3.146000
C	-3.934905	-2.004366	4.028506
C	-2.851692	0.361190	0.017885
H	0.133015	5.871306	-0.632566
H	-0.301963	4.917130	1.629576
H	-0.974192	4.892480	-2.640166
H	-3.082483	1.786257	-2.565011
H	-3.669474	4.727485	-3.368555
H	-4.697123	3.733406	-2.292627
H	-4.503102	3.275580	-4.014240
H	-2.333015	2.218029	-4.849809
H	-0.908383	2.104982	-3.767627
H	-1.475098	3.709635	-4.373080
H	-2.264930	1.796513	2.256068
H	-4.058511	3.588190	2.295833
H	-2.897204	4.733221	3.037506
H	-3.412839	3.266711	3.936565
H	0.109495	2.349945	2.849238
H	-1.014129	2.395150	4.238621
H	-0.435090	3.929314	3.527959
H	-4.997608	2.873939	-0.110463
H	-6.157307	0.325064	0.138109
H	-4.557185	-4.547574	-1.634934
H	-4.966411	-5.529135	0.619831
H	-4.987227	-4.067523	2.639041
H	-3.544322	-1.000900	-2.233138
H	-6.183937	-2.444023	-2.997638
H	-5.425899	-1.087982	-3.898331



H	-6.071225	-0.820535	-2.248420
H	-2.409958	-3.149498	-2.873831
H	-3.196323	-2.305827	-4.238632
H	-3.967798	-3.760664	-3.545311
H	-4.098619	-0.419376	2.595811
H	-6.624622	-0.523655	2.311943
H	-6.163115	-0.377761	4.037055
H	-6.677634	-1.963078	3.372745
H	-4.461724	-2.916686	4.380969
H	-3.924503	-1.286729	4.875210
H	-2.884908	-2.262450	3.789330
Cl	-0.959430	-0.277138	-2.317966
N	0.873056	-1.373609	0.034737
C	1.167228	-2.344933	0.931688
C	1.813208	-0.996989	-0.860488
C	2.417705	-2.975829	0.950176
C	3.094078	-1.575952	-0.908383
C	3.395163	-2.587317	0.021806
H	0.374589	-2.576817	1.659587
H	2.617687	-3.762110	1.693420
H	1.501544	-0.218304	-1.575197
H	4.391534	-3.058463	0.024238
C	4.083034	-1.125701	-1.979420
H	3.922059	-1.735663	-2.895124
H	3.875335	-0.073107	-2.246019
N	5.486622	-1.294714	-1.623141
H	5.949000	-2.150627	-1.949203
C	6.254928	-0.590749	-0.739753
C	5.763092	0.722127	-0.169199
C	7.512961	-1.036699	-0.363586
C	6.655465	1.488135	0.750256
C	8.405593	-0.305533	0.535888
C	7.895459	1.010520	1.083797
Cl	8.101419	-2.569953	-0.986502
O	9.524217	-0.726140	0.851950
O	4.641876	1.144312	-0.468135
C	8.822822	1.744079	2.008726
H	9.047958	2.763143	1.625799
H	8.361854	1.881513	3.011185
H	9.768235	1.181215	2.121567
C	6.114924	2.788470	1.284215
H	5.118700	3.000110	0.853394
H	6.019960	2.758776	2.391413
H	6.795841	3.633800	1.047273

112

IPrCl2Py5isomer--DMFnodisp SCF Done: -3716.67055012 A.U.

Pd	-1.322631	0.118600	-0.537202
N	-3.702325	-1.050874	0.852248
C	-2.875577	-5.158261	0.166567
N	-3.671601	1.130725	0.985778
C	-3.830120	-4.496493	-0.615367
C	-4.113800	-3.127246	-0.426986
Cl	-2.522489	-0.424551	-2.479487
C	-3.389899	-2.444957	0.589062
C	-2.433536	-3.096403	1.416336
C	-2.188936	-4.463327	1.171448
C	-1.745006	-2.388659	2.583961
C	-2.582910	-2.538446	3.875521
C	-0.298676	-2.860280	2.817225
C	-5.206567	-2.460963	-1.266614
C	-6.610601	-2.813533	-0.722065
C	-5.109499	-2.816064	-2.763264
C	-4.839780	-0.667497	1.566396
C	-4.824455	0.696974	1.643232
C	-3.322618	2.536899	0.878042
C	-2.768649	3.189253	2.014137
C	-2.486892	4.566604	1.896791
C	-2.745721	5.264925	0.710607
C	-3.310591	4.599723	-0.385701
C	-3.622521	3.225174	-0.329885
C	-2.523611	2.480589	3.348610
C	-3.664399	2.781050	4.349000
C	-1.159446	2.835699	3.972311
C	-4.329546	2.552339	-1.506139
C	-5.857820	2.764765	-1.403933
C	-3.796944	3.010579	-2.875713
C	-2.967458	0.055968	0.484879
H	-2.668208	-6.226948	-0.004283
H	-4.369735	-5.052126	-1.397601
H	-1.449230	-4.994492	1.788921
H	-1.677626	-1.309156	2.337894
H	-2.672167	-3.605839	4.172153
H	-3.610492	-2.137842	3.754293
H	-2.105131	-1.990384	4.715068
H	0.192408	-2.206128	3.566189
H	0.294421	-2.805075	1.882756
H	-0.248232	-3.900773	3.204499
H	-5.061724	-1.363809	-1.189601

H	-6.737932	-2.524991	0.341258
H	-6.801425	-3.905880	-0.793160
H	-7.398282	-2.294470	-1.308227
H	-4.101116	-2.579799	-3.155047
H	-5.848721	-2.223052	-3.341329
H	-5.331411	-3.887786	-2.953953
H	-5.549773	-1.403785	1.952879
H	-5.526030	1.401231	2.098732
H	-2.050761	5.099659	2.755608
H	-2.511916	6.339679	0.642118
H	-3.523892	5.159971	-1.308697
H	-2.510228	1.389101	3.149621
H	-3.708691	3.865631	4.586131
H	-3.502951	2.233180	5.301470
H	-4.659456	2.488021	3.956705
H	-0.339888	2.643408	3.252922
H	-0.980059	2.210828	4.872205
H	-1.113307	3.896582	4.298906
H	-4.129373	1.463200	-1.451149
H	-6.267045	2.372928	-0.449438
H	-6.378971	2.242635	-2.234101
H	-6.119242	3.843571	-1.462502
H	-4.039991	4.073572	-3.091278
H	-4.254067	2.397945	-3.679266
H	-2.699001	2.874823	-2.939833
Cl	-0.072333	0.644705	1.399990
N	0.533697	-1.571399	-1.232599
C	0.368590	-2.353035	-2.315497
C	1.696706	-1.626907	-0.565279
C	1.367885	-3.231812	-2.769075
C	2.769281	-2.463774	-0.942960
C	2.587432	-3.283002	-2.075170
H	-0.605128	-2.250576	-2.828300
H	1.190786	-3.861082	-3.655062
H	1.762634	-0.968792	0.323112
H	3.394650	-3.958686	-2.405077
C	4.072386	-2.431663	-0.171213
H	3.881511	-2.323987	0.915382
H	4.624566	-3.389374	-0.291044
N	4.888874	-1.304693	-0.644397
H	4.557418	-0.837729	-1.497181
C	6.010946	-0.748772	-0.118061
C	6.650137	-1.358523	1.112035
C	6.620272	0.362259	-0.689977

C	7.847393	-0.697488	1.703746
C	7.803298	1.015743	-0.143680
C	8.396942	0.410584	1.113254
Cl	5.932989	1.063275	-2.150396
O	8.316359	2.019139	-0.656109
O	6.178998	-2.391062	1.599512
O	0.268850	1.273108	-1.901875
N	1.922770	2.856245	-2.129815
C	2.856499	3.762176	-1.478752
H	3.909036	3.463017	-1.678757
H	2.713910	4.805595	-1.836948
H	2.688527	3.741348	-0.384010
C	1.958449	2.765712	-3.582998
H	1.184448	2.044681	-3.906265
H	1.754251	3.757688	-4.041763
H	2.955895	2.419391	-3.931678
C	1.064446	2.087737	-1.405167
H	1.129612	2.236430	-0.297660
C	8.418171	-1.322630	2.949760
H	8.434650	-0.597485	3.791638
H	7.819281	-2.202650	3.249873
H	9.469166	-1.648036	2.791839
C	9.613225	1.096725	1.663305
H	9.885857	1.954702	1.020571
H	9.432937	1.461058	2.698308
H	10.474956	0.397036	1.724485
100			
<b>IPrCl2Py6</b> SCF Done: -3468.35394974 A.U.			
Pd	1.091017	-0.000498	-0.433670
N	3.738431	-0.999968	0.608709
C	2.861388	-5.141287	0.279781
N	3.678534	1.181709	0.577609
C	2.371404	-4.406475	1.367532
C	2.642124	-3.029086	1.504257
Cl	0.233386	0.558436	1.684017
C	3.415172	-2.411871	0.482025
C	3.943726	-3.135247	-0.622380
C	3.644697	-4.512049	-0.695883
C	4.851082	-2.501805	-1.679820
C	6.337234	-2.810147	-1.382038
C	4.491862	-2.936126	-3.114539
C	2.182046	-2.276364	2.752880
C	3.237137	-2.406308	3.876515
C	0.794578	-2.716348	3.253581

C	4.967833	-0.551817	1.095451
C	4.933351	0.814803	1.068487
C	3.277222	2.571410	0.428013
C	3.369724	3.175594	-0.856576
C	3.005192	4.534183	-0.959410
C	2.590966	5.265001	0.162038
C	2.538332	4.650617	1.419297
C	2.878397	3.291832	1.587491
C	3.919317	2.433600	-2.075402
C	5.450287	2.629639	-2.177521
C	3.229425	2.827928	-3.393773
C	2.857038	2.676363	2.988805
C	4.126847	3.068948	3.779873
C	1.592711	3.050730	3.786922
C	2.929697	0.065092	0.287179
H	2.635435	-6.216466	0.195273
H	1.768441	-4.912951	2.136118
H	4.032107	-5.099915	-1.542014
H	4.703378	-1.403174	-1.631845
H	6.532338	-3.903038	-1.427620
H	6.649137	-2.460523	-0.376671
H	6.995248	-2.317993	-2.129134
H	5.100273	-2.364117	-3.845899
H	3.423864	-2.736712	-3.328877
H	4.700659	-4.013057	-3.289721
H	2.087087	-1.203161	2.489050
H	4.230316	-2.024542	3.561388
H	3.367340	-3.466959	4.181903
H	2.923481	-1.830251	4.772678
H	0.039112	-2.659487	2.444890
H	0.460049	-2.042991	4.068888
H	0.800279	-3.750012	3.661777
H	5.747369	-1.247607	1.417546
H	5.682237	1.560715	1.348739
H	3.055689	5.030320	-1.940299
H	2.311945	6.325657	0.055462
H	2.219669	5.235990	2.295287
H	3.718317	1.351690	-1.937269
H	5.708116	3.701244	-2.319885
H	5.857785	2.063441	-3.041646
H	5.976289	2.277117	-1.266244
H	2.128140	2.731226	-3.316578
H	3.565447	2.153543	-4.207622
H	3.472281	3.866731	-3.705421

H	2.845069	1.573536	2.867808
H	5.059415	2.765593	3.261716
H	4.126101	2.588924	4.781330
H	4.175537	4.168452	3.932245
H	1.564239	4.131847	4.040940
H	1.571607	2.491156	4.745396
H	0.678420	2.789402	3.219348
Cl	1.940190	-0.546192	-2.559376
N	-0.885321	-0.078955	-1.209268
C	-1.827988	0.797308	-0.791570
C	-1.228247	-1.009724	-2.132140
C	-3.136451	0.783383	-1.291857
C	-2.521309	-1.096999	-2.658594
C	-3.508995	-0.182031	-2.244593
H	-1.507662	1.505934	-0.011979
H	-3.863431	1.522474	-0.922575
H	-0.416756	-1.679395	-2.456454
H	-2.751276	-1.887793	-3.389731
C	-4.905463	-0.230469	-2.854205
H	-4.868195	0.266207	-3.848897
H	-5.182469	-1.287643	-3.027361
N	-5.942597	0.452188	-2.095560
H	-6.186046	1.405020	-2.387676
C	-6.572962	0.078154	-0.942155
C	-6.341874	-1.295871	-0.351853
C	-7.451038	0.931328	-0.291780
C	-7.063989	-1.674888	0.897598
C	-8.177796	0.580108	0.929019
C	-7.926889	-0.798797	1.501847
Cl	-7.728374	2.538188	-0.942054
O	-8.960242	1.358247	1.485431
O	-5.565434	-2.082017	-0.904539
C	-8.670647	-1.136352	2.761161
H	-9.296227	-2.045283	2.626344
H	-7.966868	-1.361377	3.592049
H	-9.318113	-0.290022	3.057486
C	-6.785402	-3.049630	1.445582
H	-6.073774	-3.588977	0.793365
H	-6.354079	-2.992978	2.468324
H	-7.718863	-3.646883	1.527904
100			
<b>IPrCl2Py6del2</b> SCF Done: -3468.35624953 A.U.			
Pd	-1.170639	-0.367423	-0.122214
N	-3.285221	1.743930	0.278724

C	-0.621734	5.043192	0.500546
N	-4.178598	-0.238500	0.092446
C	-0.806562	4.216398	1.616807
C	-1.683136	3.112512	1.575881
Cl	-1.262291	-1.175328	2.084548
C	-2.356254	2.860206	0.348305
C	-2.205830	3.693463	-0.794173
C	-1.321976	4.787513	-0.685016
C	-2.995505	3.485927	-2.088863
C	-4.208239	4.443732	-2.149577
C	-2.126153	3.640206	-3.352251
C	-1.941285	2.288197	2.837495
C	-3.102571	2.904491	3.652605
C	-0.691339	2.110792	3.718449
C	-4.666799	1.906759	0.398329
C	-5.226954	0.665546	0.274096
C	-4.398636	-1.666594	-0.066815
C	-4.403874	-2.212815	-1.380493
C	-4.660312	-3.594087	-1.505513
C	-4.918307	-4.392142	-0.383069
C	-4.931664	-3.820901	0.895493
C	-4.675604	-2.447181	1.089403
C	-4.222770	-1.348620	-2.628970
C	-5.593802	-0.842082	-3.135303
C	-3.454300	-2.059735	-3.757568
C	-4.763202	-1.855421	2.498426
C	-6.236721	-1.605660	2.897548
C	-4.063155	-2.727735	3.559005
C	-2.970731	0.418634	0.090969
H	0.069576	5.899306	0.558044
H	-0.262790	4.432596	2.548484
H	-1.178403	5.448232	-1.553548
H	-3.374249	2.443149	-2.084791
H	-3.877256	5.504195	-2.163230
H	-4.887188	4.320786	-1.281151
H	-4.801858	4.263130	-3.070584
H	-2.715620	3.367806	-4.252590
H	-1.244792	2.971254	-3.305924
H	-1.779104	4.685765	-3.495478
H	-2.242283	1.267702	2.523514
H	-4.038410	2.969160	3.059928
H	-2.850605	3.931651	3.994071
H	-3.315985	2.289321	4.552296
H	0.158769	1.705018	3.134564

H	-0.907616	1.390995	4.534077
H	-0.370335	3.062145	4.195236
H	-5.118594	2.888901	0.562863
H	-6.270143	0.338513	0.294898
H	-4.663183	-4.050218	-2.506864
H	-5.116245	-5.469021	-0.507067
H	-5.142182	-4.455426	1.769962
H	-3.608479	-0.468216	-2.348959
H	-6.246152	-1.689730	-3.437242
H	-5.462125	-0.182452	-4.018942
H	-6.136332	-0.262047	-2.360315
H	-2.485806	-2.458329	-3.395355
H	-3.233992	-1.339123	-4.571263
H	-4.035774	-2.894491	-4.204727
H	-4.232003	-0.881474	2.485401
H	-6.759467	-0.932123	2.188122
H	-6.294587	-1.143277	3.905616
H	-6.806341	-2.559056	2.929477
H	-4.586962	-3.694595	3.717265
H	-4.053980	-2.200215	4.535675
H	-3.013176	-2.929417	3.270415
Cl	-1.084431	0.413604	-2.338445
N	0.774517	-1.194767	-0.341467
C	1.087431	-2.381608	0.227945
C	1.726462	-0.539287	-1.049256
C	2.359961	-2.954550	0.102537
C	3.025662	-1.039547	-1.196582
C	3.364624	-2.278456	-0.615561
H	0.287100	-2.853148	0.819013
H	2.557230	-3.931408	0.572425
H	1.402018	0.398645	-1.526128
H	3.766826	-0.469971	-1.778937
C	4.775016	-2.846655	-0.732486
H	4.751084	-3.937480	-0.525559
H	5.161568	-2.704271	-1.757545
N	5.702095	-2.235076	0.212938
H	5.590789	-2.471644	1.213621
C	6.579391	-1.208227	0.080952
C	7.152225	-0.830020	1.450766
C	7.020790	-0.502406	-1.025402
C	8.161185	0.246948	1.565650
C	8.011073	0.578594	-0.926437
C	8.566590	0.919022	0.443036
Cl	6.458819	-0.805849	-2.664707



O	8.400271	1.207159	-1.916607
O	6.741041	-1.451674	2.437358
C	8.686381	0.554696	2.943333
H	8.453755	1.601216	3.236757
H	8.238519	-0.126080	3.690771
H	9.792012	0.452831	2.983823
C	9.577344	2.026848	0.490086
H	9.227649	2.858000	1.140643
H	10.537581	1.673454	0.925050
H	9.760896	2.416946	-0.528149
100			
<b>IPrCl2Py6del3</b> SCF Done: -3468.35562319 A.U.			
Pd	1.084553	0.040746	-0.427806
N	3.606644	-1.070612	0.798035
C	2.441545	-5.154606	0.757331
N	3.738177	1.094633	0.553793
C	1.995503	-4.310348	1.782587
C	2.359696	-2.948313	1.822830
Cl	0.225682	0.744811	1.648227
C	3.181623	-2.461494	0.769285
C	3.668849	-3.299205	-0.272071
C	3.274623	-4.653401	-0.250717
C	4.631771	-2.810660	-1.356818
C	6.089021	-3.190790	-1.004970
C	4.265886	-3.329190	-2.761332
C	1.938943	-2.077086	3.006411
C	2.961346	-2.208841	4.159585
C	0.512647	-2.374176	3.504234
C	4.850678	-0.678769	1.296706
C	4.935710	0.676671	1.137587
C	3.476053	2.485705	0.220881
C	3.735959	2.927177	-1.106508
C	3.503845	4.288640	-1.392166
C	3.055128	5.174747	-0.403942
C	2.838317	4.717713	0.901912
C	3.045106	3.366348	1.251155
C	4.321355	2.008584	-2.180064
C	5.866405	2.081874	-2.166169
C	3.775986	2.293631	-3.591061
C	2.865347	2.922906	2.704728
C	4.115468	3.278629	3.543231
C	1.598161	3.506971	3.358162
C	2.905745	0.020409	0.339941
H	2.141683	-6.214850	0.747535

H	1.352417	-4.716089	2.577901
H	3.627897	-5.326650	-1.046594
H	4.558046	-1.704430	-1.397051
H	6.211653	-4.294234	-0.960837
H	6.405658	-2.782579	-0.023510
H	6.790315	-2.803119	-1.773924
H	4.921215	-2.854929	-3.521500
H	3.216979	-3.077273	-3.011570
H	4.405677	-4.427562	-2.851918
H	1.930977	-1.020797	2.667843
H	3.987262	-1.930895	3.840554
H	3.000595	-3.251668	4.541828
H	2.680709	-1.546601	5.005797
H	-0.221807	-2.315177	2.676552
H	0.217531	-1.622162	4.264265
H	0.430439	-3.374340	3.981642
H	5.555031	-1.401809	1.717368
H	5.734071	1.383047	1.381066
H	3.685304	4.660826	-2.411572
H	2.879910	6.233803	-0.652803
H	2.497674	5.424576	1.673861
H	4.019093	0.968586	-1.939811
H	6.220109	3.108507	-2.402900
H	6.295426	1.391442	-2.922903
H	6.288454	1.802133	-1.178991
H	2.668454	2.270258	-3.605612
H	4.133658	1.514216	-4.294591
H	4.117344	3.274410	-3.986961
H	2.742903	1.820351	2.702868
H	5.041099	2.821595	3.137609
H	3.996410	2.925316	4.589349
H	4.273863	4.378055	3.573245
H	1.665695	4.607589	3.493670
H	1.454530	3.063633	4.365592
H	0.700545	3.271619	2.754061
Cl	1.941766	-0.668537	-2.499365
N	-0.883962	0.058971	-1.245039
C	-1.794693	0.971155	-0.832486
C	-1.256671	-0.851314	-2.176747
C	-3.100187	1.008202	-1.338507
C	-2.547605	-0.882881	-2.715713
C	-3.503707	0.064542	-2.300073
H	-1.452095	1.663828	-0.048018
H	-3.800895	1.769637	-0.964142

H	-0.469775	-1.551782	-2.497221
H	-2.800447	-1.658245	-3.455931
C	-4.903574	0.065558	-2.907084
H	-4.862137	0.594180	-3.885185
H	-5.205051	-0.977080	-3.124594
N	-5.922527	0.724971	-2.112247
H	-6.088349	1.734003	-2.252751
C	-6.580792	0.295186	-1.000724
C	-7.355206	1.446039	-0.363009
C	-6.650396	-0.952039	-0.408761
C	-8.168040	1.214676	0.852974
C	-7.439981	-1.195873	0.809445
C	-8.202681	-0.033482	1.416349
Cl	-5.831609	-2.371308	-1.035412
O	-7.502692	-2.310005	1.338155
O	-7.267716	2.561260	-0.892944
C	-8.992543	-0.336204	2.655439
H	-10.072952	-0.122806	2.502418
H	-8.870145	-1.399460	2.933226
H	-8.664951	0.303097	3.503926
C	-8.914694	2.394047	1.418800
H	-8.728426	3.299561	0.812037
H	-10.009111	2.202284	1.443333
H	-8.605937	2.599040	2.466382

100

**IPrCl<sub>2</sub>Py<sub>6</sub>deI<sub>5</sub>** SCF Done: -3468.35624975 A.U.

Pd	-1.170783	-0.367553	-0.121852
N	-3.285261	1.744063	0.278083
C	-0.621545	5.043162	0.499818
N	-4.178787	-0.238324	0.091975
C	-0.806649	4.216588	1.616194
C	-1.683310	3.112771	1.575314
Cl	-1.263115	-1.174880	2.085080
C	-2.356229	2.860280	0.347659
C	-2.205551	3.693346	-0.794924
C	-1.321614	4.787333	-0.685812
C	-2.995047	3.485668	-2.089701
C	-4.207633	4.443638	-2.150825
C	-2.125480	3.639562	-3.352989
C	-1.941828	2.288784	2.837067
C	-3.103241	2.905424	3.651737
C	-0.692124	2.111482	3.718373
C	-4.666860	1.907053	0.397238
C	-5.227114	0.665876	0.273110

C	-4.398945	-1.666437	-0.067058
C	-4.403906	-2.212945	-1.380623
C	-4.660322	-3.594241	-1.505386
C	-4.918589	-4.392044	-0.382825
C	-4.932269	-3.820517	0.895605
C	-4.676230	-2.446758	1.089266
C	-4.222533	-1.349007	-2.629232
C	-5.593427	-0.842513	-3.135978
C	-3.453915	-2.060383	-3.757569
C	-4.764156	-1.854704	2.498146
C	-6.237774	-1.604743	2.896786
C	-4.064508	-2.726857	3.559110
C	-2.970867	0.418684	0.090675
H	0.069829	5.899226	0.557274
H	-0.263051	4.432906	2.547947
H	-1.177842	5.447883	-1.554440
H	-3.373934	2.442945	-2.085454
H	-3.876490	5.504048	-2.164653
H	-4.886751	4.320978	-1.282493
H	-4.801126	4.262928	-3.071894
H	-2.714788	3.366899	-4.253350
H	-1.244124	2.970632	-3.306310
H	-1.778409	4.685082	-3.496450
H	-2.242864	1.268242	2.523277
H	-4.038897	2.970173	3.058781
H	-2.851168	3.932596	3.993089
H	-3.317031	2.290452	4.551475
H	0.158096	1.705491	3.134805
H	-0.908675	1.391912	4.534130
H	-0.371162	3.062913	4.195030
H	-5.118592	2.889268	0.561506
H	-6.270331	0.338929	0.293743
H	-4.662973	-4.050607	-2.506631
H	-5.116485	-5.468952	-0.506638
H	-5.143014	-4.454844	1.770164
H	-3.608238	-0.468591	-2.349268
H	-6.245702	-1.690211	-3.437942
H	-5.461507	-0.183049	-4.019705
H	-6.136166	-0.262321	-2.361257
H	-2.485534	-2.459048	-3.395133
H	-3.233394	-1.339926	-4.571341
H	-4.035417	-2.895143	-4.204690
H	-4.232869	-0.880806	2.485073
H	-6.760286	-0.931349	2.187053

H	-6.295916	-1.142119	3.904729
H	-6.807466	-2.558095	2.928771
H	-4.588440	-3.693640	3.717426
H	-4.055578	-2.199132	4.535673
H	-3.014461	-2.928696	3.270876
Cl	-1.084012	0.413173	-2.338195
N	0.774452	-1.195150	-0.340396
C	1.087297	-2.381640	0.229790
C	1.726505	-0.540102	-1.048446
C	2.359870	-2.954617	0.104981
C	3.025736	-1.040440	-1.195261
C	3.364640	-2.278947	-0.613364
H	0.286869	-2.852824	0.821014
H	2.557093	-3.931167	0.575527
H	1.402116	0.397526	-1.525958
H	3.766992	-0.471212	-1.777842
C	4.775088	-2.847142	-0.729607
H	4.751259	-3.937747	-0.521509
H	5.161691	-2.705815	-1.754793
N	5.702039	-2.234399	0.215192
H	5.590729	-2.469871	1.216135
C	6.579661	-1.208000	0.082001
C	7.152671	-0.828391	1.451369
C	7.021247	-0.503582	-1.025181
C	8.161844	0.248513	1.565000
C	8.011949	0.577132	-0.927505
C	8.567549	0.919036	0.441568
Cl	6.459019	-0.808661	-2.664091
O	8.401414	1.204352	-1.918430
O	6.741364	-1.448815	2.438681
C	9.578367	2.026859	0.487314
H	10.537063	1.675366	0.927081
H	9.764997	2.412964	-0.531881
H	9.226419	2.860827	1.133096
C	8.686747	0.558063	2.942393
H	8.453057	1.604631	3.234819
H	8.239504	-0.122402	3.690486
H	9.792476	0.457349	2.982990
100			
<b>IPrCl2Py6isomer</b> SCF Done: -3468.35518037 A.U.			
Pd	1.099429	0.016585	-0.422784
N	3.656121	-1.025278	0.787301
C	2.599662	-5.138517	0.734363
N	3.728728	1.143485	0.548739

C	2.133643	-4.310202	1.763679
C	2.461515	-2.939063	1.808007
Cl	0.235061	0.708379	1.654862
C	3.267867	-2.426822	0.754588
C	3.773496	-3.247047	-0.292002
C	3.415912	-4.611452	-0.274384
C	4.716476	-2.726776	-1.379596
C	6.187182	-3.055443	-1.031872
C	4.366178	-3.258731	-2.783054
C	2.019043	-2.083050	2.994748
C	3.045319	-2.191187	4.146869
C	0.601118	-2.418433	3.491944
C	4.890826	-0.601876	1.283029
C	4.939214	0.755747	1.127060
C	3.429669	2.528396	0.220438
C	3.667574	2.978342	-1.108239
C	3.401613	4.334651	-1.388967
C	2.940908	5.208159	-0.395037
C	2.744913	4.743371	0.911363
C	2.985628	3.396403	1.255837
C	4.263307	2.075134	-2.189062
C	5.806751	2.177043	-2.184757
C	3.703574	2.354791	-3.595533
C	2.825258	2.944923	2.709174
C	4.071237	3.328296	3.541499
C	1.548130	3.496480	3.371620
C	2.924776	0.047863	0.334706
H	2.328301	-6.206386	0.721407
H	1.503113	-4.735647	2.558771
H	3.783846	-5.272021	-1.074211
H	4.602740	-1.623871	-1.420724
H	6.347713	-4.153927	-0.985672
H	6.493233	-2.634006	-0.052763
H	6.871974	-2.645734	-1.804252
H	5.002053	-2.760762	-3.544587
H	3.308264	-3.045777	-3.031478
H	4.546255	-4.351207	-2.874280
H	1.983061	-1.026375	2.659442
H	4.063256	-1.885379	3.827748
H	3.112455	-3.233625	4.526352
H	2.747930	-1.538864	4.995036
H	-0.134912	-2.374340	2.664721
H	0.287332	-1.677279	4.255138
H	0.544338	-3.422384	3.965022

H	5.615588	-1.306939	1.699415
H	5.719876	1.482098	1.369317
H	3.565772	4.712735	-2.409091
H	2.739213	6.263411	-0.639991
H	2.393558	5.440303	1.687543
H	3.981914	1.028852	-1.950983
H	6.139822	3.210920	-2.419835
H	6.243679	1.497402	-2.946714
H	6.240067	1.901529	-1.201286
H	2.596438	2.313889	-3.602727
H	4.068784	1.582812	-4.303332
H	4.026366	3.341862	-3.991324
H	2.728632	1.839791	2.704559
H	5.005169	2.894601	3.129388
H	3.966787	2.969715	4.587388
H	4.203382	4.431132	3.573288
H	1.590048	4.597961	3.510388
H	1.420912	3.046679	4.378385
H	0.652942	3.241567	2.771813
Cl	1.960537	-0.673100	-2.499642
N	-0.872798	-0.026130	-1.224673
C	-1.801779	0.871540	-0.822023
C	-1.229548	-0.962044	-2.137255
C	-3.110877	0.869466	-1.320585
C	-2.522720	-1.034016	-2.666185
C	-3.498078	-0.101302	-2.261172
H	-1.470681	1.585471	-0.051786
H	-3.827382	1.621449	-0.957694
H	-0.428078	-1.648902	-2.451012
H	-2.761790	-1.827903	-3.391301
C	-4.901323	-0.147422	-2.858596
H	-4.863384	0.297420	-3.877741
H	-5.204953	-1.204266	-2.987150
N	-5.916496	0.573520	-2.115754
H	-6.078858	1.570707	-2.327617
C	-6.607118	0.214577	-0.999278
C	-7.405282	1.398181	-0.463677
C	-6.692322	-0.986610	-0.322391
C	-8.263364	1.257861	0.738673
C	-7.531363	-1.145499	0.876983
C	-8.320835	0.049457	1.383115
Cl	-5.839511	-2.440637	-0.806739
O	-7.617584	-2.219414	1.479872
O	-7.306610	2.478418	-1.059861

C	-9.123108	-0.237817	2.617699
H	-9.761386	0.609496	2.925011
H	-9.752108	-1.138378	2.462986
H	-8.445484	-0.498535	3.458902
C	-8.988453	2.515696	1.138131
H	-8.263087	3.319333	1.386621
H	-9.587750	2.904612	0.288699
H	-9.655227	2.365319	2.005567
112			
<b>IPrCl2Py6isomer--DMFnodisp</b> SCF Done: -3716.66853716 A.U.			
Pd	1.750785	0.487902	-0.218913
N	3.098567	-2.117241	0.356970
C	-0.091081	-4.675682	-0.784132
N	4.385093	-0.419005	0.844857
C	-0.104398	-4.057407	0.473494
C	0.937576	-3.198930	0.880717
Cl	1.239611	0.975199	2.017071
C	1.991362	-2.967023	-0.046940
C	2.044984	-3.599388	-1.319367
C	0.976426	-4.454622	-1.662933
C	3.226359	-3.442613	-2.280258
C	4.187285	-4.649720	-2.167170
C	2.788780	-3.245852	-3.744789
C	0.951408	-2.621227	2.296224
C	1.708073	-3.568196	3.257270
C	-0.452045	-2.307947	2.844171
C	4.303066	-2.639555	0.832764
C	5.109663	-1.577548	1.132511
C	4.936574	0.910125	1.049112
C	5.499795	1.594342	-0.063538
C	6.065110	2.864045	0.174970
C	6.087188	3.422211	1.460135
C	5.549467	2.713073	2.540953
C	4.964142	1.441182	2.367640
C	5.575149	0.969973	-1.457106
C	6.900469	0.191654	-1.629766
C	5.394699	1.992259	-2.593667
C	4.449379	0.675915	3.589120
C	5.620129	0.012529	4.351780
C	3.619993	1.559616	4.541494
C	3.135066	-0.738992	0.357698
H	-0.917134	-5.343260	-1.077986
H	-0.940146	-4.249688	1.162621
H	0.984452	-4.955057	-2.643394



H	3.777667	-2.526142	-1.984481
H	3.677886	-5.591959	-2.462433
H	4.570688	-4.791135	-1.136092
H	5.062942	-4.514435	-2.836693
H	3.675509	-3.036046	-4.378916
H	2.094730	-2.387895	-3.835262
H	2.299616	-4.152645	-4.160473
H	1.490329	-1.651453	2.264637
H	2.751005	-3.751925	2.927051
H	1.199255	-4.553767	3.328573
H	1.750955	-3.132353	4.277830
H	-1.029302	-1.679258	2.137635
H	-0.364613	-1.746749	3.796738
H	-1.039785	-3.227451	3.056059
H	4.468727	-3.717173	0.914923
H	6.131751	-1.535487	1.519150
H	6.502577	3.423178	-0.665854
H	6.533170	4.416913	1.621301
H	5.579169	3.156197	3.548051
H	4.735718	0.251800	-1.555001
H	7.776648	0.869683	-1.541149
H	6.942075	-0.290456	-2.629498
H	7.016319	-0.606069	-0.867416
H	4.470201	2.586980	-2.452824
H	5.308169	1.462650	-3.564387
H	6.254217	2.692094	-2.674115
H	3.772834	-0.122330	3.221148
H	6.199705	-0.684289	3.712261
H	5.241385	-0.564252	5.221977
H	6.328638	0.777610	4.735429
H	4.242462	2.332008	5.041663
H	3.172145	0.934551	5.342150
H	2.796032	2.057556	3.994067
Cl	2.226953	0.026627	-2.490091
N	-0.801469	0.259672	-0.721564
C	-1.710734	0.561668	0.222129
C	-1.238867	-0.240043	-1.891904
C	-3.091465	0.369651	0.041159
C	-2.598314	-0.459678	-2.165742
C	-3.560303	-0.158097	-1.179656
H	-1.296636	0.964408	1.164798
H	-3.790430	0.627655	0.852627
H	-0.451063	-0.464031	-2.634250
H	-2.903448	-0.865796	-3.144210

C	-5.027863	-0.453707	-1.427427
H	-5.233823	-0.428485	-2.523370
H	-5.268909	-1.488800	-1.113714
N	-5.895758	0.471128	-0.710181
H	-5.532929	1.424863	-0.584453
C	-7.157373	0.312826	-0.221296
C	-7.911178	-0.984221	-0.426829
C	-7.802437	1.341421	0.455006
C	-9.263546	-1.136996	0.184157
C	-9.139689	1.229541	1.030296
C	-9.850173	-0.097327	0.856140
Cl	-6.966900	2.867380	0.689984
O	-9.686907	2.155446	1.641642
O	-7.411521	-1.894409	-1.097804
O	0.945983	2.656614	-0.814817
N	0.789903	4.399255	-2.307522
C	0.990111	4.874105	-3.665907
H	0.032464	5.217078	-4.117619
H	1.705991	5.725835	-3.692821
H	1.397901	4.054012	-4.289204
C	0.259927	5.334616	-1.324942
H	0.190979	4.813963	-0.351449
H	0.928145	6.217650	-1.223586
H	-0.749303	5.693227	-1.624877
C	1.095079	3.118270	-1.955951
H	1.503722	2.488615	-2.786750
C	-9.944165	-2.467406	-0.006595
H	-9.294839	-3.156121	-0.578390
H	-10.190182	-2.935923	0.970574
H	-10.904994	-2.353520	-0.553652
C	-11.219007	-0.197624	1.463745
H	-11.258321	-1.003596	2.228848
H	-11.492441	0.763437	1.938119
H	-11.980791	-0.457605	0.697006

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**IPrCl2Py6del2Isomer** SCF Done: -3468.35351083 A.U.

Pd	-1.056681	-0.192006	-0.404496
N	-3.471498	1.374279	0.504780
C	-1.820152	5.232964	-0.136786
N	-3.824679	-0.773711	0.653552
C	-1.689182	4.615160	1.113470
C	-2.221888	3.331972	1.357649
Cl	-0.208325	-0.146563	1.788314
C	-2.883290	2.684681	0.277420

C	-3.063471	3.301490	-0.991793
C	-2.506701	4.584712	-1.171638
C	-3.889813	2.663268	-2.109769
C	-5.351544	3.165505	-2.054687
C	-3.293983	2.888363	-3.511697
C	-2.141327	2.727812	2.760994
C	-3.287047	3.273515	3.645628
C	-0.778247	2.951820	3.442009
C	-4.767540	1.207840	0.996760
C	-4.988569	-0.138352	1.090705
C	-3.695821	-2.221773	0.606908
C	-4.146338	-2.908431	-0.554341
C	-4.038054	-4.314894	-0.556865
C	-3.520860	-5.007855	0.545011
C	-3.114891	-4.306382	1.687832
C	-3.198912	-2.900024	1.754487
C	-4.800192	-2.193506	-1.738163
C	-6.341157	-2.237214	-1.609035
C	-4.355774	-2.750887	-3.103476
C	-2.835486	-2.172616	3.049918
C	-4.045923	-2.143093	4.012371
C	-1.599711	-2.764190	3.752236
C	-2.876969	0.153249	0.287103
H	-1.390858	6.233964	-0.303876
H	-1.162186	5.140520	1.924278
H	-2.618694	5.086348	-2.144764
H	-3.887911	1.566518	-1.943455
H	-5.402588	4.262886	-2.222499
H	-5.830216	2.955088	-1.076402
H	-5.962095	2.673197	-2.840977
H	-3.872861	2.311237	-4.262114
H	-2.245200	2.535833	-3.558373
H	-3.330909	3.955016	-3.820522
H	-2.266326	1.629710	2.661916
H	-4.286474	3.073653	3.207773
H	-3.196895	4.372925	3.779985
H	-3.260009	2.805250	4.652277
H	0.047903	2.563191	2.815074
H	-0.748757	2.408445	4.409166
H	-0.590800	4.023881	3.665527
H	-5.407465	2.062664	1.232114
H	-5.862229	-0.704647	1.425371
H	-4.369318	-4.876035	-1.443789
H	-3.441864	-6.106560	0.516655

H	-2.725094	-4.861356	2.554475
H	-4.476076	-1.133007	-1.710436
H	-6.713323	-3.283714	-1.639944
H	-6.818163	-1.683139	-2.444994
H	-6.695839	-1.786159	-0.659670
H	-3.252832	-2.728671	-3.200482
H	-4.776284	-2.126323	-3.918827
H	-4.714468	-3.789075	-3.270736
H	-2.571056	-1.128745	2.784083
H	-4.930065	-1.650646	3.558277
H	-3.792038	-1.587991	4.940173
H	-4.349132	-3.171584	4.304179
H	-1.789425	-3.781832	4.156053
H	-1.311344	-2.121522	4.609619
H	-0.733726	-2.806432	3.062999
Cl	-1.891218	-0.255667	-2.603048
N	0.907057	-0.557810	-1.149653
C	1.784075	-1.316958	-0.451625
C	1.308933	-0.026563	-2.328973
C	3.080683	-1.577628	-0.911729
C	2.595237	-0.229836	-2.841812
C	3.513285	-1.026956	-2.132579
H	1.422617	-1.692597	0.517913
H	3.753336	-2.199725	-0.301470
H	0.550284	0.560179	-2.869048
H	2.876692	0.247924	-3.792980
C	4.902067	-1.305515	-2.696064
H	4.850581	-2.226761	-3.317165
H	5.194004	-0.474316	-3.365345
N	5.934747	-1.548096	-1.697452
H	6.187085	-2.524474	-1.510219
C	6.503687	-0.677995	-0.810185
C	6.267086	0.810390	-0.941027
C	7.335476	-1.122398	0.205598
C	6.916890	1.733127	0.034718
C	7.990184	-0.237667	1.170637
C	7.725213	1.246324	1.028137
Cl	7.628043	-2.843895	0.385554
O	8.723288	-0.660916	2.071038
O	5.547711	1.242560	-1.847861
C	6.630665	3.201842	-0.134221
H	7.569903	3.785743	-0.239470
H	6.000764	3.373025	-1.026813
H	6.100187	3.610336	0.753131

C	8.394161	2.136458	2.034838
H	9.056311	2.877916	1.536907
H	7.644740	2.722657	2.609923
H	8.994760	1.529279	2.737593
100			
<b>IPrCl2Py6del2Isomer180</b> SCF Done: -3468.35609836 A.U.			
Pd	-1.312885	0.129703	-0.246914
N	-4.169873	0.785433	0.448725
C	-3.695039	5.004846	0.522553
N	-3.880398	-1.371353	0.280839
C	-3.340956	4.241113	1.642465
C	-3.483601	2.837927	1.648465
Cl	-0.738244	-0.397352	1.973032
C	-3.982054	2.227653	0.464218
C	-4.373427	2.978442	-0.679032
C	-4.212780	4.378598	-0.618321
C	-5.006765	2.341768	-1.918138
C	-6.548456	2.455608	-1.862716
C	-4.474065	2.933284	-3.237615
C	-3.184778	2.042880	2.919674
C	-4.431855	2.004574	3.833936
C	-1.958918	2.564389	3.691509
C	-5.402809	0.186911	0.715282
C	-5.223012	-1.163880	0.603560
C	-3.320859	-2.701488	0.098347
C	-3.212948	-3.221442	-1.221298
C	-2.701061	-4.528124	-1.361533
C	-2.332935	-5.290930	-0.245405
C	-2.479904	-4.763546	1.043578
C	-2.980295	-3.460934	1.251480
C	-3.702257	-2.453168	-2.449247
C	-5.178892	-2.803659	-2.747122
C	-2.826474	-2.673761	-3.695827
C	-3.195616	-2.952577	2.678781
C	-4.506932	-3.522805	3.268707
C	-2.008802	-3.261481	3.611945
C	-3.217844	-0.170536	0.181038
H	-3.573324	6.099834	0.541971
H	-2.948613	4.743193	2.539578
H	-4.498771	4.988662	-1.488605
H	-4.731858	1.266943	-1.917609
H	-6.868237	3.519718	-1.870736
H	-6.974345	1.988875	-0.951229
H	-7.008177	1.957687	-2.742544

H	-4.876440	2.358709	-4.097888
H	-3.368979	2.874344	-3.277389
H	-4.785675	3.990244	-3.378905
H	-2.939267	1.003253	2.621223
H	-5.312419	1.566582	3.320130
H	-4.713649	3.026342	4.168176
H	-4.231975	1.393501	4.739461
H	-1.068867	2.628297	3.034765
H	-1.711950	1.866579	4.517550
H	-2.138298	3.562293	4.146475
H	-6.288871	0.778930	0.960450
H	-5.921788	-1.996792	0.720911
H	-2.596296	-4.956653	-2.369531
H	-1.934762	-6.309296	-0.381615
H	-2.198951	-5.375100	1.914558
H	-3.641006	-1.369867	-2.218905
H	-5.292337	-3.881989	-2.990866
H	-5.551029	-2.217645	-3.613964
H	-5.840697	-2.584653	-1.883875
H	-1.761593	-2.455477	-3.481240
H	-3.149620	-1.989262	-4.506561
H	-2.904385	-3.709952	-4.090155
H	-3.284383	-1.848012	2.629075
H	-5.393276	-3.270677	2.651274
H	-4.681996	-3.121916	4.289509
H	-4.460119	-4.630398	3.343825
H	-1.900313	-4.350359	3.803563
H	-2.164737	-2.772259	4.596007
H	-1.063110	-2.873537	3.186108
Cl	-1.895985	0.646973	-2.467829
N	0.742886	0.471615	-0.700640
C	1.717052	-0.247061	-0.096039
C	1.103320	1.425579	-1.593227
C	3.077464	-0.038620	-0.359803
C	2.441081	1.695363	-1.899265
C	3.467274	0.957253	-1.274517
H	1.372013	-0.986439	0.643714
H	3.828863	-0.653176	0.157956
H	0.271555	1.952086	-2.086751
H	2.674248	2.483698	-2.632587
C	4.923546	1.273767	-1.569281
H	5.019581	1.556446	-2.644330
H	5.229116	2.167774	-0.989353
N	5.826906	0.184878	-1.255392

H	5.648190	-0.733711	-1.695936
C	7.017407	0.162365	-0.599852
C	7.644706	-1.229941	-0.702768
C	7.701493	1.134743	0.108939
C	8.947434	-1.511910	-0.058104
C	9.002552	0.873924	0.743272
C	9.596521	-0.515946	0.622060
Cl	7.112551	2.773104	0.346521
O	9.614406	1.746615	1.368007
O	7.028318	-2.092314	-1.340356
C	9.497690	-2.907162	-0.196496
H	9.657292	-3.375701	0.798365
H	8.805371	-3.541937	-0.779990
H	10.485793	-2.900679	-0.705186
C	10.922851	-0.729425	1.290015
H	10.855891	-1.523714	2.065355
H	11.687943	-1.070631	0.559179
H	11.264738	0.209227	1.764084
100			
<b>IPrCl2Py6del6Isomer</b> SCF Done: -3468.35394971 A.U.			
Pd	1.091120	-0.000443	-0.433570
N	3.738666	-0.999869	0.608363
C	2.861589	-5.141136	0.279019
N	3.678732	1.181803	0.577579
C	2.371633	-4.406439	1.366865
C	2.642363	-3.029063	1.503735
Cl	0.233606	0.558542	1.684110
C	3.415382	-2.411750	0.481548
C	3.943879	-3.134989	-0.622957
C	3.644863	-4.511790	-0.696602
C	4.851167	-2.501428	-1.680380
C	6.337335	-2.809774	-1.382666
C	4.491879	-2.935619	-3.115123
C	2.182341	-2.276456	2.752452
C	3.237455	-2.406616	3.876037
C	0.794831	-2.716367	3.253122
C	4.968143	-0.551774	1.094986
C	4.933612	0.814854	1.068217
C	3.277298	2.571479	0.428234
C	3.369530	3.175785	-0.856323
C	3.004898	4.534352	-0.958979
C	2.590798	5.265032	0.162614
C	2.538420	4.650536	1.419824
C	2.878620	3.291755	1.587840

C	3.918982	2.433900	-2.075276
C	5.449954	2.629888	-2.177517
C	3.228976	2.828377	-3.393543
C	2.857602	2.676155	2.989103
C	4.127570	3.068789	3.779915
C	1.593427	3.050312	3.787544
C	2.929860	0.065196	0.287115
H	2.635627	-6.216305	0.194400
H	1.768682	-4.912993	2.135408
H	4.032245	-5.099558	-1.542816
H	4.703469	-1.402801	-1.632298
H	6.532448	-3.902661	-1.428314
H	6.649271	-2.460222	-0.377280
H	6.995329	-2.317571	-2.129748
H	5.100306	-2.363592	-3.846455
H	3.423885	-2.736109	-3.329392
H	4.700596	-4.012550	-3.290385
H	2.087482	-1.203214	2.488745
H	4.230650	-2.024876	3.560920
H	3.367602	-3.467317	4.181275
H	2.923873	-1.830660	4.772292
H	0.039380	-2.659399	2.444427
H	0.460350	-2.043036	4.068470
H	0.800462	-3.750053	3.661258
H	5.747763	-1.247592	1.416814
H	5.682561	1.560719	1.348432
H	3.055201	5.030594	-1.939824
H	2.311674	6.325676	0.056183
H	2.219861	5.235814	2.295916
H	3.717973	1.351981	-1.937228
H	5.707835	3.701498	-2.319751
H	5.857335	2.063788	-3.041763
H	5.976028	2.277204	-1.266343
H	2.127694	2.731722	-3.316241
H	3.564875	2.154051	-4.207491
H	3.471852	3.867196	-3.705122
H	2.845755	1.573336	2.868001
H	5.060037	2.765608	3.261477
H	4.127121	2.588635	4.781308
H	4.176171	4.168280	3.932416
H	1.564902	4.131408	4.041641
H	1.572622	2.490684	4.745993
H	0.679028	2.788929	3.220171
Cl	1.940020	-0.546086	-2.559397



N	-0.885209	-0.078964	-1.208983
C	-1.827781	0.797527	-0.791564
C	-1.228251	-1.010097	-2.131442
C	-3.136258	0.783535	-1.291806
C	-2.521359	-1.097499	-2.657765
C	-3.508928	-0.182246	-2.244123
H	-1.507365	1.506399	-0.012234
H	-3.863182	1.522818	-0.922797
H	-0.416833	-1.679946	-2.455558
H	-2.751465	-1.888606	-3.388518
C	-4.905388	-0.230667	-2.853736
H	-4.868082	0.266058	-3.848409
H	-5.182395	-1.287831	-3.026997
N	-5.942483	0.452060	-2.095109
H	-6.186870	1.404394	-2.388030
C	-6.573153	0.078003	-0.941897
C	-6.340981	-1.295469	-0.350743
C	-7.452362	0.930690	-0.292410
C	-7.063103	-1.674420	0.898725
C	-8.179164	0.579499	0.928365
C	-7.926944	-0.798745	1.502224
Cl	-7.731185	2.536801	-0.943880
O	-8.962696	1.357136	1.483952
O	-5.563692	-2.081218	-0.902794
C	-8.670624	-1.136172	2.761622
H	-9.295785	-2.045441	2.627077
H	-7.966821	-1.360566	3.592648
H	-9.318584	-0.290073	3.057528
C	-6.783299	-3.048540	1.447649
H	-6.071786	-3.587983	0.795384
H	-6.351188	-2.990757	2.470004
H	-7.716326	-3.646282	1.531226

79

**IPrCl<sub>2</sub>PEPPSI** SCF Done: -2915.17569782 A.U.

Pd	0.661096	-0.584370	0.223122
N	-1.011137	1.908053	-0.084461
C	2.105683	4.717220	0.566306
N	-2.217439	0.108392	-0.354208
C	1.439085	4.146708	1.658494
C	0.404069	3.205721	1.476993
Cl	0.004367	-0.885518	2.461362
C	0.078220	2.845561	0.140128
C	0.719080	3.426243	-0.989025
C	1.741846	4.365190	-0.739693

C	0.301971	3.122313	-2.429613
C	-0.663807	4.208542	-2.958698
C	1.501848	2.960420	-3.382437
C	-0.370900	2.677276	2.684615
C	-1.515886	3.648992	3.055556
C	0.523275	2.398543	3.906616
C	-2.318459	2.327572	-0.338596
C	-3.073058	1.200357	-0.512077
C	-2.674028	-1.267854	-0.473325
C	-2.553086	-1.917992	-1.732944
C	-3.025232	-3.243981	-1.823469
C	-3.608915	-3.886745	-0.723933
C	-3.747985	-3.207758	0.493157
C	-3.291016	-1.882560	0.651172
C	-2.020116	-1.209489	-2.979409
C	-3.187623	-0.580870	-3.776003
C	-1.172935	-2.122546	-3.884432
C	-3.533942	-1.148601	1.971644
C	-4.974600	-0.587594	2.022400
C	-3.252962	-2.021909	3.209101
C	-0.936947	0.534867	-0.090018
H	2.912323	5.448682	0.734843
H	1.722706	4.441001	2.680188
H	2.263648	4.827988	-1.591020
H	-0.231409	2.149276	-2.423214
H	-0.168469	5.202810	-2.983994
H	-1.572689	4.306755	-2.330748
H	-0.992612	3.967750	-3.991752
H	1.148432	2.626410	-4.380149
H	2.207746	2.196916	-3.001690
H	2.048666	3.915520	-3.534299
H	-0.819226	1.703185	2.400869
H	-2.217221	3.809327	2.210819
H	-1.116484	4.642764	3.352013
H	-2.102874	3.249989	3.909644
H	1.354699	1.713973	3.647199
H	-0.073723	1.909610	4.703597
H	0.948557	3.329078	4.340123
H	-2.586478	3.387361	-0.369137
H	-4.135659	1.070932	-0.735596
H	-2.936917	-3.780432	-2.780209
H	-3.967223	-4.924346	-0.819603
H	-4.221643	-3.716426	1.346498
H	-1.346919	-0.393211	-2.646706

H	-3.895045	-1.361469	-4.129609
H	-2.804109	-0.040094	-4.666924
H	-3.766243	0.142775	-3.165705
H	-0.346893	-2.593849	-3.316423
H	-0.717152	-1.523299	-4.699087
H	-1.779465	-2.920351	-4.364388
H	-2.822617	-0.298198	2.016641
H	-5.190970	0.094635	1.175092
H	-5.139199	-0.020087	2.962690
H	-5.722620	-1.408492	1.986663
H	-3.973418	-2.862497	3.303384
H	-3.345473	-1.410267	4.130685
H	-2.223998	-2.429970	3.176454
Cl	1.322648	-0.290968	-2.011940
N	2.387841	-1.792957	0.570660
C	2.329858	-2.845488	1.421063
C	3.550708	-1.505656	-0.055342
C	3.445066	-3.657316	1.669403
C	4.707711	-2.271915	0.165767
C	4.664755	-3.371862	1.038108
H	1.362362	-2.998287	1.923092
H	3.354249	-4.508414	2.360778
H	3.532680	-0.666023	-0.767457
H	5.564531	-3.980769	1.211434
Cl	6.185974	-1.842102	-0.655985

91

**IPrCl<sub>2</sub>PEPPSI+DMF SCF Done: -3163.51078636 A.U.**

Pd	0.141111	-0.147571	-0.603543
N	-2.500033	-0.829819	0.686817
C	-2.266142	-5.043998	0.224081
N	-2.159928	1.326421	0.665775
C	-2.638944	-4.240275	-0.861386
C	-2.718855	-2.837154	-0.742718
Cl	-0.806681	0.570675	-2.631166
C	-2.384191	-2.269296	0.518094
C	-2.017979	-3.059994	1.641982
C	-1.967234	-4.458105	1.460331
C	-1.733462	-2.467497	3.024519
C	-2.972086	-2.593529	3.942049
C	-0.500878	-3.098081	3.701921
C	-3.223701	-1.994348	-1.914334
C	-4.764315	-1.866741	-1.862304
C	-2.766224	-2.521348	-3.286428
C	-3.610179	-0.235739	1.290707

C	-3.392879	1.114168	1.285032
C	-1.607549	2.657292	0.468415
C	-0.623553	3.130390	1.379717
C	-0.137292	4.439715	1.184747
C	-0.617386	5.248987	0.147038
C	-1.604201	4.764074	-0.720169
C	-2.125173	3.460229	-0.585063
C	-0.149759	2.309121	2.578740
C	-1.016810	2.623697	3.820297
C	1.346078	2.497735	2.890419
C	-3.237165	2.992840	-1.527626
C	-4.607106	3.562216	-1.090556
C	-2.954472	3.348136	-3.000929
C	-1.595301	0.128531	0.294434
H	-2.212698	-6.138261	0.106029
H	-2.882297	-4.711219	-1.825538
H	-1.681668	-5.098930	2.308519
H	-1.505103	-1.390725	2.884278
H	-3.232737	-3.660140	4.111952
H	-3.867854	-2.099054	3.514338
H	-2.772988	-2.131967	4.932317
H	-0.264685	-2.553020	4.639762
H	0.384856	-3.038104	3.039956
H	-0.673400	-4.160272	3.978026
H	-2.788349	-0.978414	-1.818026
H	-5.112690	-1.412135	-0.911899
H	-5.252087	-2.860893	-1.956998
H	-5.129395	-1.227712	-2.694011
H	-1.667148	-2.660098	-3.317914
H	-3.031527	-1.788485	-4.075340
H	-3.251879	-3.484568	-3.553778
H	-4.448324	-0.830663	1.663600
H	-3.994573	1.943733	1.666398
H	0.633561	4.831020	1.865178
H	-0.220335	6.268266	0.014731
H	-1.978849	5.408785	-1.529879
H	-0.278889	1.235844	2.331119
H	-0.920690	3.691084	4.114945
H	-0.699035	2.002167	4.684163
H	-2.093026	2.422769	3.638243
H	1.972567	2.317464	1.994184
H	1.657167	1.773502	3.671109
H	1.570073	3.514852	3.278875
H	-3.282471	1.885892	-1.468722

H	-4.874889	3.272064	-0.053958
H	-5.413338	3.196996	-1.761423
H	-4.608112	4.672424	-1.134046
H	-2.996403	4.443616	-3.180890
H	-3.718731	2.881230	-3.656870
H	-1.960474	2.970515	-3.310730
Cl	1.073868	-0.902858	1.423274
N	2.014249	-0.425457	-1.575989
C	2.421087	0.439150	-2.533384
C	2.815413	-1.454444	-1.223521
C	3.655284	0.297239	-3.181598
C	4.059003	-1.653485	-1.842703
C	4.498125	-0.769692	-2.841108
H	1.712441	1.241229	-2.786113
H	3.951725	1.027543	-3.948908
H	2.457451	-2.103922	-0.410209
H	5.473532	-0.917625	-3.328082
Cl	5.052605	-3.006001	-1.346290
O	4.120840	1.866810	-0.012207
N	5.740206	0.894648	1.332929
C	7.124630	0.908382	1.764828
H	7.204314	1.014126	2.870397
H	7.651613	-0.029126	1.474961
H	7.652494	1.763225	1.294921
C	4.874842	-0.161184	1.840415
H	3.836406	0.026847	1.505181
H	5.198776	-1.157592	1.464671
H	4.899376	-0.183142	2.951574
C	5.261608	1.818553	0.437744
H	6.063156	2.559956	0.148817
136			
<b>DimerIPrCl<sub>2</sub></b> SCF Done: -4415.10573618 A.U.			
Pd	1.697096	-0.176234	-0.523006
N	4.191238	1.164678	0.477245
C	3.124678	5.134030	-0.581406
N	4.236283	-0.987912	0.851704
C	4.000053	4.404641	-1.395394
Cl	-0.525683	-0.413615	-1.540800
C	4.362870	3.078344	-1.080473
Cl	2.698564	0.013806	-2.610084
C	3.800767	2.512574	0.096593
C	2.928831	3.236002	0.956847
C	2.599727	4.554892	0.581603
C	2.420758	2.667807	2.282978

C	3.389208	3.041770	3.430096
C	0.981238	3.095699	2.621723
C	5.366477	2.339016	-1.968083
C	6.812264	2.791817	-1.656709
C	5.064384	2.500834	-3.470803
C	5.408160	0.883315	1.100209
C	5.439982	-0.465074	1.327546
C	3.905379	-2.401294	0.947897
C	3.413518	-2.899391	2.186131
C	3.146778	-4.282089	2.265417
C	3.363436	-5.129374	1.171352
C	3.866063	-4.611882	-0.029562
C	4.157584	-3.239404	-0.172674
C	3.220467	-2.018246	3.423171
C	4.442170	-2.121648	4.366948
C	1.925468	-2.338383	4.195839
C	4.786374	-2.718399	-1.465057
C	6.323872	-2.879411	-1.418988
C	4.203019	-3.373610	-2.730503
C	3.457755	0.012605	0.318749
H	2.852192	6.166494	-0.853196
H	4.411411	4.871288	-2.303480
H	1.921434	5.139882	1.220460
H	2.406201	1.561983	2.196074
H	3.438362	4.143744	3.564171
H	4.421159	2.681464	3.238512
H	3.047438	2.597395	4.388617
H	0.623116	2.544251	3.514398
H	0.281820	2.868453	1.792956
H	0.910147	4.179566	2.855026
H	5.280255	1.256818	-1.739932
H	7.086804	2.632570	-0.593717
H	6.945578	3.873217	-1.873672
H	7.539325	2.229868	-2.280317
H	4.022304	2.200835	-3.695525
H	5.742839	1.853389	-4.064656
H	5.223123	3.544016	-3.818437
H	6.132181	1.670795	1.327188
H	6.203678	-1.102969	1.780952
H	2.757057	-4.700090	3.205808
H	3.140833	-6.205061	1.256569
H	4.041562	-5.287934	-0.879786
H	3.143086	-0.966019	3.076592
H	4.564813	-3.160693	4.740425

H	4.310252	-1.458606	5.247825
H	5.389464	-1.834230	3.867416
H	1.041197	-2.314275	3.529931
H	1.767849	-1.587526	4.997564
H	1.971985	-3.333055	4.687946
H	4.554496	-1.636686	-1.545728
H	6.772198	-2.349357	-0.553100
H	6.785513	-2.467700	-2.341301
H	6.613204	-3.949761	-1.342456
H	4.471537	-4.448774	-2.812590
H	4.601240	-2.865551	-3.632457
H	3.099098	-3.281452	-2.757132
Pd	-1.697174	-0.176204	0.523228
N	-4.235982	-0.988639	-0.851720
C	-3.362246	-5.129959	-1.170790
N	-4.191474	1.164010	-0.477513
C	-3.864845	-4.612382	0.030099
Cl	0.525672	-0.412834	1.541172
C	-4.156648	-3.239945	0.173024
Cl	-2.698877	0.014719	2.610115
C	-3.904753	-2.401961	-0.947711
C	-3.412894	-2.900144	-2.185912
C	-3.145878	-4.282799	-2.265009
C	-3.220082	-2.019150	-3.423100
C	-4.441750	-2.123020	-4.366870
C	-1.925005	-2.339095	-4.195722
C	-4.785378	-2.718857	1.465402
C	-6.322856	-2.880100	1.419543
C	-4.201773	-3.373796	2.730875
C	-5.439715	-0.466125	-1.327826
C	-5.408229	0.882298	-1.100643
C	-3.801375	2.512030	-0.096932
C	-2.929161	3.235439	-0.956918
C	-2.600387	4.554428	-0.581733
C	-3.125935	5.133688	0.580944
C	-4.001596	4.404324	1.394646
C	-4.364087	3.077925	1.079786
C	-2.420504	2.667149	-2.282783
C	-3.388564	3.040886	-3.430305
C	-0.980901	3.095157	-2.621022
C	-5.367975	2.338617	1.967093
C	-6.813665	2.791440	1.655293
C	-5.066318	2.500443	3.469901
C	-3.457768	0.012110	-0.318749

H	-3.139427	-6.205613	-1.255866
H	-4.040101	-5.288332	0.880453
H	-2.756157	-4.700866	-3.205370
H	-3.142962	-0.966845	-3.076694
H	-4.564123	-3.162160	-4.740171
H	-5.389125	-1.835761	-3.867401
H	-4.309990	-1.460095	-5.247859
H	-1.767571	-1.588330	-4.997571
H	-1.040734	-2.314676	-3.529825
H	-1.971286	-3.333857	-4.687668
H	-4.553661	-1.637099	1.545907
H	-6.771369	-2.350208	0.553653
H	-6.612047	-3.950500	1.343176
H	-6.784436	-2.468344	2.341866
H	-3.097854	-3.281547	2.757324
H	-4.599898	-2.865611	3.632799
H	-4.470175	-4.448972	2.813193
H	-6.203197	-1.104247	-1.781271
H	-6.132388	1.669582	-1.327861
H	-1.921893	5.139404	-1.220389
H	-2.853706	6.166232	0.852690
H	-4.413437	4.871070	2.302463
H	-2.405862	1.561339	-2.195768
H	-3.437782	4.142840	-3.564522
H	-3.046389	2.596436	-4.388647
H	-4.420550	2.680496	-3.239058
H	-0.281771	2.868054	-1.791972
H	-0.622384	2.543668	-3.513511
H	-0.909827	4.179014	-2.854385
H	-5.281722	1.256419	1.738960
H	-7.087896	2.632208	0.592218
H	-7.540918	2.229505	2.278689
H	-6.947026	3.872842	1.872219
H	-5.225167	3.543629	3.817476
H	-5.744937	1.852997	4.063567
H	-4.024292	2.200474	3.694914

**BP86-d3/def2SVP**

32			
Py1	SCF Done: -1335.79729368 A.U.		
N	-4.422144	-0.387863	-0.657077
C	-5.324723	-0.067850	0.284614
C	-3.141935	-0.556886	-0.275005
C	-5.004208	0.095110	1.645412



C	-2.715334	-0.419331	1.059992
C	-3.668168	-0.086881	2.036192
H	-6.366166	0.065686	-0.062045
H	-5.784817	0.358127	2.375825
H	-1.657178	-0.559266	1.325155
H	-3.367545	0.032391	3.089298
C	-2.183777	-0.885520	-1.417222
H	-2.619759	-1.726029	-1.995793
H	-2.154071	-0.017622	-2.105571
N	-0.841042	-1.266918	-1.022214
H	-0.621270	-2.271423	-0.940766
C	0.233986	-0.521357	-0.664486
C	1.415210	-1.426117	-0.331671
C	0.382627	0.856683	-0.545358
C	2.704006	-0.808118	0.052719
C	1.646161	1.503831	-0.147061
C	2.817681	0.599654	0.139596
Cl	-0.932870	1.978236	-0.836865
O	1.763679	2.728238	-0.042867
O	1.256081	-2.649911	-0.393800
C	4.046909	1.173506	0.507773
C	5.153248	0.352301	0.784758
C	3.815063	-1.630295	0.333981
C	5.038859	-1.049321	0.698119
H	4.105208	2.270980	0.569421
H	6.114352	0.808078	1.071276
H	5.908375	-1.689095	0.915732
H	3.692254	-2.721458	0.258433
32			
<b>Py2</b> SCF Done: -1335.79292026 A.U.			
N	-3.509351	0.081226	2.047160
C	-4.364014	-0.954725	1.969978
C	-2.911026	0.480352	0.912567
C	-4.661175	-1.629141	0.771270
C	-3.128103	-0.121535	-0.348705
C	-4.027891	-1.203093	-0.406476
H	-4.843304	-1.266427	2.916359
H	-5.374207	-2.468394	0.763674
H	-2.216977	1.337462	0.994685
H	-4.233207	-1.704141	-1.367982
C	-2.362396	0.345287	-1.576740
H	-2.905137	0.050613	-2.498743
H	-2.263918	1.445242	-1.583417
N	-1.030734	-0.259705	-1.647070

H	-1.006183	-1.268155	-1.875098
C	0.108369	0.069852	-0.983427
C	1.036698	-1.137927	-0.889282
C	0.525476	1.279109	-0.439237
C	2.346020	-0.986863	-0.215767
C	1.811645	1.459005	0.261985
C	2.714405	0.256685	0.349861
Cl	-0.420446	2.753201	-0.556771
O	2.156912	2.538232	0.750327
O	0.658702	-2.208980	-1.374977
C	3.954695	0.382584	0.999715
C	3.217350	-2.092761	-0.129628
C	4.453496	-1.958470	0.519549
C	4.820678	-0.720662	1.083873
H	2.899934	-3.046649	-0.577577
H	5.134901	-2.820768	0.588972
H	5.791339	-0.616083	1.594149
H	4.214644	1.362045	1.429437
32			
<b>Py2isom</b> SCF Done: -1335.79427088 A.U.			
N	-4.747078	-1.601407	0.722859
C	-4.509196	-0.973773	1.888137
C	-4.064146	-1.181281	-0.354374
C	-3.597268	0.090297	2.024392
C	-3.122932	-0.129085	-0.339713
C	-2.890863	0.519015	0.891012
H	-5.076794	-1.336053	2.765074
H	-3.446638	0.574296	3.002089
H	-4.277471	-1.708272	-1.305399
H	-2.173066	1.353073	0.949907
C	-2.350952	0.243732	-1.595294
H	-2.886913	-0.127930	-2.492935
H	-2.259304	1.340393	-1.689869
N	-1.016247	-0.358100	-1.614180
H	-0.980288	-1.373560	-1.806739
C	0.119805	0.012623	-0.970965
C	1.069014	-1.177484	-0.843308
C	0.522968	1.245451	-0.469257
C	2.379206	-0.983391	-0.182766
C	1.804315	1.465943	0.226800
C	2.729182	0.282839	0.342977
Cl	-0.448451	2.701131	-0.625854
O	2.129032	2.562486	0.691303
O	0.705911	-2.268912	-1.292230

C	3.971015	0.449263	0.980704
C	4.856895	-0.635730	1.091431
C	3.270183	-2.071083	-0.069413
C	4.507915	-1.896083	0.566836
H	4.216528	1.445408	1.379477
H	5.829013	-0.498926	1.591206
H	5.204820	-2.743949	0.656776
H	2.966659	-3.043276	-0.486602
32			
<b>Py2isom90</b> SCF Done: -1335.79292013 A.U.			
N	-3.508956	0.081298	2.047347
C	-4.363231	-0.954999	1.970370
C	-2.910891	0.480479	0.912628
C	-4.660228	-1.629728	0.771805
C	-3.127851	-0.121647	-0.348538
C	-4.027220	-1.203575	-0.406055
H	-4.842170	-1.266858	2.916883
H	-5.372972	-2.469225	0.764355
H	-2.217276	1.337960	0.994536
H	-4.232441	-1.704851	-1.367466
C	-2.362552	0.345181	-1.576848
H	-2.905456	0.050016	-2.498596
H	-2.264495	1.445178	-1.583882
N	-1.030765	-0.259459	-1.647422
H	-1.005988	-1.267755	-1.876077
C	0.108293	0.069986	-0.983675
C	1.036751	-1.137708	-0.889852
C	0.525242	1.279208	-0.439269
C	2.345892	-0.986730	-0.215971
C	1.811198	1.458970	0.262346
C	2.714016	0.256690	0.350125
Cl	-0.420520	2.753295	-0.557257
O	2.156262	2.538097	0.751080
O	0.658975	-2.208639	-1.375992
C	3.954144	0.382507	1.000303
C	4.820217	-0.720680	1.084325
C	3.217309	-2.092566	-0.129966
C	4.453291	-1.958353	0.519542
H	4.213898	1.361863	1.430380
H	5.790752	-0.616154	1.594851
H	5.134764	-2.820606	0.588866
H	2.900086	-3.046353	-0.578268
32			
<b>Py2isom-90</b> SCF Done: -1335.79427076 A.U.			

N	-4.747188	-1.601165	0.723236
C	-4.509201	-0.973333	1.888394
C	-4.064200	-1.181378	-0.354072
C	-3.597218	0.090717	2.024379
C	-3.122869	-0.129278	-0.339671
C	-2.890738	0.519086	0.890901
H	-5.076899	-1.335314	2.765387
H	-3.446567	0.574959	3.001953
H	-4.277561	-1.708573	-1.304987
H	-2.172878	1.353097	0.949664
C	-2.350898	0.243123	-1.595413
H	-2.886868	-0.128994	-2.492866
H	-2.259340	1.339753	-1.690460
N	-1.016187	-0.358624	-1.614098
H	-0.980042	-1.374037	-1.806813
C	0.119831	0.012308	-0.970976
C	1.069262	-1.177637	-0.843302
C	0.522819	1.245263	-0.469431
C	2.379355	-0.983320	-0.182646
C	1.804054	1.465960	0.226722
C	2.729091	0.282995	0.343054
Cl	-0.448685	2.700838	-0.626456
O	2.128596	2.562582	0.691187
O	0.706397	-2.269116	-1.292295
C	3.970853	0.449645	0.980857
C	4.856890	-0.635209	1.091703
C	3.270492	-2.070872	-0.069181
C	4.508147	-1.895646	0.567152
H	4.216185	1.445849	1.379591
H	5.828952	-0.498221	1.591537
H	5.205176	-2.743400	0.657190
H	2.967149	-3.043129	-0.486352

32

**Py3** SCF Done: -1335.79385543 A.U.

N	-4.282443	-0.321271	2.187651
C	-3.174627	-1.070249	2.051501
C	-4.731801	0.306667	1.085344
C	-2.480060	-1.230670	0.838575
C	-4.111080	0.219744	-0.172302
C	-2.956178	-0.573263	-0.310032
H	-2.809835	-1.577086	2.964073
H	-1.573828	-1.855123	0.794922
H	-5.638996	0.926388	1.209975
H	-4.517951	0.776688	-1.032128

C	-2.270864	-0.716170	-1.663878
H	-2.769319	-1.527783	-2.236690
H	-2.412786	0.214051	-2.248694
N	-0.861555	-1.065571	-1.591153
H	-0.605900	-2.061205	-1.677562
C	0.153363	-0.381533	-0.995358
C	1.323362	-1.307949	-0.700133
C	0.241118	0.957540	-0.639941
C	2.543155	-0.745959	-0.078210
C	1.427450	1.544599	0.017463
C	2.590054	0.622584	0.278984
Cl	-1.035512	2.109539	-0.967732
O	1.488614	2.734869	0.334215
O	1.209550	-2.506614	-0.981655
C	3.747009	1.140608	0.886404
C	3.649438	-1.584434	0.171244
C	4.801384	-1.058690	0.775075
C	4.848480	0.303216	1.132713
H	3.579206	-2.644386	-0.116769
H	5.666734	-1.711202	0.970191
H	5.752669	0.715085	1.608372
H	3.755168	2.208005	1.155087

32

**Py3isom** SCF Done: -1335.79385564 A.U.

N	-4.282826	-0.318930	2.187590
C	-3.175063	-1.068184	2.052441
C	-4.731956	0.307847	1.084589
C	-2.480342	-1.229941	0.839800
C	-4.111016	0.219529	-0.172898
C	-2.956196	-0.573712	-0.309612
H	-2.810479	-1.574037	2.965631
H	-1.574157	-1.854519	0.796929
H	-5.639113	0.927789	1.208357
H	-4.517773	0.775619	-1.033331
C	-2.270668	-0.718211	-1.663189
H	-2.768958	-1.530632	-2.235000
H	-2.412635	0.211266	-2.249189
N	-0.861355	-1.067418	-1.589868
H	-0.605382	-2.062975	-1.676053
C	0.153527	-0.382662	-0.994896
C	1.323877	-1.308542	-0.699312
C	0.241010	0.956719	-0.640552
C	2.543498	-0.745809	-0.077733
C	1.427105	1.544497	0.016561

C	2.589962	0.622947	0.278702
Cl	-1.035882	2.108202	-0.969325
O	1.487962	2.734979	0.332596
O	1.210490	-2.507377	-0.980261
C	3.746752	1.141667	0.885834
C	4.848498	0.304765	1.132582
C	3.650063	-1.583789	0.172141
C	4.801849	-1.057346	0.775665
H	3.754578	2.209220	1.153910
H	5.752555	0.717186	1.608013
H	5.667421	-1.709467	0.971100
H	3.580175	-2.643915	-0.115315
32			
<b>Py3isom90</b> SCF Done: -1335.79383584 A.U.			
N	-4.457272	-0.980337	2.000258
C	-4.671354	-1.579445	0.815860
C	-3.583727	0.043527	2.019530
C	-4.034885	-1.195795	-0.378988
C	-2.893979	0.508125	0.885672
C	-3.121320	-0.124509	-0.353364
H	-5.393785	-2.416690	0.812445
H	-4.254200	-1.727425	-1.320047
H	-3.421169	0.529829	2.999066
H	-2.195408	1.356380	0.961765
C	-2.355029	0.291530	-1.601562
H	-2.893561	-0.048728	-2.509721
H	-2.262062	1.390742	-1.655139
N	-1.023080	-0.312360	-1.637273
H	-0.991604	-1.325090	-1.844927
C	0.112996	0.040013	-0.981375
C	1.052074	-1.158772	-0.867544
C	0.522072	1.261957	-0.460178
C	2.360801	-0.984783	-0.198830
C	1.804259	1.463056	0.242136
C	2.718990	0.271204	0.345722
Cl	-0.438368	2.725572	-0.598097
O	2.136052	2.551145	0.720419
O	0.682111	-2.240615	-1.334345
C	3.959448	0.418820	0.990668
C	4.835809	-0.674940	1.090378
C	3.242274	-2.081242	-0.096540
C	4.478632	-1.925099	0.547295
H	4.211492	1.407290	1.404166
H	5.806746	-0.553107	1.596248

H	5.167999	-2.779926	0.628994
H	2.932602	-3.045240	-0.527949
32			
<b>Py3isom-90</b> SCF Done: -1335.79383585 A.U.			
N	-4.456865	-0.980991	2.000231
C	-3.583412	0.042959	2.019685
C	-4.671027	-1.579775	0.815685
C	-2.893849	0.507945	0.885874
C	-4.034748	-1.195714	-0.379132
C	-3.121283	-0.124344	-0.353314
H	-3.420779	0.528989	2.999340
H	-2.195333	1.356228	0.962160
H	-5.393372	-2.417095	0.812108
H	-4.254117	-1.727101	-1.320316
C	-2.355128	0.292115	-1.601445
H	-2.893729	-0.047819	-2.509680
H	-2.262188	1.391348	-1.654662
N	-1.023173	-0.311754	-1.637477
H	-0.991740	-1.324440	-1.845362
C	0.112937	0.040380	-0.981486
C	1.051901	-1.158501	-0.867910
C	0.522097	1.262172	-0.459993
C	2.360600	-0.984793	-0.199065
C	1.804362	1.463048	0.242256
C	2.718922	0.271057	0.345713
Cl	-0.438235	2.725887	-0.597563
O	2.136332	2.551062	0.720583
O	0.681859	-2.240209	-1.334963
C	3.959352	0.418397	0.990777
C	4.835542	-0.675507	1.090404
C	3.241908	-2.081393	-0.096872
C	4.478229	-1.925532	0.547101
H	4.211514	1.406772	1.404428
H	5.806451	-0.553897	1.596382
H	5.167462	-2.780474	0.628733
H	2.932139	-3.045276	-0.528471
32			
<b>Py4</b> SCF Done: -1260.82315622 A.U.			
N	-4.027023	-0.362022	-0.754859
C	-4.957009	0.001643	0.143286
C	-2.762325	-0.530467	-0.323876
C	-4.680698	0.210764	1.507431
C	-2.379461	-0.348383	1.019175
C	-3.360739	0.029337	1.949596

H	-5.984585	0.133232	-0.243279
H	-5.482372	0.508425	2.200812
H	-1.332585	-0.488159	1.326104
H	-3.094305	0.184301	3.007261
C	-1.769326	-0.907276	-1.420727
H	-2.203235	-1.749687	-1.997912
H	-1.692750	-0.054382	-2.124491
N	-0.451581	-1.307873	-0.966799
H	-0.255944	-2.313228	-0.847865
C	0.616897	-0.567959	-0.576671
C	1.773640	-1.475720	-0.161311
C	0.787661	0.803711	-0.486272
C	3.058992	-0.884089	0.273007
C	2.050429	1.404998	-0.035412
C	3.193446	0.477051	0.331695
Cl	-0.477302	1.958582	-0.870824
O	2.205925	2.627985	0.055927
O	1.593790	-2.699211	-0.200931
C	4.470622	1.131068	0.770081
H	4.742509	0.817193	1.801609
H	5.316973	0.823184	0.118277
H	4.370684	2.231882	0.742161
C	4.170233	-1.830361	0.643815
H	4.499472	-1.668328	1.692757
H	3.845117	-2.881584	0.533737
H	5.063479	-1.665576	0.003554
32			
<b>Py5</b> SCF Done: -1260.81914962 A.U.			
N	-3.271607	0.518148	1.889688
C	-4.217444	-0.437903	1.857629
C	-2.574039	0.741608	0.763466
C	-4.511494	-1.202081	0.713212
C	-2.777188	0.034477	-0.444429
C	-3.773798	-0.960121	-0.455911
H	-4.777177	-0.605510	2.796332
H	-5.302190	-1.968188	0.740114
H	-1.805543	1.535681	0.806150
H	-3.972091	-1.536894	-1.375542
C	-1.897029	0.295019	-1.656950
H	-2.416298	-0.030381	-2.582232
H	-1.676128	1.372588	-1.757035
N	-0.639046	-0.449068	-1.580103
H	-0.710774	-1.473462	-1.699703
C	0.490406	-0.160973	-0.880481



C	1.290457	-1.433541	-0.599385
C	0.999789	1.044260	-0.428789
C	2.577312	-1.356366	0.127706
C	2.264346	1.134862	0.317859
C	3.030320	-0.146306	0.580280
Cl	0.232384	2.595855	-0.732609
O	2.717242	2.211666	0.720478
O	0.821639	-2.509461	-0.990182
C	4.312812	-0.013361	1.347463
H	5.171831	-0.390556	0.750758
H	4.494959	1.043476	1.616396
H	4.284463	-0.626396	2.274589
C	3.324919	-2.643026	0.358097
H	3.444481	-2.843603	1.444740
H	2.791586	-3.496416	-0.100196
H	4.349657	-2.590354	-0.068105
32			
<b>Py5isom</b> SCF Done: -1260.82046912 A.U.			
N	-4.563240	-1.208384	0.658499
C	-4.325460	-0.503417	1.778791
C	-3.794399	-0.944707	-0.410395
C	-3.329239	0.486814	1.875908
C	-2.763670	0.019768	-0.431276
C	-2.533276	0.751954	0.751724
H	-4.964701	-0.737097	2.650130
H	-3.183228	1.040757	2.816499
H	-4.008365	-1.533183	-1.324538
H	-1.746142	1.522752	0.779653
C	-1.896380	0.207665	-1.665732
H	-2.421135	-0.184022	-2.561474
H	-1.687179	1.278356	-1.839673
N	-0.631238	-0.520387	-1.555379
H	-0.689170	-1.548422	-1.648478
C	0.496786	-0.195915	-0.872380
C	1.321414	-1.448389	-0.566494
C	0.989852	1.028020	-0.451978
C	2.609337	-1.331710	0.153314
C	2.249950	1.156865	0.294659
C	3.041681	-0.104015	0.577924
Cl	0.191773	2.560042	-0.783443
O	2.678627	2.248871	0.683969
O	0.870388	-2.540435	-0.930953
C	3.381912	-2.599061	0.407003
H	3.512002	-2.773565	1.496947

H	2.861860	-3.472090	-0.028984
H	4.402854	-2.536848	-0.026965
C	4.325069	0.068423	1.335842
H	4.318225	-0.535692	2.269109
H	5.189170	-0.293820	0.737056
H	4.483430	1.132290	1.591816
32			
<b>Py6</b> SCF Done: -1260.81758680 A.U.			
N	-4.059976	0.512923	1.843345
C	-3.092333	-0.417166	1.931575
C	-4.308376	1.018438	0.621380
C	-2.346989	-0.879731	0.832368
C	-3.620892	0.629810	-0.541950
C	-2.616576	-0.350557	-0.444624
H	-2.892035	-0.822689	2.940650
H	-1.556832	-1.634643	0.974382
H	-5.098003	1.790303	0.562017
H	-3.855601	1.099350	-1.510740
C	-1.860415	-0.826920	-1.677860
H	-2.384644	-1.708031	-2.106955
H	-1.867830	-0.031720	-2.447043
N	-0.493350	-1.261094	-1.401214
H	-0.355569	-2.271125	-1.290044
C	0.496632	-0.532653	-0.800374
C	0.469528	0.978077	-0.875716
C	1.556969	-1.138886	-0.147137
C	1.587541	1.748048	-0.257248
C	2.673944	-0.404577	0.454902
C	2.627852	1.104309	0.357876
Cl	1.583585	-2.888413	0.013169
O	3.607800	-0.969825	1.034051
O	-0.462924	1.552272	-1.446195
C	3.772070	1.849368	0.981516
H	4.286331	2.488066	0.230965
H	3.410891	2.534508	1.779203
H	4.501983	1.142296	1.417711
C	1.511713	3.249009	-0.347527
H	0.607327	3.564488	-0.900095
H	1.486663	3.707155	0.664843
H	2.406628	3.663264	-0.859614
11			
<b>PEPPSIorg</b> SCF Done: -707.611445747 A.U.			
N	1.549112	-1.256182	-0.000020
C	2.231564	-0.097149	-0.000058

C	0.209006	-1.202241	0.000085
C	1.610935	1.165765	0.000038
C	-0.500980	0.017231	-0.000010
C	0.208649	1.230016	0.000018
H	3.333733	-0.176217	-0.000159
H	2.214189	2.087205	0.000113
H	-0.344798	-2.158071	0.000111
H	-0.330113	2.189365	-0.000008
Cl	-2.251285	0.009957	-0.000021
66			
<b>IPr</b> SCF Done: -1287.32550290 A.U.			
Pd	0.000033	0.000406	-1.816116
N	1.083234	-0.022422	0.976826
C	5.103567	-0.082932	-0.306713
N	-1.083285	0.023349	0.976882
C	4.390763	-1.285398	-0.190203
C	3.047727	-1.293917	0.237715
C	2.453973	-0.044502	0.539835
C	3.145528	1.187970	0.428692
C	4.486199	1.140360	-0.001551
C	2.436039	2.518329	0.672902
C	3.301499	3.536551	1.436944
C	1.929418	3.091523	-0.668701
C	2.256952	-2.597656	0.310300
C	2.966440	-3.667347	1.162462
C	1.940350	-3.106130	-1.111168
C	0.684696	-0.015260	2.315185
C	-0.684675	0.016130	2.315225
C	-2.454050	0.044589	0.539923
C	-3.048686	1.293639	0.238007
C	-4.391647	1.284224	-0.190107
C	-5.103562	0.081255	-0.306938
C	-4.485371	-1.141637	-0.001865
C	-3.144719	-1.188355	0.428553
C	-2.258754	2.597872	0.310915
C	-2.969905	3.667752	1.161446
C	-1.940568	3.105662	-1.110456
C	-2.434422	-2.518284	0.672783
C	-3.299154	-3.536798	1.437277
C	-1.927859	-3.091497	-0.668822
C	-0.000052	0.000417	0.115077
H	6.152401	-0.097721	-0.643840
H	4.883065	-2.237517	-0.443937
H	5.054630	2.076924	-0.109409

H	1.540608	2.311846	1.297471
H	4.168592	3.879041	0.833126
H	3.694929	3.112179	2.384157
H	2.704522	4.439236	1.683741
H	1.348304	4.023872	-0.505124
H	1.274240	2.352434	-1.183839
H	2.782275	3.325906	-1.341130
H	1.283911	-2.373394	0.795851
H	3.185977	-3.293797	2.184399
H	3.927713	-3.986356	0.706581
H	2.330736	-4.572941	1.254414
H	1.376080	-2.323727	-1.670193
H	1.318235	-4.025007	-1.071714
H	2.870783	-3.340094	-1.671399
H	1.410971	-0.030524	3.133426
H	-1.410906	0.031435	3.133504
H	-4.884615	2.236020	-0.443751
H	-6.152354	0.095349	-0.644225
H	-5.053119	-2.078593	-0.109917
H	-1.286249	2.374384	0.797910
H	-3.930543	3.986268	0.703888
H	-2.334622	4.573588	1.253893
H	-3.190921	3.294676	2.183236
H	-1.375194	2.323181	-1.668314
H	-1.318990	4.024895	-1.070774
H	-2.870444	3.338743	-1.671975
H	-1.538930	-2.311234	1.297079
H	-3.692476	-3.112448	2.384543
H	-2.701666	-4.439157	1.684038
H	-4.166282	-3.879791	0.833798
H	-2.780751	-3.326398	-1.341028
H	-1.346308	-4.023563	-0.505181
H	-1.273105	-2.352229	-1.184225
68			
<b>IPrCl2</b> SCF Done: -2207.64986720 A.U.			
Pd	-0.000069	-0.000017	-1.698163
N	1.090994	-0.053008	1.030971
C	5.096356	-0.275724	-0.283419
N	-1.090920	0.053672	1.031023
C	4.347724	-1.451743	-0.129558
C	3.008931	-1.408655	0.308037
Cl	-0.330984	-2.264027	-1.935786
C	2.465747	-0.128537	0.583144
C	3.191695	1.080333	0.441190

C	4.525985	0.973370	0.000964
C	2.585069	2.433412	0.804491
C	2.899728	2.780623	2.277075
C	3.035314	3.569369	-0.130410
C	2.205904	-2.687561	0.530232
C	2.423962	-3.207766	1.968549
C	2.506608	-3.780938	-0.508092
C	0.684070	-0.035577	2.365628
C	-0.683908	0.036620	2.365662
C	-2.465718	0.128649	0.583243
C	-3.009455	1.408518	0.308091
C	-4.348240	1.451003	-0.129586
C	-5.096339	0.274648	-0.283470
C	-4.525441	-0.974191	0.000985
C	-3.191133	-1.080554	0.441284
C	-2.206999	2.687779	0.530253
C	-2.425939	3.208395	1.968286
C	-2.507624	3.780697	-0.508579
C	-2.583911	-2.433345	0.804692
C	-2.897453	-2.780035	2.277639
C	-3.034551	-3.569816	-0.129386
C	0.000013	0.000203	0.209399
H	6.139514	-0.333327	-0.632831
H	4.809207	-2.423686	-0.358359
H	5.126166	1.886328	-0.127244
H	1.483997	2.343827	0.693405
H	3.995947	2.874662	2.430641
H	2.530697	2.004220	2.977521
H	2.429336	3.745532	2.560680
H	2.452169	4.488096	0.085526
H	2.863057	3.300593	-1.190530
H	4.108084	3.821891	0.009534
H	1.131553	-2.436396	0.412610
H	2.138749	-2.451731	2.728714
H	3.491265	-3.466779	2.136147
H	1.816232	-4.118795	2.151651
H	2.384738	-3.391043	-1.537601
H	1.794503	-4.622027	-0.383201
H	3.530975	-4.195968	-0.395582
H	1.409012	-0.076653	3.182790
H	-1.408788	0.077880	3.182869
H	-4.810140	2.422740	-0.358427
H	-6.139497	0.331778	-0.632963
H	-5.125201	-1.887418	-0.127272

H	-1.132505	2.436953	0.413215
H	-3.493427	3.467026	2.135302
H	-1.818672	4.119739	2.151359
H	-2.140775	2.452745	2.728852
H	-2.385057	3.390518	-1.537896
H	-1.795942	4.622128	-0.383585
H	-3.532229	4.195322	-0.396733
H	-1.482936	-2.343545	0.692794
H	-2.528115	-2.003270	2.977518
H	-2.426615	-3.744711	2.561298
H	-3.993539	-2.874291	2.431998
H	-4.107137	-3.822589	0.011506
H	-2.450974	-4.488283	0.086486
H	-2.863194	-3.301452	-1.189756
Cl	0.330975	2.264089	-1.935212
68			
<b>IPrCl<sub>2</sub>isomer</b> SCF Done: -2207.63262178 A.U.			
Pd	-0.299656	0.705000	1.293663
N	-1.007293	-0.401588	-1.335696
C	-5.026433	-0.409244	-0.060031
N	1.155414	-0.259537	-1.201550
C	-4.264118	-1.582747	0.026813
C	-2.916016	-1.605385	-0.383431
Cl	0.503778	-1.273135	2.154622
C	-2.387671	-0.403403	-0.912370
C	-3.118007	0.808648	-0.981971
C	-4.456481	0.778010	-0.546151
C	-2.441234	2.110234	-1.409724
C	-3.387413	3.085644	-2.135921
C	-1.798809	2.803765	-0.190461
C	-2.063748	-2.864687	-0.252263
C	-2.357643	-3.842962	-1.409190
C	-2.222010	-3.537960	1.123017
C	-0.509334	-0.815700	-2.570133
C	0.857034	-0.718042	-2.486467
C	2.489938	-0.022891	-0.700717
C	2.963994	1.310268	-0.644364
C	4.278385	1.506880	-0.173920
C	5.075651	0.423331	0.217905
C	4.568017	-0.883308	0.167630
C	3.257382	-1.138903	-0.280599
C	2.109513	2.510788	-1.044085
C	2.737359	3.289761	-2.217644
C	1.844921	3.421589	0.172791

C	2.704028	-2.562168	-0.313167
C	3.164254	-3.305288	-1.586254
C	3.072297	-3.364900	0.948641
C	0.007148	-0.048083	-0.490397
H	-6.075690	-0.412986	0.274731
H	-4.717639	-2.496610	0.439425
H	-5.060409	1.696816	-0.574158
H	-1.623470	1.851540	-2.117857
H	-4.151914	3.507641	-1.450609
H	-3.917095	2.586381	-2.972828
H	-2.814561	3.941090	-2.548735
H	-1.352909	3.785146	-0.452678
H	-0.914452	2.213320	0.202201
H	-2.504700	2.931034	0.652434
H	-0.999661	-2.556097	-0.325054
H	-2.174322	-3.373486	-2.398171
H	-3.417262	-4.176076	-1.386936
H	-1.714571	-4.744742	-1.333534
H	-1.997493	-2.821402	1.937774
H	-1.508609	-4.383286	1.211409
H	-3.242376	-3.950280	1.272604
H	-1.169008	-1.132408	-3.383187
H	1.644005	-0.915498	-3.219470
H	4.680708	2.529946	-0.109147
H	6.100589	0.599600	0.580746
H	5.197040	-1.722554	0.500388
H	1.125721	2.131556	-1.392735
H	3.715631	3.732175	-1.934315
H	2.074801	4.123636	-2.531907
H	2.907172	2.632758	-3.095778
H	1.391542	2.851887	1.013281
H	1.153309	4.247012	-0.095867
H	2.784486	3.878490	0.548096
H	1.596243	-2.481971	-0.328287
H	2.853617	-2.782099	-2.513321
H	2.739460	-4.330722	-1.616708
H	4.271433	-3.393964	-1.609020
H	4.154332	-3.613719	0.981341
H	2.516110	-4.324989	0.962598
H	2.809671	-2.800053	1.864452
Cl	-0.780154	1.844388	3.256898
79			
<b>IPrCl2Py</b> SCF Done: -2455.81729069 A.U.			
Pd	0.005104	1.120990	0.000317

N	-1.081868	-1.674626	0.175317
C	-5.047211	-0.409955	0.906461
N	1.064515	-1.684673	-0.169012
C	-4.104323	-0.391847	1.944364
C	-2.775241	-0.807291	1.726754
Cl	1.082767	1.113571	2.085620
C	-2.437923	-1.235419	0.417595
C	-3.365551	-1.267189	-0.654053
C	-4.681620	-0.846627	-0.374621
C	-2.990592	-1.778438	-2.043905
C	-3.367440	-3.269792	-2.192312
C	-3.627022	-0.954525	-3.178805
C	-1.771412	-0.863913	2.874722
C	-1.877038	-2.224021	3.598838
C	-1.905431	0.311759	3.855702
C	-0.689252	-3.012367	0.120789
C	0.660157	-3.018686	-0.110418
C	2.423757	-1.257740	-0.415219
C	2.761727	-0.836194	-1.726399
C	4.093483	-0.431591	-1.947950
C	5.038355	-0.453814	-0.911936
C	4.672213	-0.884389	0.371039
C	3.353552	-1.294110	0.654403
C	1.755374	-0.888873	-2.872333
C	1.848935	-2.252258	-3.591971
C	1.896828	0.282238	-3.857735
C	2.978028	-1.799709	2.046100
C	3.344237	-3.293586	2.196055
C	3.623214	-0.978485	3.177959
C	-0.005009	-0.845732	0.002037
H	-6.080680	-0.079715	1.098608
H	-4.404714	-0.052214	2.946871
H	-5.431109	-0.853705	-1.180210
H	-1.889925	-1.675221	-2.147476
H	-4.464823	-3.406337	-2.085304
H	-2.877600	-3.906843	-1.429037
H	-3.071322	-3.651014	-3.192396
H	-3.195605	-1.259476	-4.154702
H	-3.430581	0.125958	-3.038751
H	-4.724449	-1.116353	-3.242861
H	-0.751618	-0.785432	2.447937
H	-1.703408	-3.070336	2.901832
H	-2.884313	-2.358508	4.048799
H	-1.124358	-2.293067	4.412463



H	-1.867593	1.278982	3.316065
H	-1.059548	0.298922	4.572271
H	-2.846164	0.265683	4.445549
H	-1.406343	-3.825592	0.257990
H	1.369968	-3.838712	-0.245029
H	4.394373	-0.097248	-2.952077
H	6.073863	-0.131857	-1.107147
H	5.423325	-0.895153	1.175077
H	0.737035	-0.801037	-2.443965
H	2.854198	-2.396217	-4.043503
H	1.094091	-2.318117	-4.403854
H	1.670029	-3.094829	-2.891780
H	1.867858	1.251644	-3.321500
H	1.049345	0.273650	-4.572471
H	2.835966	0.226367	-4.449281
H	1.878436	-1.688226	2.152088
H	2.848373	-3.928042	1.434469
H	3.047212	-3.671253	3.197220
H	4.440386	-3.438278	2.087145
H	4.719619	-1.148013	3.239560
H	3.192068	-1.278618	4.155466
H	3.434076	0.103112	3.036411
Cl	-1.074788	1.122383	-2.083880
N	0.018795	3.238451	-0.002401
C	1.107587	3.918078	0.430252
C	-1.060393	3.931795	-0.437398
C	1.157446	5.318804	0.434100
C	-1.090530	5.333054	-0.446136
C	0.038504	6.043227	-0.007278
H	1.940363	3.301738	0.802025
H	-1.901787	3.326005	-0.807130
H	2.067785	5.825831	0.786966
H	-1.993656	5.851605	-0.800789
H	0.046248	7.144680	-0.009230

91

**IPrCl2Py+DMF SCF Done: -2704.18581783 A.U.**

Pd	-0.031240	0.957124	0.002541
N	-2.183890	-1.048930	0.592544
C	-5.435102	1.507022	-0.279022
N	-0.223593	-1.990741	0.560911
C	-4.727179	1.672863	0.918655
C	-3.625881	0.849403	1.233348
Cl	0.766278	0.909445	2.224644
C	-3.277551	-0.149592	0.295672

C	-3.955785	-0.328793	-0.939223
C	-5.048829	0.519935	-1.198380
C	-3.547395	-1.403947	-1.946395
C	-4.419273	-2.669424	-1.789796
C	-3.586213	-0.909308	-3.404223
C	-2.864523	1.042164	2.539750
C	-3.708144	0.577768	3.744534
C	-2.387207	2.498026	2.702215
C	-2.367525	-2.374976	0.987227
C	-1.136244	-2.971067	0.955461
C	1.166697	-2.249564	0.256082
C	1.535703	-2.335106	-1.115221
C	2.892106	-2.590416	-1.396457
C	3.825233	-2.770296	-0.364938
C	3.421140	-2.712440	0.975404
C	2.081060	-2.442660	1.321298
C	0.506775	-2.194955	-2.235396
C	-0.262677	-3.519072	-2.440279
C	1.096846	-1.683271	-3.558133
C	1.641353	-2.438533	2.784012
C	1.450560	-3.888655	3.282812
C	2.609135	-1.678144	3.708924
C	-0.860195	-0.795191	0.353173
H	-6.292132	2.161252	-0.505490
H	-5.030603	2.458738	1.627879
H	-5.600494	0.413284	-2.144547
H	-2.494552	-1.678677	-1.729638
H	-5.484294	-2.438808	-2.006133
H	-4.370278	-3.090182	-0.766083
H	-4.089309	-3.459698	-2.496716
H	-3.120459	-1.665867	-4.069835
H	-3.025592	0.038360	-3.513832
H	-4.626437	-0.755871	-3.762836
H	-1.950732	0.415941	2.506368
H	-4.002788	-0.487831	3.643744
H	-4.639511	1.176411	3.839447
H	-3.134409	0.688266	4.688810
H	-1.850055	2.831206	1.791107
H	-1.686664	2.577406	3.558123
H	-3.233298	3.195528	2.880318
H	-3.356613	-2.761149	1.246315
H	-0.822058	-3.996825	1.164246
H	3.225829	-2.624797	-2.442477
H	4.881997	-2.960486	-0.611591

H	4.160331	-2.872132	1.775025
H	-0.225300	-1.424106	-1.921901
H	0.422068	-4.328568	-2.772973
H	-1.045092	-3.389790	-3.217924
H	-0.767683	-3.858926	-1.513001
H	1.711255	-0.775236	-3.394944
H	0.270959	-1.422213	-4.250714
H	1.723988	-2.451642	-4.061064
H	0.668026	-1.907848	2.835310
H	0.737542	-4.457980	2.652658
H	1.070516	-3.900450	4.326062
H	2.415651	-4.438770	3.263464
H	3.601151	-2.173890	3.775244
H	2.194758	-1.638149	4.737730
H	2.749839	-0.637174	3.361768
Cl	-0.930374	1.035422	-2.153610
N	0.894876	2.840277	-0.326270
C	0.914871	3.783938	0.644917
C	1.498660	3.099135	-1.511999
C	1.532803	5.028025	0.461790
C	2.152818	4.313948	-1.759561
C	2.167797	5.300271	-0.761309
H	0.438935	3.503959	1.596873
H	1.515968	5.765255	1.278233
H	1.460730	2.298903	-2.266066
H	2.669228	6.266192	-0.931650
O	3.371505	0.567857	-2.420184
N	4.417435	0.577311	-0.359291
C	4.267544	0.582310	1.084065
H	4.779081	-0.292646	1.541701
H	4.697993	1.510089	1.523876
H	3.192177	0.536948	1.349747
C	5.759111	0.635054	-0.911154
H	5.679728	0.631530	-2.015236
H	6.287998	1.557156	-0.581540
H	6.357108	-0.243580	-0.579791
C	3.330618	0.518198	-1.188264
H	2.365486	0.424459	-0.612283
H	2.644195	4.467804	-2.731513
91			
<b>IPrCl2Py--DMF SCF Done: -2704.16163269 A.U.</b>			
Pd	0.071710	-0.807290	-0.399783
N	-0.874436	1.686929	0.915821
C	-4.987908	0.733917	0.709013

N	1.284325	1.697307	0.622378
C	-4.318895	1.197631	-0.433133
C	-2.947486	1.514739	-0.396219
Cl	0.542356	0.014007	-2.553718
C	-2.275864	1.333755	0.843035
C	-2.917850	0.851417	2.010401
C	-4.295650	0.562883	1.914271
C	-2.181090	0.680915	3.337150
C	-2.410005	1.906990	4.248637
C	-2.572701	-0.614127	4.073049
C	-2.227538	2.071042	-1.621666
C	-2.125953	3.610690	-1.546975
C	-2.846653	1.626122	-2.954974
C	-0.392785	2.870955	1.478600
C	0.964961	2.873170	1.302587
C	2.613791	1.303472	0.215201
C	3.328410	0.404574	1.045814
C	4.606039	0.001068	0.608465
C	5.137275	0.471620	-0.601352
C	4.409684	1.372847	-1.392186
C	3.129118	1.815466	-1.002981
C	2.778172	-0.048203	2.394090
C	3.294738	0.884763	3.510599
C	3.075261	-1.524081	2.700635
C	2.364988	2.842585	-1.835811
C	2.733239	4.276426	-1.390494
C	2.587340	2.686082	-3.350429
C	0.156427	0.948490	0.391592
H	-6.060749	0.490110	0.652815
H	-4.873107	1.307770	-1.376066
H	-4.829244	0.186722	2.800151
H	-1.098585	0.598482	3.104500
H	-3.487151	2.013229	4.499929
H	-2.087546	2.853198	3.769504
H	-1.846612	1.799308	5.199499
H	-1.913326	-0.761274	4.953418
H	-2.453668	-1.493298	3.410457
H	-3.617825	-0.581164	4.448674
H	-1.196729	1.663110	-1.621111
H	-1.595165	3.947545	-0.633372
H	-3.134987	4.076368	-1.546698
H	-1.565978	4.002066	-2.422379
H	-2.991725	0.528312	-2.980884
H	-2.164351	1.893624	-3.786941

H	-3.825307	2.115238	-3.152840
H	-1.064012	3.600857	1.938256
H	1.732070	3.592651	1.600291
H	5.194773	-0.691199	1.229000
H	6.135855	0.139351	-0.928619
H	4.842605	1.736301	-2.335833
H	1.673357	0.035654	2.360556
H	4.402441	0.839519	3.588039
H	2.868210	0.592701	4.493349
H	3.014158	1.941192	3.317181
H	2.700460	-2.163159	1.878215
H	2.544958	-1.832111	3.624172
H	4.159207	-1.715788	2.855493
H	1.283430	2.677127	-1.645733
H	2.527815	4.449037	-0.315686
H	2.153963	5.025789	-1.970054
H	3.813677	4.472196	-1.560289
H	3.612453	2.990392	-3.653001
H	1.879177	3.336306	-3.904301
H	2.413561	1.639922	-3.667686
Cl	-0.260467	-1.732295	1.743234
N	-2.160117	-1.848673	-1.192745
C	-2.413695	-2.010412	-2.503339
C	-3.156458	-2.025754	-0.309633
C	-3.686291	-2.356310	-2.990700
C	-4.462611	-2.369315	-0.699796
C	-4.732134	-2.536784	-2.068108
H	-1.555797	-1.833268	-3.176237
H	-3.850999	-2.476509	-4.072853
H	-2.883659	-1.873579	0.749714
H	-5.744505	-2.802786	-2.413140
H	-5.250329	-2.490876	0.059360
O	0.743092	-2.923082	-1.133344
N	2.797180	-3.582768	-0.336746
C	4.241575	-3.431806	-0.379185
H	4.642503	-3.261906	0.643357
H	4.728998	-4.338053	-0.802867
H	4.505465	-2.553941	-1.001267
C	2.234143	-4.631156	0.506044
H	2.694311	-4.585595	1.515342
H	1.144479	-4.460924	0.593489
H	2.423723	-5.638256	0.073002
C	1.982706	-2.785615	-1.075300
H	2.517744	-1.977397	-1.637280

87

**IPrCl2Py+K3PO4** SCF Done: -4898.14066568 A.U.

Pd	-0.472317	-0.643675	-0.446143
N	-2.864407	0.884319	0.393168
C	-5.305440	-2.550577	0.057585
N	-1.140301	2.208437	0.447363
C	-4.831769	-1.915669	-1.099670
C	-4.025700	-0.761809	-1.018611
Cl	-0.034618	0.540588	-2.456725
C	-3.706222	-0.285306	0.276861
C	-4.168707	-0.903428	1.467302
C	-4.982759	-2.044157	1.324623
C	-3.829005	-0.355125	2.852679
C	-4.966275	0.551177	3.375748
C	-3.520762	-1.456881	3.884220
C	-3.595011	-0.021789	-2.281711
C	-4.740475	0.892889	-2.767020
C	-3.107676	-0.963960	-3.394794
C	-3.345986	2.152111	0.712474
C	-2.261546	2.982446	0.760991
C	0.188282	2.781045	0.418518
C	1.122563	2.423795	1.433478
C	2.380106	3.065582	1.393462
C	2.671373	4.043290	0.428526
C	1.726600	4.377986	-0.553467
C	0.468157	3.737071	-0.595852
C	0.798241	1.391036	2.514967
C	-0.342002	1.845191	3.454822
C	2.027511	0.989477	3.345282
C	-0.529057	4.103894	-1.698034
C	-1.139254	5.501225	-1.450519
C	0.099415	4.038756	-3.104663
C	-1.500015	0.905829	0.211445
H	-5.934962	-3.450783	-0.028909
H	-5.101130	-2.314940	-2.089427
H	-5.355903	-2.555157	2.224877
H	-2.907899	0.255870	2.747680
H	-5.901685	-0.034391	3.503774
H	-5.192015	1.387586	2.685005
H	-4.698288	0.987589	4.361049
H	-3.134371	-0.999311	4.818942
H	-2.755838	-2.156602	3.496048
H	-4.428670	-2.036231	4.157520
H	-2.732710	0.626084	-2.028792

H	-5.043827	1.612310	-1.977518
H	-5.637751	0.298262	-3.043320
H	-4.425074	1.474497	-3.658936
H	-2.297607	-1.622965	-3.023828
H	-2.689470	-0.372063	-4.233520
H	-3.926008	-1.596502	-3.800577
H	-4.410769	2.338578	0.871950
H	-2.170897	4.044241	1.001974
H	3.164856	2.766490	2.098507
H	3.659285	4.531338	0.433637
H	1.969517	5.141219	-1.309886
H	0.468546	0.481653	1.969624
H	-0.052588	2.759149	4.017455
H	-0.556303	1.044567	4.193517
H	-1.291328	2.060697	2.927077
H	2.875413	0.690128	2.695645
H	1.761881	0.138205	4.009313
H	2.360213	1.815440	4.011939
H	-1.345097	3.352294	-1.680931
H	-1.624793	5.577587	-0.456582
H	-1.901540	5.740840	-2.221560
H	-0.354792	6.286845	-1.492963
H	0.904288	4.792797	-3.236511
H	-0.671381	4.242730	-3.877067
H	0.511310	3.029795	-3.301437
Cl	-1.011661	-1.907169	1.499095
N	0.307217	-2.403419	-1.305800
C	1.592749	-2.562300	-1.698914
C	-0.583008	-3.408706	-1.496487
C	2.028410	-3.757067	-2.296486
C	-0.218622	-4.619988	-2.097784
C	1.115406	-4.801009	-2.506653
H	2.324603	-1.758288	-1.482421
H	3.090050	-3.836475	-2.573799
H	-1.607655	-3.223403	-1.137274
H	1.433685	-5.745434	-2.976947
H	-0.975964	-5.406489	-2.233602
O	2.223270	-0.508572	0.505938
P	3.803002	-0.670419	0.425555
O	4.297708	-1.843405	1.393349
K	2.921207	1.189399	-1.599341
O	4.220376	-1.027578	-1.084927
O	4.541981	0.687544	0.797093
K	1.964840	-2.483336	2.067166

K	6.564985	-0.969747	0.443257
87			
<b>IPrCl2Py--K3PO4-21</b> SCF Done: -4898.11967599 A.U.			
Pd	-0.291159	-0.666937	-0.293614
N	-2.543543	1.198685	0.211821
C	-5.467969	-1.855082	0.214863
N	-0.681983	2.321505	0.195034
C	-4.865381	-1.468250	-0.991755
C	-3.901414	-0.440073	-1.025802
Cl	0.134992	0.238491	-2.539855
C	-3.543773	0.155171	0.208616
C	-4.146508	-0.200793	1.442557
C	-5.124278	-1.214526	1.413392
C	-3.786699	0.497237	2.753904
C	-4.816400	1.602581	3.081294
C	-3.657966	-0.468250	3.947223
C	-3.358839	0.085188	-2.350158
C	-4.329623	1.142032	-2.921591
C	-3.057855	-1.018683	-3.374664
C	-2.885522	2.545466	0.315756
C	-1.718058	3.252180	0.317590
C	0.698030	2.737139	0.234773
C	1.478928	2.399630	1.374571
C	2.792988	2.906398	1.418714
C	3.287980	3.742871	0.406915
C	2.491497	4.063645	-0.702690
C	1.179373	3.552767	-0.825982
C	0.912507	1.547301	2.511745
C	-0.134264	2.323308	3.342944
C	1.997517	0.958989	3.426865
C	0.332945	3.915091	-2.049817
C	-0.093570	5.399058	-2.004895
C	1.049533	3.606289	-3.380260
C	-1.171814	1.037849	0.119479
H	-6.222347	-2.658379	0.219149
H	-5.161201	-1.958513	-1.931761
H	-5.608384	-1.521961	2.352700
H	-2.792976	0.971885	2.614092
H	-5.823754	1.160970	3.238547
H	-4.906803	2.350450	2.268432
H	-4.531718	2.142933	4.008954
H	-3.271307	0.077701	4.833572
H	-2.957688	-1.291480	3.707660
H	-4.638145	-0.904387	4.236418



H	-2.393200	0.588924	-2.151522
H	-4.489945	1.972916	-2.202743
H	-5.322290	0.695619	-3.146832
H	-3.924751	1.576132	-3.860376
H	-2.369292	-1.773115	-2.946379
H	-2.553064	-0.582095	-4.259772
H	-3.977591	-1.532942	-3.728562
H	-3.928410	2.866184	0.375386
H	-1.516077	4.321907	0.409863
H	3.449790	2.629997	2.251586
H	4.316112	4.132635	0.477338
H	2.891830	4.719950	-1.492508
H	0.404230	0.685156	2.033614
H	0.331404	3.191384	3.857974
H	-0.569906	1.657358	4.117564
H	-0.973750	2.705648	2.728142
H	2.788259	0.455351	2.834002
H	1.536365	0.224083	4.121658
H	2.471532	1.738278	4.063840
H	-0.576748	3.280165	-2.032785
H	-0.614192	5.657277	-1.060248
H	-0.776109	5.639376	-2.847175
H	0.790549	6.067484	-2.083616
H	2.004226	4.165390	-3.481705
H	0.406123	3.894383	-4.237698
H	1.241090	2.518300	-3.472515
Cl	-1.369265	-1.729275	1.649205
N	0.029509	-2.627466	-1.088596
C	1.205146	-3.079491	-1.581712
C	-1.092591	-3.376277	-1.220790
C	1.283508	-4.321509	-2.237684
C	-1.084269	-4.618556	-1.867982
C	0.128055	-5.102057	-2.391987
H	2.115554	-2.452022	-1.417656
H	2.260032	-4.656081	-2.619708
H	-2.011168	-2.952646	-0.783485
H	0.166795	-6.073952	-2.910216
H	-2.021022	-5.189042	-1.956645
O	1.647773	-0.783843	0.504447
P	3.231575	-1.003289	0.499816
O	3.641250	-2.039345	1.645111
K	3.050698	0.785754	-1.813451
O	3.710236	-1.577051	-0.918599
O	4.034046	0.352587	0.708396

K	1.342944	-2.643934	2.346185
K	5.983130	-1.466933	0.765173
87			
<b>IPrCl2Py--K3PO4-22</b> SCF Done: -4898.12779615 A.U.			
Pd	-0.302867	-0.646791	-0.304637
N	-2.614592	1.136705	0.229576
C	-5.406231	-2.038346	0.161085
N	-0.788023	2.315794	0.240734
C	-4.815543	-1.603406	-1.034848
C	-3.896171	-0.534588	-1.044949
Cl	0.148127	0.306509	-2.494077
C	-3.573397	0.055331	0.201708
C	-4.164963	-0.349891	1.425925
C	-5.095719	-1.406077	1.373075
C	-3.842122	0.337641	2.752050
C	-4.919392	1.392486	3.093015
C	-3.681663	-0.644203	3.927981
C	-3.364668	0.030542	-2.357443
C	-4.382385	1.039046	-2.933750
C	-2.990666	-1.048897	-3.384381
C	-2.997925	2.469219	0.369161
C	-1.851925	3.210821	0.388961
C	0.580635	2.769777	0.276204
C	1.389385	2.421895	1.394340
C	2.690876	2.962644	1.430610
C	3.145383	3.841537	0.435266
C	2.322519	4.169532	-0.653114
C	1.024107	3.623669	-0.770746
C	0.869412	1.517689	2.512910
C	-0.209129	2.219646	3.368536
C	1.986524	0.958660	3.407183
C	0.155707	3.978762	-1.980911
C	-0.323970	5.445162	-1.908479
C	0.874789	3.716983	-3.320091
C	-1.240310	1.021405	0.133117
H	-6.124421	-2.874027	0.146779
H	-5.084963	-2.089703	-1.984794
H	-5.569651	-1.752574	2.303939
H	-2.868091	0.855488	2.627325
H	-5.908402	0.906198	3.234521
H	-5.036825	2.151562	2.294098
H	-4.663630	1.926227	4.032822
H	-3.315413	-0.101514	4.824782
H	-2.953088	-1.438816	3.676968

H	-4.646771	-1.118839	4.206958
H	-2.429747	0.582500	-2.141082
H	-4.595919	1.853464	-2.209818
H	-5.346660	0.542053	-3.175653
H	-3.989283	1.501737	-3.863774
H	-2.271329	-1.769673	-2.948827
H	-2.494847	-0.580612	-4.258277
H	-3.876398	-1.607464	-3.756839
H	-4.049851	2.756448	0.439741
H	-1.682478	4.283453	0.508795
H	3.371063	2.677562	2.241485
H	4.163176	4.258475	0.501096
H	2.692711	4.855528	-1.432219
H	0.402033	0.644324	2.013781
H	0.217639	3.092149	3.909171
H	-0.611551	1.510917	4.122886
H	-1.067522	2.581829	2.768009
H	2.797536	0.509980	2.797091
H	1.565440	0.183507	4.083380
H	2.425521	1.743172	4.062744
H	-0.731125	3.312012	-1.968245
H	-0.856771	5.665761	-0.961055
H	-1.012446	5.676944	-2.748313
H	0.535436	6.146552	-1.971155
H	1.796776	4.327601	-3.426006
H	0.208464	3.975878	-4.169325
H	1.126402	2.642147	-3.420275
Cl	-1.274561	-1.727779	1.647468
N	0.096014	-2.591797	-1.114415
C	1.285687	-2.986762	-1.623629
C	-0.988152	-3.397360	-1.228429
C	1.417093	-4.225895	-2.276350
C	-0.927044	-4.640561	-1.871359
C	0.300626	-5.064731	-2.410851
H	2.169311	-2.321335	-1.471654
H	2.404562	-4.512145	-2.669172
H	-1.920656	-3.020014	-0.778646
H	0.381372	-6.036025	-2.925362
H	-1.834861	-5.258202	-1.944060
O	1.741694	-0.761210	0.499535
P	3.324908	-0.957689	0.474335
O	3.763611	-2.041897	1.564378
K	3.051942	0.921329	-1.741250
O	3.801205	-1.453875	-0.974494

O	4.104327	0.403110	0.744653
K	1.469162	-2.656031	2.275775
K	6.085433	-1.373063	0.699381
87			
<b>IPrCl2Py--K3PO4-23</b> SCF Done: -4898.13298529 A.U.			
Pd	0.326476	0.637133	-0.325376
N	2.658882	-1.092059	0.274215
C	5.366836	2.152183	0.111091
N	0.855276	-2.305901	0.300958
C	4.794193	1.661180	-1.071621
C	3.902310	0.569454	-1.049272
Cl	-0.136007	-0.367247	-2.470526
C	3.590844	0.012004	0.215428
C	4.162231	0.476887	1.428074
C	5.064492	1.555495	1.343012
C	3.845417	-0.169109	2.776191
C	4.932346	-1.201445	3.153547
C	3.676061	0.849653	3.918846
C	3.386868	-0.047399	-2.345166
C	4.431635	-1.043618	-2.893486
C	2.984120	0.993354	-3.401240
C	3.066871	-2.412192	0.456123
C	1.934689	-3.175061	0.486406
C	-0.505605	-2.786162	0.319202
C	-1.345653	-2.431681	1.412394
C	-2.638188	-2.995844	1.429349
C	-3.053863	-3.901503	0.440657
C	-2.201022	-4.233860	-0.623152
C	-0.910566	-3.666157	-0.721695
C	-0.872780	-1.488999	2.519827
C	0.222913	-2.128691	3.402450
C	-2.020934	-0.958444	3.391691
C	-0.010773	-4.023854	-1.907642
C	0.501914	-5.476693	-1.797803
C	-0.710626	-3.804472	-3.264354
C	1.284797	-1.007786	0.161261
H	6.063035	3.005452	0.071212
H	5.055723	2.122203	-2.036237
H	5.522279	1.948046	2.263518
H	2.875490	-0.698007	2.666719
H	5.916508	-0.700873	3.278204
H	5.057503	-1.986646	2.381864
H	4.681061	-1.704497	4.111256
H	3.310387	0.334128	4.831645

H	2.943729	1.632001	3.641728
H	4.637897	1.338103	4.184933
H	2.466600	-0.617423	-2.112967
H	4.666470	-1.831651	-2.147327
H	5.382275	-0.527423	-3.148664
H	4.052123	-1.541665	-3.810730
H	2.239515	1.701395	-2.987536
H	2.508358	0.487027	-4.265036
H	3.853753	1.569620	-3.784062
H	4.123247	-2.677066	0.545554
H	1.784321	-4.246851	0.635794
H	-3.343422	-2.705695	2.216696
H	-4.065179	-4.335998	0.491959
H	-2.541269	-4.939689	-1.398101
H	-0.437170	-0.607897	2.005511
H	-0.173953	-3.007949	3.954840
H	0.583169	-1.388993	4.148142
H	1.105749	-2.465045	2.822959
H	-2.840202	-0.546883	2.766458
H	-1.637263	-0.158807	4.061654
H	-2.438987	-1.749794	4.052785
H	0.860441	-3.336858	-1.890457
H	1.028595	-5.664030	-0.839931
H	1.205552	-5.710232	-2.624487
H	-0.340188	-6.199168	-1.854719
H	-1.606069	-4.451332	-3.381871
H	-0.016946	-4.047716	-4.096152
H	-1.002964	-2.741967	-3.381644
Cl	1.210854	1.756680	1.628079
N	-0.130581	2.552679	-1.156349
C	-1.333289	2.915455	-1.659593
C	0.931675	3.386094	-1.279553
C	-1.500219	4.149311	-2.314035
C	0.834743	4.625491	-1.925244
C	-0.406956	5.016658	-2.457563
H	-2.202196	2.233062	-1.500894
H	-2.497910	4.408289	-2.699785
H	1.876266	3.034927	-0.834004
H	-0.516346	5.984530	-2.973218
H	1.725771	5.266261	-2.004723
O	-1.816531	0.740357	0.503399
P	-3.397952	0.922349	0.453066
O	-3.862616	2.025758	1.513396
K	-3.041269	-0.996553	-1.706592

O	-3.857744	1.383392	-1.013616
O	-4.167766	-0.441493	0.741211
K	-1.566784	2.659441	2.223340
K	-6.163603	1.313572	0.626429
87			
<b>IPrCl2Py--K3PO4-24</b> SCF Done: -4898.13620625 A.U.			
Pd	0.348317	0.629974	-0.345438
N	2.701098	-1.041866	0.319916
C	5.332380	2.259239	0.063348
N	0.921739	-2.290906	0.358992
C	4.779947	1.714399	-1.105141
C	3.912602	0.604217	-1.050676
Cl	-0.114086	-0.426959	-2.451670
C	3.607114	0.082050	0.230723
C	4.155004	0.604798	1.430520
C	5.032136	1.701071	1.313703
C	3.836781	0.003115	2.798704
C	4.927290	-1.009463	3.216897
C	3.658126	1.060117	3.904588
C	3.412545	-0.061425	-2.328611
C	4.474996	-1.056315	-2.844321
C	2.996382	0.941204	-3.416264
C	3.133559	-2.348056	0.541804
C	2.016069	-3.132442	0.580609
C	-0.429895	-2.798955	0.359606
C	-1.301230	-2.440877	1.427197
C	-2.584038	-3.028442	1.423926
C	-2.960663	-3.957214	0.440720
C	-2.077699	-4.291503	-0.597586
C	-0.795368	-3.702917	-0.675363
C	-0.876588	-1.463280	2.524024
C	0.234204	-2.039771	3.431309
C	-2.054543	-0.965644	3.375253
C	0.137624	-4.066235	-1.833557
C	0.675132	-5.506356	-1.682049
C	-0.535730	-3.888543	-3.209472
C	1.327986	-0.989701	0.189497
H	6.009278	3.126352	-0.001848
H	5.037209	2.148369	-2.083331
H	5.471438	2.138143	2.222967
H	2.869162	-0.532681	2.701858
H	5.908414	-0.499585	3.326956
H	5.058841	-1.821356	2.474853
H	4.674596	-1.478770	4.191173

H	3.283989	0.575803	4.830844
H	2.929088	1.833754	3.595948
H	4.618230	1.556218	4.162634
H	2.500640	-0.639120	-2.082442
H	4.719077	-1.819362	-2.075518
H	5.418394	-0.532435	-3.110399
H	4.107307	-1.585749	-3.748663
H	2.242688	1.652456	-3.024555
H	2.528139	0.402247	-4.264246
H	3.858943	1.516506	-3.816016
H	4.193845	-2.589927	0.648771
H	1.885522	-4.202766	0.756967
H	-3.314094	-2.735391	2.187229
H	-3.965347	-4.408449	0.476130
H	-2.387328	-5.015438	-1.368569
H	-0.473637	-0.574712	1.995516
H	-0.130082	-2.928293	3.991334
H	0.546414	-1.273199	4.171236
H	1.142288	-2.342145	2.872777
H	-2.880789	-0.590030	2.736525
H	-1.708751	-0.145432	4.040992
H	-2.450980	-1.765191	4.039820
H	0.995788	-3.363167	-1.810423
H	1.186044	-5.662963	-0.710311
H	1.399071	-5.744266	-2.489736
H	-0.152208	-6.245640	-1.739203
H	-1.408857	-4.563382	-3.336947
H	0.184317	-4.125152	-4.020556
H	-0.858056	-2.837944	-3.350350
Cl	1.152841	1.792161	1.604528
N	-0.168007	2.512335	-1.198526
C	-1.385093	2.843211	-1.689451
C	0.872380	3.370441	-1.339618
C	-1.589217	4.069218	-2.347840
C	0.738109	4.603418	-1.990682
C	-0.519201	4.962008	-2.509195
H	-2.238443	2.145300	-1.518093
H	-2.598142	4.301138	-2.721258
H	1.830419	3.045027	-0.903298
H	-0.658419	5.924483	-3.027728
H	1.612459	5.264894	-2.084050
O	-1.894603	0.713062	0.504506
P	-3.474856	0.881364	0.436275
O	-3.960572	1.999183	1.471780

K	-3.019951	-1.059853	-1.674681
O	-3.920701	1.314033	-1.044439
O	-4.234149	-0.485757	0.738261
K	-1.661720	2.646831	2.181967
K	-6.242290	1.253803	0.550151
87			
<b>IPrCl2Py--K3PO4-25</b> SCF Done: -4898.13817612 A.U.			
Pd	-0.372270	-0.630650	-0.365267
N	-2.740290	0.999318	0.340712
C	-5.305288	-2.350742	0.055932
N	-0.980069	2.275003	0.386268
C	-4.773626	-1.777732	-1.108601
C	-3.928280	-0.651228	-1.044593
Cl	0.082445	0.459042	-2.447375
C	-3.624965	-0.140643	0.241934
C	-4.150318	-0.693252	1.438345
C	-5.005041	-1.806004	1.312264
C	-3.830848	-0.106253	2.812616
C	-4.933853	0.882351	3.254788
C	-3.626046	-1.176524	3.901173
C	-3.446743	0.037967	-2.317332
C	-4.532023	1.014037	-2.821312
C	-3.012768	-0.946404	-3.414953
C	-3.191589	2.294737	0.586010
C	-2.085741	3.095565	0.629361
C	0.363595	2.805599	0.377158
C	1.255099	2.450205	1.429372
C	2.528797	3.058018	1.414739
C	2.877733	4.001880	0.435468
C	1.975582	4.332640	-0.587212
C	0.701428	3.725238	-0.653361
C	0.864354	1.451144	2.519604
C	-0.258235	1.983651	3.439114
C	2.061299	0.982673	3.360912
C	-0.251462	4.086471	-1.795935
C	-0.809989	5.515909	-1.620821
C	0.408186	3.936178	-3.181653
C	-1.368447	0.971241	0.199807
H	-5.964843	-3.230502	-0.016856
H	-5.029279	-2.203019	-2.091014
H	-5.426286	-2.266527	2.218442
H	-2.872614	0.446321	2.715665
H	-5.905768	0.355232	3.365049
H	-5.084259	1.703133	2.526298



H	-4.680381	1.340856	4.233966
H	-3.248579	-0.700368	4.830261
H	-2.890047	-1.936036	3.574405
H	-4.576624	-1.689175	4.162181
H	-2.546767	0.633415	-2.068824
H	-4.790737	1.764716	-2.045143
H	-5.464351	0.471813	-3.089611
H	-4.178754	1.559339	-3.721951
H	-2.245552	-1.647384	-3.030790
H	-2.555950	-0.390885	-4.258448
H	-3.865099	-1.533972	-3.818672
H	-4.254635	2.518922	0.703371
H	-1.970657	4.164941	0.821623
H	3.275078	2.766465	2.162857
H	3.876123	4.467482	0.461606
H	2.263585	5.068256	-1.355408
H	0.487708	0.555863	1.982531
H	0.080961	2.878870	4.004236
H	-0.538739	1.201127	4.174947
H	-1.180694	2.260240	2.891215
H	2.894384	0.633385	2.716093
H	1.742615	0.149649	4.024309
H	2.438112	1.789887	4.027577
H	-1.098161	3.369772	-1.770566
H	-1.312586	5.652606	-0.641820
H	-1.546227	5.752212	-2.417774
H	0.005072	6.268742	-1.677639
H	1.264138	4.631791	-3.313627
H	-0.327203	4.164063	-3.981403
H	0.753946	2.895171	-3.336157
Cl	-1.110572	-1.819057	1.585838
N	0.207352	-2.484132	-1.222424
C	1.439589	-2.775632	-1.700768
C	-0.802482	-3.377070	-1.371862
C	1.691335	-3.995969	-2.352714
C	-0.620504	-4.606272	-2.018198
C	0.653514	-4.924423	-2.522290
H	2.270802	-2.054634	-1.522081
H	2.712206	-4.193952	-2.712748
H	-1.775140	-3.083677	-0.945368
H	0.830192	-5.883543	-3.035566
H	-1.471295	-5.296826	-2.118160
O	1.970083	-0.670815	0.507529
P	3.549381	-0.834502	0.430587

O	4.045283	-1.963338	1.448846
K	2.987895	1.103128	-1.645308
O	3.984627	-1.248716	-1.059307
O	4.301806	0.533791	0.743635
K	1.740751	-2.614705	2.155315
K	6.317209	-1.184682	0.507000
87			
<b>IPrCl2Py--K3PO4-27</b> SCF Done: -4898.14021664 A.U.			
Pd	-0.424124	-0.639468	-0.409582
N	-2.811319	0.928991	0.367921
C	-5.297696	-2.476883	0.063331
N	-1.075852	2.238037	0.416667
C	-4.799578	-1.870492	-1.098985
C	-3.978965	-0.726237	-1.028265
Cl	0.017442	0.500561	-2.453744
C	-3.668448	-0.230762	0.262236
C	-4.156968	-0.819144	1.457229
C	-4.986204	-1.950150	1.324772
C	-3.826993	-0.250226	2.836668
C	-4.951037	0.692834	3.322573
C	-3.562912	-1.336198	3.896792
C	-3.526712	-0.010623	-2.297549
C	-4.648176	0.927410	-2.794273
C	-3.059904	-0.974223	-3.400608
C	-3.284597	2.208284	0.651963
C	-2.193572	3.029610	0.697469
C	0.257348	2.797527	0.395427
C	1.174341	2.446415	1.427680
C	2.436291	3.079133	1.398224
C	2.749162	4.041801	0.424923
C	1.821877	4.369144	-0.575996
C	0.558837	3.737703	-0.627647
C	0.825817	1.426336	2.513274
C	-0.310207	1.908103	3.444118
C	2.044074	1.002239	3.348019
C	-0.420284	4.097164	-1.748383
C	-1.011508	5.508313	-1.535699
C	0.222182	3.992961	-3.146291
C	-1.443236	0.932918	0.204672
H	-5.938356	-3.369989	-0.014897
H	-5.061603	-2.284151	-2.084742
H	-5.379246	-2.438295	2.229191
H	-2.889554	0.335743	2.732976
H	-5.902302	0.131972	3.444808

H	-5.144762	1.521177	2.612926
H	-4.689764	1.141417	4.304237
H	-3.180879	-0.867470	4.827789
H	-2.809361	-2.063298	3.537760
H	-4.489574	-1.886543	4.167041
H	-2.648901	0.617287	-2.048373
H	-4.934005	1.662815	-2.012997
H	-5.559851	0.352487	-3.065273
H	-4.316958	1.491220	-3.691873
H	-2.268472	-1.650214	-3.020491
H	-2.623744	-0.399899	-4.242400
H	-3.892296	-1.589234	-3.804841
H	-4.349729	2.408445	0.791323
H	-2.096338	4.095843	0.915306
H	3.204928	2.788314	2.123881
H	3.739699	4.524339	0.438626
H	2.081677	5.120021	-1.339271
H	0.482241	0.520720	1.970502
H	-0.004086	2.815714	4.008294
H	-0.549165	1.113154	4.181341
H	-1.249723	2.145553	2.907707
H	2.887558	0.685826	2.700223
H	1.760232	0.156730	4.011676
H	2.391499	1.822188	4.014841
H	-1.248183	3.358827	-1.725114
H	-1.504379	5.612309	-0.547856
H	-1.763542	5.742978	-2.318243
H	-0.215475	6.281645	-1.587096
H	1.048867	4.722672	-3.280330
H	-0.533944	4.205238	-3.930856
H	0.607057	2.969543	-3.322678
Cl	-1.053442	-1.869483	1.539477
N	0.276409	-2.439221	-1.264645
C	1.540184	-2.653285	-1.700052
C	-0.666384	-3.399326	-1.436497
C	1.896069	-3.860306	-2.326490
C	-0.380748	-4.619394	-2.061977
C	0.928432	-4.857467	-2.518381
H	2.318463	-1.884432	-1.501921
H	2.941399	-3.989843	-2.644455
H	-1.669726	-3.169310	-1.044065
H	1.185702	-5.808935	-3.011334
H	-1.179386	-5.366827	-2.181064
O	2.112885	-0.570220	0.511717

P	3.691604	-0.736639	0.432469
O	4.187435	-1.888943	1.423730
K	2.938433	1.156844	-1.609877
O	4.114429	-1.123001	-1.069446
O	4.438680	0.626390	0.773070
K	1.866688	-2.532042	2.111845
K	6.455755	-1.059881	0.466988
100			
<b>IPrCl2Py1</b> SCF Done: -3543.52672415 A.U.			
Pd	1.289895	0.974051	-0.034512
N	1.224482	-1.928261	0.610194
C	-2.974831	-2.281811	0.219380
N	3.282737	-1.250093	0.413795
C	-2.404217	-2.176282	1.492047
C	-1.009622	-2.036760	1.656160
Cl	0.916212	1.181469	2.271687
C	-0.217031	-2.011125	0.482913
C	-0.767481	-2.107432	-0.828953
C	-2.166738	-2.235935	-0.927154
C	0.113855	-2.107888	-2.078009
C	0.820180	-3.467817	-2.278606
C	-0.631100	-1.707468	-3.361617
C	-0.404968	-1.982583	3.056877
C	-0.330609	-3.405241	3.655555
C	-1.168274	-1.037685	4.003206
C	2.041122	-3.006484	0.959227
C	3.336037	-2.577013	0.843286
C	4.436886	-0.486886	-0.006810
C	4.928777	-0.706560	-1.320738
C	6.071514	0.021015	-1.704697
C	6.681818	0.928977	-0.825857
C	6.156929	1.135462	0.457031
C	5.015480	0.433281	0.896965
C	4.270508	-1.702605	-2.275052
C	4.946454	-3.088816	-2.183654
C	4.247903	-1.218134	-3.735769
C	4.462022	0.642959	2.301767
C	5.341579	-0.081895	3.341857
C	4.287301	2.134480	2.639310
C	1.986308	-0.832067	0.297467
H	-4.066935	-2.384724	0.116139
H	-3.056465	-2.171277	2.377097
H	-2.636908	-2.307108	-1.918468
H	0.900258	-1.338430	-1.933635

H	0.079385	-4.281524	-2.432146
H	1.456746	-3.742436	-1.414386
H	1.478268	-3.427544	-3.172156
H	0.101393	-1.515711	-4.171271
H	-1.225227	-0.782431	-3.222989
H	-1.321815	-2.503930	-3.713581
H	0.624841	-1.579559	2.961399
H	0.244869	-4.103331	3.013456
H	-1.349075	-3.832223	3.776860
H	0.152207	-3.384590	4.655240
H	-1.234025	-0.021475	3.573873
H	-0.635762	-0.970247	4.974674
H	-2.198932	-1.393531	4.211164
H	1.620992	-3.974271	1.245027
H	4.288564	-3.082361	1.022989
H	6.483777	-0.116714	-2.715458
H	7.573394	1.488988	-1.150460
H	6.638778	1.857251	1.134355
H	3.212545	-1.809991	-1.957749
H	6.008893	-3.026908	-2.502267
H	4.431540	-3.816918	-2.845441
H	4.928960	-3.498624	-1.154685
H	3.822631	-0.198696	-3.805817
H	3.617790	-1.898059	-4.346641
H	5.261979	-1.219738	-4.189841
H	3.447893	0.197342	2.344245
H	5.411054	-1.168493	3.124380
H	4.920006	0.037599	4.362112
H	6.375553	0.325588	3.347991
H	5.260716	2.662671	2.725859
H	3.750048	2.245608	3.602704
H	3.679336	2.637134	1.860306
Cl	1.898198	0.960493	-2.311282
N	0.301028	2.816624	-0.323172
C	0.766416	3.961020	0.221117
C	-0.883549	2.812667	-0.984263
C	0.070824	5.171832	0.116576
C	-1.637208	3.989499	-1.120833
C	-1.155735	5.183909	-0.567788
H	1.715899	3.879559	0.770901
H	0.484943	6.080938	0.576170
H	-2.602214	3.942826	-1.646403
H	-1.735560	6.115304	-0.663638
C	-1.327527	1.484615	-1.571092

H	-0.790503	1.346366	-2.533683
H	-0.946772	0.667129	-0.917274
N	-2.750812	1.349903	-1.809770
H	-3.076167	1.269056	-2.783965
C	-3.714997	0.913417	-0.952419
C	-4.948420	0.465405	-1.709745
C	-3.692469	0.831559	0.434149
C	-6.090557	-0.091191	-0.946741
C	-4.783740	0.226573	1.216954
C	-6.009459	-0.214265	0.460920
Cl	-2.316123	1.332992	1.377963
O	-4.711242	0.058367	2.439155
O	-4.955926	0.559237	-2.943167
C	-7.088055	-0.769106	1.171327
C	-8.240174	-1.192202	0.486347
C	-7.246358	-0.518509	-1.631642
C	-8.320689	-1.067112	-0.914561
H	-6.994387	-0.856357	2.264633
H	-9.083067	-1.624587	1.048578
H	-9.224147	-1.401955	-1.447881
H	-7.274713	-0.412977	-2.726897
100			
<b>IPrCl2Py1isomer</b> SCF Done: -3543.52374264 A.U.			
Pd	-1.255678	0.089158	-0.979870
N	-1.369942	0.392766	1.961725
C	2.730731	1.435143	2.038263
N	-3.317358	-0.240132	1.231751
C	2.352540	0.084633	2.061994
C	0.992074	-0.289845	2.048297
Cl	-0.966681	-2.231865	-0.955813
C	0.031441	0.754543	1.996262
C	0.381732	2.128903	1.970114
C	1.757181	2.441715	1.989237
C	-0.673827	3.230951	1.989205
C	-1.009696	3.621541	3.446304
C	-0.268136	4.473986	1.178999
C	0.576981	-1.752760	2.161543
C	0.453913	-2.148975	3.649558
C	1.513529	-2.705610	1.403788
C	-2.198418	0.277746	3.078686
C	-3.427494	-0.114594	2.617762
C	-4.396766	-0.628648	0.350926
C	-5.161345	0.397164	-0.260126
C	-6.204937	-0.005603	-1.117550

C	-6.467442	-1.363940	-1.348206
C	-5.693808	-2.352590	-0.723440
C	-4.634885	-2.010253	0.141525
C	-4.914872	1.871115	0.050172
C	-5.781555	2.310505	1.251396
C	-5.136203	2.793792	-1.159550
C	-3.823488	-3.087361	0.857025
C	-4.513210	-3.490649	2.179343
C	-3.561315	-4.326497	-0.016988
C	-2.053257	0.072092	0.815668
H	3.796674	1.709064	2.046720
H	3.128478	-0.695465	2.093043
H	2.074001	3.494821	1.964292
H	-1.587133	2.820782	1.510306
H	-0.111932	4.024439	3.962000
H	-1.374628	2.756956	4.035869
H	-1.798058	4.403004	3.467880
H	-1.127470	5.171462	1.105571
H	0.022136	4.194937	0.147240
H	0.566743	5.030403	1.656148
H	-0.420823	-1.856829	1.688527
H	-0.269662	-1.504488	4.189636
H	1.434417	-2.060006	4.164726
H	0.109779	-3.200283	3.744836
H	1.605432	-2.399550	0.343479
H	1.094977	-3.732599	1.416998
H	2.525332	-2.754435	1.859626
H	-1.834628	0.480694	4.089357
H	-4.367447	-0.313087	3.139316
H	-6.821554	0.759048	-1.613034
H	-7.286405	-1.656041	-2.024952
H	-5.910193	-3.414035	-0.915178
H	-3.847641	1.981934	0.332653
H	-6.862713	2.209391	1.015610
H	-5.583673	3.372522	1.508590
H	-5.576508	1.699033	2.154183
H	-4.535409	2.458010	-2.027337
H	-4.809619	3.823686	-0.908760
H	-6.205512	2.848609	-1.456836
H	-2.830555	-2.649664	1.091289
H	-4.655640	-2.624502	2.856301
H	-3.908847	-4.248615	2.721075
H	-5.514861	-3.928882	1.981044
H	-4.487875	-4.912058	-0.199878

H	-2.842982	-5.000746	0.493364
H	-3.118323	-4.034960	-0.989011
Cl	-1.653230	2.399988	-1.214625
N	-0.161551	0.147886	-2.779994
C	-0.662539	-0.363462	-3.925126
C	1.084227	0.682143	-2.761851
C	0.058009	-0.344970	-5.124875
C	1.862743	0.732474	-3.929306
C	1.345868	0.217127	-5.124816
H	-1.668286	-0.804411	-3.854658
H	-0.386554	-0.771006	-6.036008
H	2.874379	1.159341	-3.870628
H	1.945468	0.245113	-6.048252
C	1.562446	1.222716	-1.428218
H	0.997843	2.155364	-1.213949
H	1.257343	0.509588	-0.631690
N	2.986861	1.527281	-1.342333
H	3.217346	2.519347	-1.226903
C	3.950185	0.701155	-0.843439
C	3.748027	-0.791605	-0.941525
C	5.131934	1.185217	-0.292624
C	4.733377	-1.670028	-0.253211
C	6.141160	0.357721	0.377916
C	5.875828	-1.124000	0.380003
Cl	5.369034	2.922447	-0.190693
O	7.129971	0.831721	0.946493
O	2.795062	-1.252087	-1.572464
C	6.785312	-1.976887	1.030345
C	6.558349	-3.363162	1.051862
C	4.518711	-3.063270	-0.243938
C	5.427005	-3.907230	0.412450
H	7.663506	-1.521851	1.513651
H	7.270270	-4.026402	1.568391
H	5.253418	-4.994557	0.427161
H	3.626468	-3.458324	-0.751978

112

**IPrCl2Py1isomer+DMF** SCF Done: -3791.89172060 A.U.

Pd	-0.975315	-0.557443	0.104257
N	-0.405001	2.356635	0.210571
C	3.674659	1.987786	-0.860173
N	-2.532780	2.008393	0.491532
C	3.317069	2.086256	0.489995
C	1.963368	2.179644	0.880751
Cl	-0.357031	-0.545824	2.356591



C	0.988239	2.180000	-0.146718
C	1.318362	2.061597	-1.526858
C	2.684895	1.956542	-1.854760
C	0.245138	2.084390	-2.612673
C	-0.186640	3.529768	-2.944851
C	0.652191	1.335351	-3.891386
C	1.598016	2.321532	2.354512
C	1.822214	3.772773	2.830956
C	2.368839	1.322246	3.235879
C	-0.984844	3.597918	0.483133
C	-2.324126	3.377557	0.665571
C	-3.830766	1.371846	0.448396
C	-4.538216	1.397466	-0.781949
C	-5.806233	0.784555	-0.800304
C	-6.321135	0.153132	0.342216
C	-5.591912	0.141151	1.538807
C	-4.327640	0.759067	1.623674
C	-3.985561	2.109861	-2.016591
C	-4.492916	3.568301	-2.071899
C	-4.303971	1.384279	-3.335077
C	-3.552583	0.810818	2.934047
C	-3.965889	2.061141	3.741275
C	-3.688390	-0.474184	3.767381
C	-1.353737	1.366376	0.235158
H	4.735324	1.927659	-1.147517
H	4.103327	2.084860	1.259895
H	2.988505	1.846777	-2.905627
H	-0.640532	1.547624	-2.216499
H	0.666114	4.116486	-3.348512
H	-0.576692	4.060247	-2.053482
H	-0.993631	3.522874	-3.707678
H	-0.233335	1.204409	-4.545083
H	1.044738	0.324402	-3.661020
H	1.425015	1.881735	-4.473482
H	0.521798	2.072812	2.458418
H	1.228833	4.501628	2.241530
H	2.891577	4.059392	2.735620
H	1.532727	3.882639	3.897231
H	2.248098	0.292671	2.845359
H	1.969968	1.343123	4.271081
H	3.451481	1.565084	3.291125
H	-0.389061	4.514178	0.510529
H	-3.145957	4.058643	0.901266
H	-6.393406	0.790347	-1.730663

H	-7.304623	-0.341470	0.296459
H	-5.997764	-0.372773	2.421800
H	-2.879458	2.129289	-1.920752
H	-5.598444	3.592079	-2.178822
H	-4.051782	4.103578	-2.939092
H	-4.233754	4.136137	-1.156632
H	-3.964470	0.332156	-3.296941
H	-3.775278	1.880532	-4.175240
H	-5.388736	1.407557	-3.573214
H	-2.476647	0.905024	2.682784
H	-3.798800	2.997164	3.167978
H	-3.377107	2.128337	4.680266
H	-5.042888	2.020301	4.012657
H	-4.699728	-0.572775	4.218925
H	-2.953913	-0.458695	4.598087
H	-3.494402	-1.369916	3.144752
Cl	-1.734922	-0.728078	-2.136316
N	-0.263068	-2.537115	0.015798
C	-0.868721	-3.560624	0.658014
C	0.915744	-2.730992	-0.625963
C	-0.322065	-4.850655	0.656193
C	1.516012	-3.998004	-0.665815
C	0.889294	-5.072722	-0.019502
H	-1.808810	-3.324353	1.184480
H	-0.843805	-5.659177	1.188577
H	2.478638	-4.110499	-1.185430
H	1.348238	-6.073962	-0.034052
C	1.510858	-1.502767	-1.286357
H	0.888325	-1.260419	-2.174188
H	1.377883	-0.642233	-0.593680
N	2.896390	-1.609036	-1.725123
H	3.041317	-1.562975	-2.738937
C	3.995702	-1.216831	-1.018701
C	3.943213	-1.246739	0.490926
C	5.170323	-0.820023	-1.647717
C	5.135092	-0.749794	1.233551
C	6.356594	-0.304193	-0.956204
C	6.285077	-0.293377	0.546094
Cl	5.200138	-0.723037	-3.400654
O	7.342905	0.139934	-1.553583
O	2.944643	-1.669360	1.075108
C	7.383576	0.196970	1.274576
C	7.341103	0.226050	2.678416
C	5.104521	-0.736585	2.642489

C	6.203923	-0.246191	3.363020
H	8.259513	0.551426	0.709853
H	8.202278	0.615085	3.244569
H	6.175056	-0.230142	4.463750
H	4.202874	-1.110008	3.149305
O	-4.034945	-2.898486	1.399055
N	-5.165126	-2.785747	-0.612661
C	-5.175333	-2.299916	-1.980298
H	-5.164857	-3.148596	-2.700822
H	-6.079550	-1.683944	-2.179995
H	-4.275352	-1.677829	-2.154906
C	-6.257127	-3.637844	-0.177540
H	-6.072973	-3.924699	0.875559
H	-7.228031	-3.097720	-0.249865
H	-6.323740	-4.555112	-0.803940
C	-4.151009	-2.463768	0.248062
H	-3.413734	-1.752207	-0.211162

100

**IPrCl2Py2** SCF Done: -3543.51344066 A.U.

Pd	-1.175457	-0.725168	-0.458287
N	-2.099000	1.643794	1.097130
C	1.105932	4.091051	-0.168114
N	-3.654582	0.123252	1.034968
C	1.350278	3.058789	0.747576
C	0.304920	2.222680	1.191947
Cl	-1.021714	-2.082350	1.458634
C	-0.988470	2.473480	0.677967
C	-1.265336	3.496758	-0.267096
C	-0.186454	4.307504	-0.668325
C	-2.669982	3.744720	-0.818836
C	-3.327456	4.949546	-0.111114
C	-2.696391	3.932159	-2.347098
C	0.585343	1.112241	2.198421
C	0.832869	1.704751	3.601315
C	1.755709	0.216572	1.749474
C	-3.127852	2.085237	1.929891
C	-4.112628	1.135092	1.881134
C	-4.462930	-0.981362	0.570843
C	-4.988287	-0.898984	-0.748472
C	-5.783561	-1.975189	-1.188582
C	-6.052628	-3.069062	-0.351721
C	-5.532824	-3.109513	0.948591
C	-4.720138	-2.067536	1.442101
C	-4.768873	0.331613	-1.627886

C	-5.808248	1.424010	-1.292738
C	-4.747596	0.023101	-3.132271
C	-4.194873	-2.106650	2.874587
C	-5.293821	-1.662579	3.865303
C	-3.639660	-3.489113	3.265051
C	-2.405309	0.421871	0.560095
H	1.942041	4.722424	-0.508565
H	2.379103	2.882744	1.095099
H	-0.361283	5.112083	-1.399393
H	-3.283114	2.846073	-0.601684
H	-2.758776	5.881529	-0.316784
H	-3.360060	4.818367	0.989502
H	-4.368287	5.097279	-0.469336
H	-3.746892	4.004517	-2.700403
H	-2.216723	3.071337	-2.851104
H	-2.181701	4.864970	-2.661414
H	-0.307555	0.459103	2.261280
H	-0.035297	2.306166	3.944253
H	1.724529	2.367807	3.603342
H	1.005489	0.895542	4.342190
H	1.603592	-0.135455	0.709045
H	1.819992	-0.678660	2.400285
H	2.721505	0.758224	1.795931
H	-3.062094	3.036518	2.464240
H	-5.096085	1.083503	2.355250
H	-6.204663	-1.953712	-2.204464
H	-6.678025	-3.898669	-0.718746
H	-5.753521	-3.971461	1.596317
H	-3.765066	0.741507	-1.399111
H	-6.839303	1.075129	-1.516256
H	-5.614509	2.338133	-1.892883
H	-5.771143	1.711566	-0.221925
H	-4.023481	-0.784271	-3.360123
H	-4.420991	0.924796	-3.688873
H	-5.747390	-0.267493	-3.521487
H	-3.347692	-1.392389	2.934328
H	-5.684599	-0.650806	3.632740
H	-4.902276	-1.645433	4.904312
H	-6.156496	-2.362389	3.836980
H	-4.442275	-4.253917	3.339920
H	-3.146465	-3.433376	4.257707
H	-2.887073	-3.828133	2.526896
Cl	-1.305891	0.631088	-2.367753
N	0.297426	-1.914482	-1.394573

C	0.336287	-3.258091	-1.249245
C	1.298253	-1.289828	-2.056409
C	1.385424	-4.026221	-1.775219
C	2.394046	-1.980033	-2.596499
C	2.431578	-3.380591	-2.449155
H	-0.485748	-3.703522	-0.669080
H	1.375773	-5.118577	-1.645826
H	1.199330	-0.198246	-2.154273
H	3.274529	-3.962092	-2.859011
C	3.526693	-1.217910	-3.271441
H	3.765447	-1.689318	-4.247260
H	3.221390	-0.176008	-3.473547
N	4.758760	-1.237089	-2.485995
H	5.346657	-2.083897	-2.564146
C	5.083291	-0.579190	-1.342480
C	6.224981	-1.299231	-0.630372
C	4.566130	0.586160	-0.787051
C	6.752352	-0.734741	0.630757
C	5.074666	1.173948	0.463720
C	6.189650	0.448123	1.165713
Cl	3.301928	1.523880	-1.553596
O	4.620632	2.219984	0.944032
O	6.667273	-2.338572	-1.131585
C	6.685093	0.965629	2.375134
C	7.805846	-1.388282	1.302654
C	8.295748	-0.864488	2.508409
C	7.733570	0.311103	3.043891
H	8.220686	-2.306575	0.860038
H	9.117297	-1.373788	3.035898
H	8.116888	0.720946	3.991766
H	6.228359	1.886280	2.768752

100

**IPrCl2Py2isomer** SCF Done: -3543.51262216 A.U.

Pd	0.881624	-0.739639	-0.273568
N	2.299171	1.368662	1.296994
C	-1.279183	3.398364	2.248754
N	3.730944	0.123101	0.236260
C	-0.414744	3.919955	1.274924
C	0.776436	3.252920	0.926569
Cl	0.224387	0.935817	-1.782348
C	1.073120	2.058602	1.632512
C	0.232135	1.513173	2.632581
C	-0.961686	2.207365	2.916736
C	0.638813	0.271165	3.415919

C	1.460839	0.679976	4.658029
C	-0.551434	-0.623187	3.797219
C	1.727623	3.839969	-0.117410
C	2.589870	4.954289	0.516352
C	1.013502	4.359716	-1.377710
C	3.568628	1.778089	1.707090
C	4.470473	0.999542	1.032592
C	4.309458	-0.755984	-0.755843
C	4.913133	-1.966523	-0.338422
C	5.491664	-2.774264	-1.339856
C	5.458075	-2.392953	-2.687229
C	4.851250	-1.185965	-3.067731
C	4.266026	-0.332082	-2.112610
C	4.987469	-2.377948	1.129496
C	6.370703	-2.024918	1.719505
C	4.668244	-3.869360	1.343198
C	3.661472	1.012501	-2.514537
C	4.679186	2.157336	-2.315878
C	3.085549	1.029540	-3.938488
C	2.388778	0.332848	0.404839
H	-2.219877	3.921906	2.480515
H	-0.681853	4.855428	0.759918
H	-1.655985	1.802162	3.666748
H	1.294762	-0.343157	2.767447
H	0.855440	1.307991	5.346588
H	2.364084	1.261156	4.377234
H	1.796147	-0.219859	5.215572
H	-0.181509	-1.601284	4.166240
H	-1.210515	-0.801297	2.925836
H	-1.173844	-0.173984	4.601069
H	2.406016	3.028094	-0.452736
H	3.150002	4.592301	1.401763
H	1.951928	5.800048	0.850829
H	3.325517	5.347774	-0.216444
H	0.420979	3.551254	-1.847699
H	1.762972	4.708328	-2.118813
H	0.348607	5.221433	-1.157185
H	3.704698	2.585136	2.431640
H	5.563508	0.989555	1.031984
H	5.970189	-3.723295	-1.054475
H	5.909891	-3.043653	-3.452962
H	4.834814	-0.899872	-4.129553
H	4.208169	-1.805533	1.673908
H	7.176194	-2.582650	1.195292

H	6.417205	-2.290061	2.796854
H	6.603250	-0.944379	1.625479
H	3.698097	-4.130716	0.877557
H	4.596726	-4.088720	2.428706
H	5.458914	-4.529293	0.926234
H	2.799700	1.205785	-1.844778
H	5.034094	2.217533	-1.267130
H	4.213559	3.134006	-2.566977
H	5.566468	2.019191	-2.970155
H	3.877698	0.984176	-4.716792
H	2.516544	1.968075	-4.096665
H	2.383208	0.186654	-4.094351
Cl	1.506361	-2.427740	1.235950
N	-0.809399	-1.875057	-0.835928
C	-1.229086	-1.965542	-2.119139
C	-1.588094	-2.368034	0.151512
C	-2.454698	-2.558213	-2.451836
C	-2.853930	-2.926389	-0.088505
C	-3.289607	-3.020649	-1.423753
H	-0.575343	-1.507105	-2.875563
H	-2.760896	-2.616908	-3.506604
H	-1.192224	-2.271168	1.173307
H	-4.292365	-3.418076	-1.651861
C	-3.780838	-3.233730	1.078135
H	-4.036563	-4.313406	1.100901
H	-3.271573	-2.987790	2.031148
N	-5.055702	-2.505454	0.968361
H	-5.892985	-3.073087	0.804685
C	-5.166157	-1.230941	0.483697
C	-4.030908	-0.262629	0.730427
C	-6.310331	-0.747515	-0.133609
C	-3.971000	0.941737	-0.128612
C	-6.400566	0.567628	-0.799603
C	-5.124853	1.364460	-0.838151
Cl	-7.708758	-1.797244	-0.283957
O	-7.427629	0.959325	-1.359126
O	-3.198378	-0.501724	1.608319
C	-5.066726	2.530380	-1.618411
C	-2.764947	1.660262	-0.231356
C	-2.707607	2.801670	-1.047559
C	-3.857271	3.242787	-1.726476
H	-1.871183	1.307026	0.302765
H	-1.751858	3.333332	-1.152347
H	-3.809842	4.144186	-2.358189

H	-5.979217	2.847711	-2.146295
108			
<b>IPrCl2Py2isomer+K3PO4</b> SCF Done: -5985.86947774 A.U.			
Pd	1.972817	-0.771438	0.442153
N	4.701401	0.006917	-0.374278
C	5.967058	-4.021623	-0.577960
N	3.497324	1.811021	-0.209737
C	5.775160	-3.414755	0.670602
C	5.346640	-2.075096	0.771413
Cl	1.970128	0.295417	2.549265
C	5.119831	-1.377142	-0.439843
C	5.295713	-1.962823	-1.720971
C	5.730147	-3.302030	-1.758716
C	5.056477	-1.182056	-3.012467
C	6.375357	-0.575907	-3.542596
C	4.388913	-2.025125	-4.115099
C	5.185710	-1.416551	2.138475
C	6.566553	-1.052872	2.723886
C	4.358365	-2.281034	3.107014
C	5.562534	1.080727	-0.588960
C	4.805328	2.214639	-0.499865
C	2.428202	2.779070	-0.087745
C	1.442092	2.858904	-1.115253
C	0.480522	3.885667	-1.001029
C	0.527507	4.817376	0.049270
C	1.517518	4.719424	1.038410
C	2.479266	3.683284	1.006707
C	1.429518	1.895038	-2.301465
C	2.640248	2.110499	-3.240441
C	0.128177	1.936768	-3.119142
C	3.525534	3.590647	2.119578
C	4.562403	4.729190	2.002210
C	2.884497	3.591707	3.522550
C	3.425491	0.444046	-0.118260
H	6.302143	-5.069695	-0.632750
H	5.964390	-3.989262	1.590459
H	5.875776	-3.794048	-2.731973
H	4.356214	-0.355232	-2.769244
H	7.096608	-1.380389	-3.801135
H	6.867015	0.084439	-2.801527
H	6.189323	0.023732	-4.458445
H	4.080776	-1.369219	-4.955765
H	3.488082	-2.541197	-3.731498
H	5.082990	-2.784741	-4.534088



H	4.619686	-0.473017	2.007353
H	7.127421	-0.376839	2.044638
H	7.187646	-1.960403	2.882256
H	6.453155	-0.541049	3.702727
H	3.382796	-2.549678	2.653569
H	4.146556	-1.713668	4.035536
H	4.888055	-3.214728	3.392041
H	6.628012	0.932313	-0.781458
H	5.058924	3.269504	-0.629836
H	-0.332210	3.954311	-1.735316
H	-0.231877	5.613254	0.102251
H	1.542400	5.453597	1.859362
H	1.522809	0.871426	-1.882949
H	2.602752	3.118805	-3.705778
H	2.617963	1.355522	-4.053392
H	3.616743	2.009281	-2.727799
H	-0.792209	1.815201	-2.504881
H	0.152085	1.126787	-3.879737
H	0.029671	2.889111	-3.684245
H	4.050758	2.619463	2.010580
H	5.064080	4.739747	1.013450
H	5.347007	4.627036	2.780820
H	4.079440	5.720562	2.135793
H	2.361721	4.547062	3.740880
H	3.665935	3.459951	4.299493
H	2.168941	2.752321	3.626005
Cl	1.864757	-1.673298	-1.743642
N	0.501621	-2.183044	1.043296
C	0.457761	-3.437472	0.518320
C	-0.585891	-1.707596	1.683515
C	-0.704972	-4.214222	0.581698
C	-1.816898	-2.388043	1.714675
C	-1.874045	-3.666633	1.145068
H	1.364785	-3.782575	0.001753
H	-0.702188	-5.224430	0.145493
H	-0.482273	-0.713232	2.128830
H	-2.836854	-4.199117	1.116757
C	-3.002021	-1.607491	2.229854
H	-2.887432	-1.438608	3.323730
H	-2.969629	-0.607708	1.738472
N	-4.329248	-2.179119	1.996216
H	-4.839332	-2.415270	2.854107
C	-5.175639	-1.646566	1.051097
C	-4.628886	-1.386650	-0.333157

C	-6.526016	-1.451530	1.307161
C	-5.569081	-0.773339	-1.324904
C	-7.457330	-0.793664	0.393223
C	-6.909060	-0.473765	-0.970501
Cl	-7.156634	-1.808459	2.918804
O	-8.612880	-0.473045	0.706624
O	-3.573746	-1.947177	-0.700616
C	-7.767278	0.140399	-1.907443
C	-7.303852	0.452453	-3.196629
C	-5.124083	-0.489859	-2.633199
C	-5.979704	0.126760	-3.559812
H	-8.800581	0.350367	-1.588953
H	-7.977523	0.930645	-3.926225
H	-5.610542	0.358568	-4.571643
H	-4.087619	-0.724083	-2.900161
O	-1.454343	0.523198	0.323001
P	-2.741626	1.316449	-0.160621
O	-2.869390	1.271582	-1.732282
K	-0.737654	2.270944	1.962844
O	-4.084097	0.664270	0.483087
O	-2.721488	2.804734	0.387941
K	-1.331355	-0.944113	-1.784607
K	-5.188073	2.650376	-0.811326

100

**IPrCl<sub>2</sub>Py<sub>3</sub>** SCF Done: -3543.50357268 A.U.

Pd	1.218052	-0.087794	-0.472551
N	3.724403	-0.710753	1.061534
C	2.740074	-4.793929	1.528948
N	3.653958	1.385655	0.490479
C	2.143587	-3.832543	2.357346
C	2.457242	-2.464696	2.225885
Cl	0.163203	1.042389	1.297049
C	3.389625	-2.109226	1.218884
C	4.014608	-3.055203	0.367142
C	3.668254	-4.409011	0.551065
C	5.056494	-2.650922	-0.674046
C	6.482228	-2.790264	-0.094848
C	4.934953	-3.446165	-1.986902
C	1.877742	-1.427964	3.183342
C	2.770097	-1.320923	4.439603
C	0.409538	-1.693262	3.552630
C	4.877523	-0.115153	1.573487
C	4.839731	1.202206	1.202461
C	3.252315	2.637388	-0.111674

C	3.485762	2.811624	-1.500062
C	3.089431	4.038390	-2.069271
C	2.498676	5.041499	-1.287197
C	2.295260	4.841627	0.085391
C	2.663938	3.632234	0.708975
C	4.210842	1.756003	-2.330203
C	5.731574	2.026226	-2.309191
C	3.677595	1.639042	-3.766630
C	2.473176	3.440109	2.212093
C	3.663043	4.042566	2.992588
C	1.145753	4.027371	2.726186
C	2.957664	0.209623	0.396839
H	2.478889	-5.857734	1.647800
H	1.421365	-4.147945	3.125011
H	4.128260	-5.174442	-0.091744
H	4.875389	-1.584172	-0.923606
H	6.694655	-3.848897	0.167107
H	6.623552	-2.186426	0.823587
H	7.240973	-2.462470	-0.836514
H	5.596635	-3.003599	-2.760075
H	3.895874	-3.419626	-2.367668
H	5.245344	-4.505576	-1.860098
H	1.889960	-0.443697	2.674199
H	3.814796	-1.054395	4.174959
H	2.798066	-2.285018	4.991684
H	2.383576	-0.540388	5.128537
H	-0.211818	-1.802313	2.641652
H	0.006660	-0.834284	4.126433
H	0.288670	-2.601890	4.180915
H	5.606578	-0.684098	2.155854
H	5.541887	2.023484	1.366633
H	3.251612	4.210709	-3.143727
H	2.195172	5.992610	-1.753414
H	1.832299	5.637617	0.687697
H	4.034200	0.767893	-1.860163
H	5.967501	3.008779	-2.771801
H	6.275839	1.239906	-2.873710
H	6.129239	2.037953	-1.273010
H	2.582290	1.471448	-3.765051
H	4.144426	0.767919	-4.269388
H	3.905458	2.539571	-4.376769
H	2.436484	2.346538	2.400835
H	4.633194	3.598172	2.692657
H	3.538708	3.877598	4.083707

H	3.730857	5.137787	2.817993
H	1.150658	5.138480	2.713574
H	0.974946	3.713303	3.776663
H	0.295171	3.664243	2.117771
Cl	2.282506	-1.220392	-2.233388
N	-0.663415	-0.409823	-1.395548
C	-1.622605	0.544573	-1.360437
C	-0.932706	-1.579679	-2.023977
C	-2.875793	0.365694	-1.957501
C	-2.168798	-1.833787	-2.627238
C	-3.170786	-0.846198	-2.607518
H	-1.367418	1.461820	-0.808287
H	-3.622375	1.171974	-1.897963
H	-0.111856	-2.312722	-2.044080
H	-2.346961	-2.812587	-3.098630
C	-4.518848	-1.085507	-3.274332
H	-4.456781	-0.762384	-4.336008
H	-4.737776	-2.171457	-3.287882
N	-5.616948	-0.345239	-2.675163
H	-5.890730	0.549740	-3.109210
C	-6.055130	-0.381908	-1.385401
C	-6.820788	0.887012	-1.042742
C	-5.888061	-1.357044	-0.412977
C	-7.411458	1.025058	0.306985
C	-6.437938	-1.240179	0.955147
C	-7.217568	0.008647	1.272745
Cl	-5.046817	-2.862426	-0.715839
O	-6.287294	-2.119778	1.805495
O	-6.913217	1.767270	-1.906357
C	-7.768240	0.159033	2.557215
C	-8.152421	2.180714	0.630261
C	-8.700918	2.321503	1.913733
C	-8.507664	1.310723	2.875976
H	-8.281718	2.954093	-0.142109
H	-9.280020	3.222874	2.168338
H	-8.936943	1.422997	3.884191
H	-7.600258	-0.646198	3.288611
100			
<b>IPrCl2Py3del2</b> SCF Done: -3543.51036813 A.U.			
Pd	-1.419959	-0.265459	-1.157724
N	-1.647346	0.882414	1.485831
C	2.062363	2.730394	0.603618
N	-3.534486	-0.123495	1.073599
C	2.024285	1.385213	0.989252

C	0.813074	0.748163	1.324311
Cl	-1.357698	-2.486409	-0.384366
C	-0.368637	1.524849	1.251468
C	-0.368436	2.897112	0.882685
C	0.874990	3.478662	0.562077
C	-1.653160	3.724149	0.867631
C	-1.890399	4.372065	2.251155
C	-1.683732	4.800717	-0.230952
C	0.822609	-0.702501	1.791252
C	1.267561	-0.771505	3.268620
C	1.708590	-1.592512	0.903469
C	-2.394195	0.938142	2.661337
C	-3.586290	0.315138	2.399799
C	-4.648266	-0.716566	0.367762
C	-5.374360	0.111911	-0.530139
C	-6.475509	-0.470284	-1.187908
C	-6.836503	-1.806231	-0.955107
C	-6.098858	-2.593589	-0.061484
C	-4.979551	-2.069796	0.618722
C	-5.013139	1.582003	-0.734064
C	-5.637138	2.457804	0.374651
C	-5.366872	2.115114	-2.130350
C	-4.197400	-2.931967	1.606226
C	-4.934879	-3.011452	2.960716
C	-3.911262	-4.342803	1.058357
C	-2.337758	0.210218	0.506782
H	3.029770	3.187569	0.339466
H	2.954525	0.804551	1.034620
H	0.911842	4.535775	0.260333
H	-2.491011	3.025704	0.658707
H	-1.075034	5.088382	2.488511
H	-1.922480	3.623798	3.067465
H	-2.851070	4.928925	2.263145
H	-2.698381	5.246501	-0.291338
H	-1.439778	4.362527	-1.217544
H	-0.976918	5.631339	-0.018917
H	-0.208967	-1.102195	1.719695
H	0.607422	-0.160970	3.919950
H	2.306143	-0.393293	3.388247
H	1.242568	-1.819080	3.636368
H	1.428798	-1.497247	-0.162418
H	1.597313	-2.658199	1.185786
H	2.778046	-1.327879	1.015757
H	-2.007861	1.411834	3.567551

H	-4.470026	0.150999	3.021983
H	-7.062232	0.134990	-1.894310
H	-7.702371	-2.238846	-1.481460
H	-6.388759	-3.641784	0.107546
H	-3.911200	1.671596	-0.655453
H	-6.747057	2.417259	0.337314
H	-5.325977	3.516776	0.250666
H	-5.318748	2.131774	1.385999
H	-4.942440	1.465925	-2.922030
H	-4.930102	3.125700	-2.262746
H	-6.464059	2.201239	-2.286592
H	-3.212115	-2.444784	1.761384
H	-5.107977	-2.008785	3.402338
H	-4.350524	-3.609188	3.691828
H	-5.928088	-3.495067	2.840662
H	-4.835853	-4.953459	0.976098
H	-3.221738	-4.881658	1.741002
H	-3.430108	-4.284155	0.062641
Cl	-1.771218	1.856256	-2.099086
N	0.221169	-0.641731	-2.462868
C	0.620809	-1.866783	-2.878044
C	1.125674	0.369212	-2.452271
C	1.947382	-2.132153	-3.243195
C	2.466676	0.176247	-2.795605
C	2.909199	-1.103511	-3.179765
H	-0.144680	-2.656927	-2.852826
H	2.226629	-3.152057	-3.552051
H	0.746693	1.352529	-2.132324
H	3.162616	1.025286	-2.738531
C	4.390806	-1.381626	-3.394263
H	4.531946	-2.225302	-4.098992
H	4.897231	-0.494690	-3.817983
N	5.034478	-1.766793	-2.132671
H	4.906305	-2.751905	-1.846052
C	5.208182	-1.004118	-1.018927
C	5.193475	-1.861377	0.240289
C	5.420363	0.363726	-0.898743
C	5.263157	-1.190831	1.559438
C	5.428619	1.070257	0.395191
C	5.341681	0.220137	1.634904
Cl	5.687845	1.402772	-2.284727
O	5.482304	2.301608	0.479785
O	5.085673	-3.084631	0.117673
C	5.312677	0.850060	2.891476

C	5.173121	-1.961869	2.736255
C	5.148395	-1.326200	3.985723
C	5.213476	0.079433	4.061687
H	5.100766	-3.055695	2.641070
H	5.065012	-1.925255	4.905700
H	5.182786	0.578066	5.043197
H	5.360000	1.949074	2.919779
100			
<b>IPrCl2Py3isomer</b> SCF Done: -3543.50390774 A.U.			
Pd	0.958060	0.096659	-0.692070
N	3.049424	-0.972017	1.155439
C	2.363990	-5.007553	0.100401
N	3.217855	1.189422	0.973874
C	1.434729	-4.337474	0.907463
C	1.628023	-2.990148	1.278025
Cl	-0.242887	1.059980	1.091483
C	2.797236	-2.352025	0.802814
C	3.749909	-2.994512	-0.032040
C	3.508346	-4.341372	-0.363353
C	5.008062	-2.283872	-0.530890
C	6.230607	-2.675414	0.328317
C	5.294946	-2.535068	-2.022565
C	0.615588	-2.282704	2.171280
C	0.697105	-2.811780	3.617970
C	-0.815392	-2.380661	1.611069
C	4.027872	-0.566399	2.064576
C	4.141690	0.792588	1.942377
C	3.130205	2.523620	0.423247
C	3.701990	2.740155	-0.861325
C	3.620096	4.044832	-1.385517
C	3.011872	5.081624	-0.661290
C	2.471263	4.835903	0.607420
C	2.511908	3.547561	1.180925
C	4.431652	1.629305	-1.615489
C	5.888650	1.500787	-1.118809
C	4.374305	1.775275	-3.143119
C	1.951052	3.304004	2.579671
C	2.959586	3.768496	3.653590
C	0.582171	3.975806	2.796309
C	2.526661	0.108524	0.494839
H	2.192862	-6.060106	-0.176664
H	0.536569	-4.867716	1.260931
H	4.224160	-4.874310	-1.007605
H	4.844243	-1.192653	-0.417230

H	6.442917	-3.761696	0.232880
H	6.071878	-2.462041	1.404566
H	7.134180	-2.119897	-0.000394
H	6.143600	-1.900477	-2.354477
H	4.410030	-2.281933	-2.636983
H	5.580951	-3.590133	-2.219558
H	0.864762	-1.203444	2.193329
H	1.717310	-2.687520	4.037713
H	0.443354	-3.892815	3.668403
H	-0.013081	-2.263511	4.272396
H	-0.850434	-2.038507	0.557004
H	-1.495152	-1.722929	2.187914
H	-1.212944	-3.417736	1.659253
H	4.552354	-1.284930	2.699801
H	4.795153	1.513053	2.441148
H	4.043723	4.254316	-2.378623
H	2.960961	6.094123	-1.092860
H	1.998768	5.658417	1.165624
H	3.915334	0.674019	-1.395269
H	6.463826	2.429216	-1.323480
H	6.397868	0.658506	-1.633358
H	5.936782	1.304366	-0.028078
H	3.328186	1.891791	-3.489919
H	4.777266	0.857231	-3.616737
H	4.974874	2.634965	-3.511598
H	1.789964	2.210996	2.684847
H	3.943972	3.267835	3.550336
H	2.574110	3.554891	4.672824
H	3.137683	4.862696	3.578523
H	0.660473	5.083802	2.818325
H	0.154695	3.658327	3.769988
H	-0.127780	3.680237	1.999726
Cl	2.131714	-0.939924	-2.437012
N	-0.825316	0.006575	-1.820493
C	-1.742396	1.000401	-1.757861
C	-1.141007	-1.133055	-2.481019
C	-3.015667	0.873135	-2.322679
C	-2.402371	-1.337368	-3.051202
C	-3.377348	-0.328315	-2.962823
H	-1.445694	1.897581	-1.194774
H	-3.738316	1.696260	-2.213023
H	-0.346090	-1.893443	-2.528109
H	-2.633122	-2.305933	-3.519429
C	-4.797761	-0.550175	-3.460385



H	-4.929405	-0.060833	-4.449213
H	-4.973863	-1.634677	-3.598928
N	-5.807828	0.032474	-2.572983
H	-6.287241	0.869325	-2.919715
C	-5.805413	-0.047669	-1.206184
C	-5.172887	-1.248936	-0.544199
C	-6.416324	0.912836	-0.410165
C	-5.056134	-1.238878	0.939194
C	-6.415970	0.909454	1.063160
C	-5.660430	-0.217534	1.712014
Cl	-7.177285	2.294730	-1.178054
O	-6.961326	1.790631	1.731815
O	-4.769687	-2.195302	-1.224961
C	-5.542866	-0.242586	3.112465
C	-4.338248	-2.271850	1.573702
C	-4.216157	-2.284790	2.971298
C	-4.819894	-1.271430	3.740039
H	-3.871500	-3.046640	0.947368
H	-3.639960	-3.083795	3.462875
H	-4.722242	-1.280980	4.837127
H	-6.023270	0.564852	3.686030

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**IPrCl2Py3del2Isomer** SCF Done: -3543.50944395 A.U.

Pd	-0.682366	-0.631576	-0.374289
N	-2.713599	1.601180	-0.289908
C	-0.390801	5.015101	-1.172627
N	-3.547410	-0.283438	0.402531
C	-0.729344	4.717335	0.156230
C	-1.446158	3.548531	0.482232
Cl	0.379553	0.465296	1.406295
C	-1.819199	2.696994	-0.591453
C	-1.440989	2.935724	-1.933440
C	-0.727139	4.123673	-2.201248
C	-1.724151	1.940475	-3.051895
C	-2.560348	2.558113	-4.188210
C	-0.394659	1.348484	-3.567178
C	-1.818290	3.242959	1.932732
C	-3.045216	4.065215	2.382393
C	-0.638304	3.459260	2.898617
C	-4.075848	1.819103	-0.064092
C	-4.596543	0.635768	0.381535
C	-3.655747	-1.614628	0.959124
C	-4.314168	-2.623696	0.215067

C	-4.419788	-3.897091	0.812833
C	-3.888452	-4.147692	2.084217
C	-3.247184	-3.123959	2.798244
C	-3.120092	-1.828819	2.259164
C	-4.937205	-2.359416	-1.153304
C	-6.458166	-2.123676	-1.017926
C	-4.654388	-3.488476	-2.162341
C	-2.488862	-0.694836	3.064975
C	-3.572518	0.146009	3.774811
C	-1.414098	-1.164807	4.056138
C	-2.382383	0.298303	-0.029055
H	0.162711	5.938698	-1.404339
H	-0.434452	5.409425	0.960034
H	-0.422306	4.345603	-3.235908
H	-2.300924	1.091566	-2.631962
H	-2.024613	3.389777	-4.694146
H	-3.522724	2.960001	-3.808266
H	-2.787794	1.791217	-4.957663
H	-0.592530	0.535139	-4.294261
H	0.181012	0.910159	-2.725582
H	0.234624	2.120543	-4.060146
H	-2.080949	2.166497	1.986099
H	-3.930384	3.877749	1.742789
H	-2.825572	5.153656	2.345303
H	-3.322811	3.807766	3.426151
H	0.254123	2.900955	2.557083
H	-0.906609	3.087451	3.909323
H	-0.377415	4.534026	3.003650
H	-4.534257	2.794735	-0.245602
H	-5.606864	0.359936	0.694274
H	-4.922756	-4.707588	0.263994
H	-3.976006	-5.152625	2.527321
H	-2.841421	-3.334745	3.798587
H	-4.465264	-1.440631	-1.559532
H	-6.962764	-3.029840	-0.619425
H	-6.907877	-1.889436	-2.005838
H	-6.695410	-1.286884	-0.329631
H	-3.568579	-3.696714	-2.221902
H	-5.002654	-3.189027	-3.172689
H	-5.187304	-4.426613	-1.896999
H	-1.960035	-0.028786	2.354587
H	-4.301923	0.571450	3.055690
H	-3.105983	0.995673	4.317258
H	-4.135699	-0.466837	4.510818

H	-1.842001	-1.731896	4.910928
H	-0.881975	-0.285147	4.471221
H	-0.658485	-1.799535	3.551273
Cl	-1.736783	-1.621588	-2.228952
N	1.104809	-1.694285	-0.782125
C	1.904193	-2.104439	0.230960
C	1.520887	-1.888999	-2.056268
C	3.170893	-2.652098	0.003696
C	2.780314	-2.419727	-2.357092
C	3.655738	-2.771982	-1.314358
H	1.529594	-1.920041	1.248511
H	3.808134	-2.901436	0.866049
H	0.815806	-1.578984	-2.842526
H	3.106632	-2.468388	-3.406454
C	5.130699	-3.059424	-1.568162
H	5.365058	-4.123513	-1.354155
H	5.366572	-2.867588	-2.633768
N	5.994393	-2.246824	-0.690909
H	6.529194	-2.761677	0.015729
C	5.618560	-0.996895	-0.268672
C	4.853184	-0.125508	-1.239041
C	5.940946	-0.467750	0.968426
C	4.031611	0.959150	-0.655366
C	5.348483	0.774789	1.513229
C	4.286244	1.414879	0.661445
Cl	6.933044	-1.408066	2.069061
O	5.632816	1.207277	2.631804
O	4.896168	-0.362625	-2.448354
C	3.508743	2.456982	1.194088
C	2.986969	1.521497	-1.414368
C	2.187683	2.528050	-0.856950
C	2.458519	3.003811	0.438567
H	2.803748	1.134287	-2.428196
H	1.337454	2.935293	-1.420214
H	1.821185	3.792268	0.865608
H	3.729528	2.799263	2.216517

112

**IPrCl2Py3isomer+DMF** SCF Done: -3791.87582890 A.U.

Pd	-1.115424	-0.405476	-0.510301
N	-1.285956	2.084723	1.007214
C	2.081886	3.582312	-1.074828
N	-3.143100	0.983585	1.294928
C	2.267958	2.659187	-0.039879
C	1.174414	2.142931	0.688948

Cl	-0.887932	-1.575347	1.524038
C	-0.113657	2.604341	0.329225
C	-0.337598	3.542861	-0.716322
C	0.791136	4.021242	-1.407577
C	-1.735953	4.056427	-1.057303
C	-2.025369	5.374890	-0.305719
C	-1.976623	4.234771	-2.566650
C	1.428864	1.152104	1.820744
C	2.163481	1.845311	2.988195
C	2.221665	-0.068974	1.318998
C	-2.001007	2.755728	1.999474
C	-3.172323	2.067750	2.177021
C	-4.256787	0.097298	1.041223
C	-5.003976	0.303258	-0.153035
C	-6.082036	-0.570718	-0.391708
C	-6.411889	-1.585085	0.520070
C	-5.673039	-1.742431	1.698891
C	-4.573622	-0.906767	1.988570
C	-4.696842	1.460713	-1.104049
C	-5.268414	2.785125	-0.549081
C	-5.168613	1.236174	-2.548552
C	-3.811641	-1.062206	3.301445
C	-4.603438	-0.413196	4.458236
C	-3.475563	-2.530142	3.623592
C	-1.972698	0.974110	0.588094
H	2.956103	3.960204	-1.628758
H	3.285399	2.327065	0.211776
H	0.655423	4.742435	-2.227399
H	-2.464032	3.297834	-0.705869
H	-1.327817	6.173417	-0.637302
H	-1.908955	5.264837	0.790859
H	-3.062123	5.718846	-0.505610
H	-3.048152	4.459692	-2.751674
H	-1.716217	3.309838	-3.115691
H	-1.391250	5.081321	-2.984669
H	0.452317	0.778586	2.191351
H	1.600729	2.727875	3.358265
H	3.172286	2.190420	2.676758
H	2.303075	1.139216	3.832563
H	1.639564	-0.641678	0.574720
H	2.471024	-0.753422	2.154371
H	3.169453	0.244846	0.843657
H	-1.609837	3.656877	2.479092
H	-4.026220	2.247501	2.835530

H	-6.676272	-0.452732	-1.309182
H	-7.258293	-2.257749	0.308494
H	-5.943509	-2.537191	2.410260
H	-3.593875	1.559552	-1.165336
H	-6.376107	2.738302	-0.478377
H	-5.001234	3.629895	-1.218291
H	-4.870434	3.020638	0.458065
H	-4.786117	0.281561	-2.958865
H	-4.774846	2.048714	-3.192162
H	-6.276267	1.245623	-2.639787
H	-2.844609	-0.530753	3.189198
H	-4.827749	0.655735	4.262694
H	-4.030195	-0.473356	5.407156
H	-5.574985	-0.929625	4.613112
H	-4.385174	-3.129847	3.841285
H	-2.826162	-2.581007	4.521898
H	-2.927095	-2.999872	2.784040
Cl	-1.540354	0.716782	-2.530957
N	0.324581	-1.682281	-1.426129
C	0.649785	-2.893669	-0.914691
C	1.216739	-1.054990	-2.233098
C	1.905685	-3.472421	-1.124602
C	2.494670	-1.568630	-2.475823
C	2.876133	-2.786166	-1.878668
H	-0.108435	-3.384515	-0.292150
H	2.121087	-4.450618	-0.667287
H	0.881697	-0.095960	-2.658269
H	3.203540	-0.998599	-3.093073
C	4.316872	-3.271506	-1.922023
H	4.351593	-4.375514	-2.015900
H	4.862917	-2.828162	-2.771995
N	5.011101	-2.940985	-0.663711
H	4.864982	-3.624058	0.089734
C	5.250051	-1.688921	-0.166087
C	5.475038	-0.533613	-1.110985
C	5.373523	-1.461598	1.203000
C	5.631062	0.828428	-0.521645
C	5.591723	-0.147362	1.825124
C	5.707846	1.015450	0.878646
Cl	5.121668	-2.790545	2.314861
O	5.623957	0.019347	3.047111
O	5.519940	-0.709805	-2.331896
C	5.853947	2.311089	1.404276
C	5.917283	3.417921	0.540863

C	5.700781	1.941575	-1.384120
C	5.840722	3.233270	-0.853487
H	5.904849	2.420688	2.498249
H	6.020376	4.432309	0.956857
H	5.887439	4.102127	-1.528343
H	5.637547	1.766386	-2.468700
O	-1.323401	-4.934980	-1.817174
N	-2.977741	-3.318982	-1.707323
C	-3.677566	-2.238414	-2.376211
H	-4.769925	-2.443991	-2.434100
H	-3.529166	-1.284911	-1.827313
H	-3.273592	-2.100345	-3.398196
C	-3.346581	-3.596110	-0.327460
H	-2.721076	-4.430541	0.040852
H	-3.173872	-2.701588	0.307161
H	-4.421653	-3.872158	-0.258771
C	-1.985356	-4.028405	-2.324773
H	-1.824372	-3.673960	-3.382820

112

**IPrCl2Py3isomer--DMF** SCF Done: -3791.84319992 A.U.

Pd	2.041480	0.617685	-0.119823
N	3.036361	-2.144900	-0.447509
C	-0.276886	-3.405829	-2.757048
N	4.303998	-1.026135	0.927772
C	-0.403338	-3.254730	-1.368827
C	0.681225	-2.822330	-0.580422
Cl	1.307571	0.547784	2.098438
C	1.904580	-2.552530	-1.250059
C	2.065835	-2.696019	-2.651365
C	0.942415	-3.125662	-3.388706
C	3.402574	-2.459441	-3.349486
C	4.150654	-3.796900	-3.549132
C	3.253629	-1.725748	-4.695311
C	0.548084	-2.710003	0.935089
C	0.930618	-4.045695	1.608069
C	-0.834407	-2.215177	1.387189
C	4.071926	-2.999467	-0.065243
C	4.875216	-2.292079	0.787629
C	4.792816	-0.023223	1.846793
C	5.481309	1.101308	1.333545
C	5.975717	2.034681	2.267842
C	5.784681	1.854133	3.644061
C	5.079111	0.738600	4.118130
C	4.556146	-0.223201	3.232246

C	5.713529	1.314807	-0.158899
C	7.185238	1.038119	-0.528443
C	5.255103	2.715583	-0.606968
C	3.789964	-1.432848	3.768418
C	4.763325	-2.514377	4.287410
C	2.776301	-1.056979	4.866142
C	3.176066	-0.917599	0.156462
H	-1.139254	-3.744306	-3.353910
H	-1.367102	-3.469403	-0.884237
H	1.029580	-3.245372	-4.479103
H	4.005422	-1.802487	-2.688846
H	3.570404	-4.475212	-4.210807
H	4.318595	-4.333396	-2.593639
H	5.141402	-3.625037	-4.020045
H	4.253570	-1.439217	-5.081990
H	2.655204	-0.802338	-4.572522
H	2.776586	-2.365853	-5.468163
H	1.262468	-1.941299	1.288165
H	1.963329	-4.353328	1.341036
H	0.241922	-4.861926	1.300397
H	0.881449	-3.949614	2.713313
H	-1.107136	-1.279592	0.860189
H	-0.809836	-1.985526	2.471198
H	-1.634071	-2.968460	1.217635
H	4.130454	-4.027919	-0.430345
H	5.797893	-2.562565	1.307358
H	6.519304	2.920392	1.904013
H	6.180061	2.596006	4.356236
H	4.917067	0.618115	5.200003
H	5.085536	0.593924	-0.718589
H	7.872166	1.737884	-0.005207
H	7.342015	1.159216	-1.621161
H	7.483927	0.005280	-0.250792
H	4.217225	2.903542	-0.269223
H	5.267996	2.783478	-1.713815
H	5.910680	3.517186	-0.202922
H	3.206234	-1.858898	2.925386
H	5.477766	-2.847038	3.508052
H	4.205741	-3.406955	4.641797
H	5.360226	-2.124441	5.139458
H	3.280396	-0.740660	5.804174
H	2.145712	-1.936056	5.115586
H	2.113423	-0.240081	4.522342
Cl	2.818715	0.765114	-2.344099

N	-0.250650	0.995735	-0.894697
C	-1.161400	1.458265	-0.014578
C	-0.652275	0.122293	-1.839250
C	-2.503486	1.050826	-0.029467
C	-1.975377	-0.333724	-1.932442
C	-2.929719	0.121306	-1.002783
H	-0.770455	2.147481	0.752172
H	-3.201684	1.441123	0.727888
H	0.132350	-0.233261	-2.530313
H	-2.246779	-1.060560	-2.713330
C	-4.336669	-0.439499	-1.011635
H	-4.564376	-0.903432	-1.997147
H	-4.402786	-1.268514	-0.276821
N	-5.312729	0.590775	-0.673330
H	-5.008279	1.561935	-0.811416
C	-6.584831	0.476872	-0.207378
C	-7.232510	-0.884624	-0.117892
C	-7.327733	1.602648	0.151637
C	-8.614006	-0.959827	0.437001
C	-8.698872	1.577189	0.668798
C	-9.319606	0.211542	0.803866
Cl	-6.578944	3.184187	0.019199
O	-9.320437	2.595535	0.988805
O	-6.633351	-1.892305	-0.503622
C	-10.628190	0.106821	1.306847
C	-11.230775	-1.154464	1.447506
C	-9.224221	-2.223504	0.577495
C	-10.528969	-2.320535	1.083820
H	-11.149463	1.036829	1.581198
H	-12.255911	-1.230512	1.843553
H	-11.003471	-3.308184	1.194597
H	-8.651878	-3.115323	0.279663
O	1.734321	3.073189	-0.083220
N	2.104814	4.729720	-1.638423
C	1.933862	5.188260	-3.005984
H	1.435463	6.182669	-3.036959
H	2.916952	5.276730	-3.519562
H	1.314087	4.462026	-3.568039
C	2.930462	5.535112	-0.749556
H	2.946689	5.053311	0.245793
H	3.970555	5.603084	-1.136645
H	2.517946	6.563635	-0.658884
C	1.582490	3.545279	-1.220322
H	0.997309	3.005489	-2.006253



100

IPrCl2Py4 SCF Done: -3468.55203490 A.U.

Pd	1.063709	0.979358	-0.042732
N	1.103881	-1.915687	0.628606
C	-3.081162	-2.394114	0.224277
N	3.137349	-1.166018	0.436312
C	-2.519719	-2.262761	1.498314
C	-1.129959	-2.085190	1.666632
Cl	0.669123	1.197244	2.259363
C	-0.333413	-2.046643	0.496329
C	-0.874993	-2.172156	-0.816807
C	-2.269760	-2.339326	-0.919356
C	0.010451	-2.159880	-2.062961
C	0.764283	-3.497129	-2.241793
C	-0.742921	-1.804872	-3.355027
C	-0.532384	-2.005563	3.069056
C	-0.414194	-3.423003	3.673320
C	-1.328930	-1.083046	4.009917
C	1.956534	-2.961222	0.990782
C	3.235843	-2.486607	0.877265
C	4.266357	-0.367649	0.013046
C	4.776455	-0.589078	-1.293561
C	5.897746	0.170748	-1.678628
C	6.470021	1.110755	-0.807946
C	5.927407	1.317591	0.467466
C	4.806378	0.583753	0.908242
C	4.160613	-1.619498	-2.239562
C	4.892211	-2.976026	-2.134105
C	4.120508	-1.148622	-3.704481
C	4.233045	0.796872	2.304498
C	5.130089	0.124958	3.364787
C	3.997421	2.286484	2.612026
C	1.827480	-0.795599	0.310434
H	-4.169909	-2.523452	0.115846
H	-3.175845	-2.266975	2.380614
H	-2.733762	-2.431600	-1.911751
H	0.768175	-1.360289	-1.928164
H	0.052528	-4.338043	-2.385908
H	1.406778	-3.737628	-1.371890
H	1.423693	-3.446975	-3.133847
H	-0.014065	-1.601207	-4.165044
H	-1.367770	-0.897979	-3.233175
H	-1.405175	-2.629503	-3.696647
H	0.484070	-1.569827	2.975294

H	0.183755	-4.105201	3.034756
H	-1.419056	-3.881162	3.794650
H	0.066015	-3.383544	4.673707
H	-1.429255	-0.071744	3.575579
H	-0.800536	-0.992920	4.981778
H	-2.346631	-1.474172	4.218841
H	1.570190	-3.941233	1.282496
H	4.205016	-2.956157	1.064928
H	6.323066	0.032961	-2.684035
H	7.345280	1.695552	-1.133256
H	6.379110	2.064687	1.138166
H	3.107636	-1.768285	-1.922688
H	5.951126	-2.874972	-2.454682
H	4.406788	-3.731770	-2.787153
H	4.892163	-3.374539	-1.100462
H	3.654452	-0.147757	-3.783290
H	3.519165	-1.858391	-4.310411
H	5.134539	-1.112991	-4.157185
H	3.235941	0.314570	2.346721
H	5.242127	-0.962047	3.167863
H	4.695507	0.246991	4.379252
H	6.148053	0.570987	3.371735
H	4.948078	2.855570	2.692649
H	3.450066	2.394436	3.570067
H	3.373649	2.748048	1.820177
Cl	1.684102	0.963703	-2.316061
N	0.000211	2.775333	-0.356492
C	0.418653	3.944064	0.174080
C	-1.182796	2.715766	-1.017728
C	-0.325371	5.124356	0.055876
C	-1.983294	3.859604	-1.167952
C	-1.551223	5.078764	-0.628463
H	1.371087	3.908154	0.723580
H	0.051568	6.054747	0.504748
H	-2.944690	3.766810	-1.693930
H	-2.168333	5.984714	-0.734976
C	-1.572354	1.364956	-1.591571
H	-1.018911	1.233898	-2.545796
H	-1.173007	0.569592	-0.921731
N	-2.986941	1.177457	-1.843412
H	-3.299423	1.057943	-2.817330
C	-3.941856	0.734531	-0.977663
C	-5.163456	0.224998	-1.722081
C	-3.928850	0.681463	0.404215

C	-6.306643	-0.339878	-0.965436
C	-5.021487	0.056633	1.161310
C	-6.240828	-0.423106	0.399302
Cl	-2.575946	1.222223	1.365582
O	-4.965889	-0.106471	2.386704
O	-5.160363	0.280484	-2.959244
C	-7.355367	-1.008511	1.216277
H	-8.297325	-0.436937	1.067411
H	-7.572476	-2.052719	0.902283
H	-7.091833	-1.001219	2.290148
C	-7.496313	-0.817252	-1.755102
H	-8.419905	-0.280390	-1.448975
H	-7.336701	-0.661850	-2.838328
H	-7.686174	-1.897619	-1.576131

100

**IPrCl2Py4isomer** SCF Done: -3468.54726630 A.U.

Pd	1.148790	0.924805	-0.448672
N	1.066907	-1.407993	1.386081
C	-3.111726	-2.035154	1.108055
N	3.131335	-0.858825	0.972974
C	-2.584512	-1.335284	2.198851
C	-1.200001	-1.081211	2.304060
Cl	0.687580	2.118907	1.511957
C	-0.368346	-1.569863	1.266747
C	-0.876118	-2.269761	0.133151
C	-2.268332	-2.481153	0.078950
C	0.041582	-2.793131	-0.970431
C	0.763721	-4.090853	-0.543095
C	-0.671108	-3.003586	-2.316146
C	-0.647508	-0.347729	3.521837
C	-0.550821	-1.300081	4.733600
C	-1.476386	0.902277	3.871272
C	1.870505	-2.218592	2.192259
C	3.169044	-1.867363	1.937420
C	4.296481	-0.359848	0.275948
C	4.814659	-1.151118	-0.783610
C	5.968522	-0.673259	-1.433742
C	6.563898	0.539690	-1.054587
C	6.012037	1.305971	-0.019081
C	4.858979	0.875433	0.670195
C	4.173177	-2.476303	-1.193790
C	4.872530	-3.667145	-0.501871
C	4.142628	-2.687165	-2.718359
C	4.274373	1.706734	1.806498

C	5.159516	1.601067	3.065722
C	4.042919	3.169777	1.387480
C	1.840515	-0.546722	0.649492
H	-4.193851	-2.227367	1.046919
H	-3.258994	-0.974370	2.989560
H	-2.711045	-2.997550	-0.784553
H	0.815206	-2.019763	-1.156844
H	0.033602	-4.902016	-0.335367
H	1.383560	-3.946328	0.363778
H	1.440480	-4.434773	-1.353290
H	0.081838	-3.162648	-3.113832
H	-1.278595	-2.121616	-2.602468
H	-1.344983	-3.887033	-2.303927
H	0.370592	0.006830	3.260876
H	0.091386	-2.180078	4.525262
H	-1.554824	-1.682481	5.017666
H	-0.126506	-0.770784	5.612592
H	-1.601927	1.547538	2.980312
H	-0.956419	1.494129	4.652487
H	-2.478238	0.637270	4.271779
H	1.438573	-2.973130	2.854869
H	4.114316	-2.236413	2.344074
H	6.400194	-1.256003	-2.261214
H	7.464227	0.895359	-1.580616
H	6.481173	2.260941	0.264107
H	3.117418	-2.450364	-0.854080
H	5.932327	-3.739929	-0.827024
H	4.367227	-4.620911	-0.763168
H	4.867165	-3.573507	0.602142
H	3.693390	-1.812784	-3.226933
H	3.530595	-3.581081	-2.961609
H	5.157396	-2.865917	-3.133866
H	3.275163	1.297983	2.057489
H	5.275746	0.545354	3.389584
H	4.712688	2.171666	3.906998
H	6.176603	2.008267	2.878874
H	4.995606	3.705373	1.188442
H	3.502247	3.713675	2.188052
H	3.412590	3.212757	0.476511
Cl	1.758517	-0.095818	-2.481882
N	0.106591	2.416965	-1.517283
C	0.565807	3.677341	-1.663852
C	-1.124045	2.083782	-1.979448
C	-0.187042	4.672098	-2.299291

C	-1.934397	3.030455	-2.624455
C	-1.462181	4.339901	-2.787472
H	1.562022	3.880047	-1.243049
H	0.222581	5.687782	-2.398674
H	-2.931667	2.722808	-2.971091
H	-2.085908	5.098448	-3.286075
C	-1.528834	0.639623	-1.766548
H	-0.896882	0.016230	-2.436075
H	-1.232266	0.353309	-0.732702
N	-2.922379	0.309696	-2.025303
H	-3.087892	-0.302196	-2.831260
C	-3.924438	0.238700	-1.099570
C	-3.846094	1.105536	0.136723
C	-5.030249	-0.575506	-1.268902
C	-4.923076	0.990440	1.160715
C	-6.102310	-0.700845	-0.280520
C	-5.995432	0.164267	0.955242
Cl	-5.096175	-1.656901	-2.652702
O	-7.038602	-1.499423	-0.408916
O	-2.908347	1.894771	0.273774
C	-7.106188	0.036179	1.957527
H	-6.712769	-0.290717	2.944759
H	-7.602678	1.015865	2.129259
H	-7.858176	-0.696229	1.609472
C	-4.783776	1.838513	2.395425
H	-4.754956	1.207268	3.309308
H	-3.857545	2.440397	2.357197
H	-5.652249	2.522103	2.510374

112

**IPrCl2Py4isomer+DMF** SCF Done: -3716.91638953 A.U.

Pd	0.793771	0.556941	0.037762
N	0.429971	-2.302932	0.718148
C	-3.516750	-2.227494	-0.812830
N	2.516883	-1.756294	0.989634
C	-3.299705	-2.015577	0.554838
C	-1.997979	-2.044584	1.100871
Cl	0.142625	0.961524	2.248011
C	-0.925285	-2.285000	0.207340
C	-1.110557	-2.502996	-1.186748
C	-2.433394	-2.462783	-1.671736
C	0.061033	-2.812006	-2.116723
C	0.447876	-4.305864	-2.043643
C	-0.179140	-2.388776	-3.574086
C	-1.778396	-1.888178	2.601256

C	-2.003137	-3.241904	3.310525
C	-2.660102	-0.788607	3.215725
C	1.068024	-3.415081	1.271008
C	2.382344	-3.069402	1.445407
C	3.781867	-1.087778	0.779655
C	4.496811	-1.404822	-0.404566
C	5.734704	-0.760438	-0.593866
C	6.214217	0.172182	0.338039
C	5.479272	0.464554	1.495217
C	4.243894	-0.166079	1.748658
C	3.997945	-2.451744	-1.400547
C	4.702748	-3.803309	-1.151250
C	4.145856	-2.019301	-2.869520
C	3.465193	0.087205	3.032514
C	3.928226	-0.896368	4.129705
C	3.540271	1.547486	3.506789
C	1.315095	-1.266201	0.562092
H	-4.538241	-2.194266	-1.220529
H	-4.157887	-1.816498	1.214536
H	-2.622383	-2.617699	-2.743710
H	0.926029	-2.213838	-1.764779
H	-0.385708	-4.948948	-2.398182
H	0.705731	-4.618182	-1.012495
H	1.333500	-4.504457	-2.683728
H	0.763088	-2.492566	-4.149675
H	-0.484204	-1.325449	-3.636641
H	-0.946017	-3.017812	-4.074951
H	-0.724684	-1.575519	2.753359
H	-1.338351	-4.035973	2.912634
H	-3.050632	-3.587999	3.177085
H	-1.808309	-3.148959	4.399616
H	-2.517367	0.170060	2.680958
H	-2.382105	-0.627319	4.277468
H	-3.736951	-1.061391	3.194542
H	0.528900	-4.342727	1.481215
H	3.234673	-3.629214	1.839459
H	6.327392	-0.985623	-1.493681
H	7.174561	0.681167	0.157148
H	5.859989	1.207985	2.210088
H	2.912550	-2.598395	-1.224010
H	5.794905	-3.715850	-1.334888
H	4.301896	-4.585983	-1.829416
H	4.566946	-4.153332	-0.107999
H	3.608919	-1.068589	-3.048950

H	3.704110	-2.790231	-3.535336
H	5.209323	-1.900185	-3.166625
H	2.395705	-0.117491	2.822000
H	3.802795	-1.953704	3.814291
H	3.338423	-0.746743	5.058514
H	5.001383	-0.742666	4.374812
H	4.541757	1.801332	3.917930
H	2.797511	1.715790	4.312770
H	3.319232	2.244281	2.674001
Cl	1.486800	0.329567	-2.212061
N	-0.037417	2.419227	-0.463179
C	0.574160	3.586093	-0.160795
C	-1.250383	2.414189	-1.068926
C	-0.003780	4.819842	-0.486690
C	-1.880289	3.615988	-1.425573
C	-1.249814	4.833569	-1.135050
H	1.547988	3.515370	0.353292
H	0.523601	5.748958	-0.226123
H	-2.868619	3.572005	-1.905582
H	-1.732433	5.786751	-1.403180
C	-1.859023	1.047478	-1.325099
H	-1.277248	0.551689	-2.131644
H	-1.696665	0.424329	-0.418205
N	-3.263230	1.040044	-1.717668
H	-3.452580	0.693094	-2.663281
C	-4.334779	0.897646	-0.883806
C	-4.219154	1.362025	0.551164
C	-5.547490	0.384854	-1.312388
C	-5.364252	1.133163	1.476713
C	-6.681278	0.136208	-0.421264
C	-6.525933	0.569796	1.019883
Cl	-5.705968	-0.186456	-2.968017
O	-7.717668	-0.422740	-0.800601
O	-3.193472	1.933601	0.928897
O	3.778523	3.287993	0.576243
N	4.920941	2.693182	-1.342338
C	4.955566	1.859377	-2.529954
H	4.894398	2.480991	-3.451613
H	5.892758	1.262200	-2.572903
H	4.092372	1.165471	-2.514952
C	5.968089	3.683031	-1.165380
H	5.764559	4.237713	-0.229335
H	6.964592	3.191409	-1.095016
H	5.993499	4.396144	-2.019181

C	3.919371	2.567415	-0.418270
H	3.218606	1.727187	-0.666469
C	-5.201802	1.604552	2.896876
H	-5.942766	2.398898	3.133718
H	-5.381418	0.778640	3.616480
H	-4.186481	2.007534	3.065850
C	-7.713083	0.353064	1.913176
H	-7.445145	-0.284828	2.783204
H	-8.073560	1.317240	2.333551
H	-8.535616	-0.127841	1.351734
108			
<b>IPrCl2Py4isomer+K3PO4</b> SCF Done: -5910.90392793 A.U.			
Pd	1.463041	-0.653548	0.290796
N	4.161981	0.435119	0.041464
C	5.611630	-3.521991	-0.297169
N	2.785605	2.121132	0.067674
C	5.217923	-3.030229	0.955362
C	4.751539	-1.707520	1.102870
Cl	1.088015	0.219252	2.468517
C	4.686513	-0.909637	-0.065564
C	5.086740	-1.372880	-1.346668
C	5.554436	-2.698710	-1.431394
C	5.042065	-0.474381	-2.580925
C	6.385011	0.268327	-2.765863
C	4.681215	-1.224029	-3.876060
C	4.404842	-1.153443	2.480960
C	5.696539	-0.723124	3.209489
C	3.569711	-2.130225	3.325770
C	4.944944	1.586010	0.093687
C	4.081437	2.646381	0.097773
C	1.619043	2.974954	-0.014008
C	0.893408	3.030862	-1.239975
C	-0.193011	3.925789	-1.293426
C	-0.515784	4.750988	-0.205976
C	0.229412	4.686951	0.980431
C	1.306528	3.779905	1.113082
C	1.280915	2.181491	-2.451038
C	2.634946	2.621950	-3.056646
C	0.216692	2.151356	-3.559318
C	2.094191	3.724349	2.424212
C	2.994706	4.969853	2.578903
C	1.179689	3.572993	3.656910
C	2.823583	0.753976	0.051276
H	5.970947	-4.559325	-0.391045



H	5.278289	-3.681574	1.840617
H	5.864233	-3.099401	-2.407801
H	4.243386	0.276223	-2.406400
H	7.207200	-0.455518	-2.950982
H	6.663445	0.867966	-1.877525
H	6.332196	0.957363	-3.634893
H	4.492699	-0.494829	-4.691132
H	3.768664	-1.835753	-3.741980
H	5.506941	-1.884918	-4.216457
H	3.781167	-0.248245	2.343108
H	6.260040	0.030482	2.620121
H	6.369331	-1.591625	3.375261
H	5.458525	-0.278149	4.198612
H	2.664474	-2.450238	2.772189
H	3.229875	-1.631347	4.255498
H	4.146693	-3.032788	3.619543
H	6.036382	1.538865	0.122193
H	4.256291	3.724975	0.098640
H	-0.833195	3.957423	-2.182994
H	-1.378973	5.429421	-0.283506
H	-0.030253	5.344936	1.825426
H	1.390867	1.140082	-2.086512
H	2.568631	3.656864	-3.456002
H	2.907467	1.949463	-3.897051
H	3.471683	2.594241	-2.331760
H	-0.778312	1.846111	-3.179153
H	0.528096	1.428660	-4.343890
H	0.111776	3.137534	-4.061092
H	2.737657	2.820584	2.397532
H	3.684360	5.096298	1.719781
H	3.608069	4.902756	3.502046
H	2.381408	5.893834	2.643839
H	0.508905	4.448263	3.789592
H	1.790562	3.483675	4.579255
H	0.566901	2.652828	3.580804
Cl	1.819257	-1.444487	-1.916149
N	0.433776	-2.494361	0.689375
C	1.241278	-3.566683	0.471131
C	-0.835135	-2.697394	1.127531
C	0.814572	-4.882244	0.667182
C	-1.332877	-3.999403	1.325521
C	-0.507462	-5.103449	1.093342
H	2.257929	-3.340907	0.115272
H	1.511195	-5.711560	0.476680

H	-2.376403	-4.104658	1.653293
H	-0.887688	-6.126389	1.242682
C	-1.661956	-1.472333	1.424786
H	-1.132547	-0.945966	2.249036
H	-1.625860	-0.786671	0.543052
N	-3.033917	-1.721105	1.844989
H	-3.236519	-1.508946	2.826790
C	-4.132147	-1.563978	1.042806
C	-3.986106	-1.823005	-0.431882
C	-5.365258	-1.167483	1.543535
C	-5.186405	-1.641894	-1.301523
C	-6.459312	-0.793781	0.667260
C	-6.386350	-1.260845	-0.759721
Cl	-5.439168	-0.567226	3.212955
O	-7.389177	-0.028296	1.016014
O	-2.954631	-2.376573	-0.876393
O	-1.194538	0.785652	-0.863200
P	-2.685422	1.190235	-1.232634
O	-3.064738	0.741374	-2.681787
K	-1.683277	1.818623	1.468598
O	-3.648942	0.437294	-0.138273
O	-3.002253	2.706608	-0.900845
K	-1.210876	-1.147219	-2.604694
K	-5.544853	2.026498	-0.749230
C	-4.955347	-1.868345	-2.765198
H	-4.359141	-2.788435	-2.935083
H	-5.892687	-1.928738	-3.347820
H	-4.350977	-0.999842	-3.128777
C	-7.651481	-1.105351	-1.572862
H	-7.564887	-0.306746	-2.344408
H	-7.893659	-2.040019	-2.120752
H	-8.497534	-0.841499	-0.910478

100

**IPrCl2Py5** SCF Done: -3468.54104247 A.U.

Pd	-1.010453	-0.802557	-0.439543
N	-1.426003	1.738450	1.058157
C	2.352681	3.203616	-0.154065
N	-3.296207	0.636113	0.908298
C	2.274831	2.208342	0.827550
C	1.036393	1.697880	1.264221
Cl	-1.282216	-2.146687	1.474005
C	-0.126835	2.252471	0.683248
C	-0.089379	3.260247	-0.316832
C	1.178239	3.725430	-0.714878

C	-1.360367	3.848380	-0.930205
C	-1.708041	5.195163	-0.258100
C	-1.281093	4.010367	-2.459181
C	0.991894	0.608813	2.330582
C	1.296402	1.203476	3.721243
C	1.940568	-0.558186	1.997739
C	-2.362710	2.429816	1.826957
C	-3.543080	1.742433	1.724142
C	-4.311359	-0.258391	0.400501
C	-4.714368	-0.089555	-0.953171
C	-5.707660	-0.962980	-1.437585
C	-6.278872	-1.942851	-0.610982
C	-5.866696	-2.072773	0.721663
C	-4.865232	-1.237546	1.259769
C	-4.152471	1.032447	-1.826009
C	-4.908985	2.352144	-1.557297
C	-4.126282	0.700137	-3.325023
C	-4.442581	-1.372727	2.720130
C	-5.453314	-0.659026	3.644814
C	-4.258321	-2.840021	3.150417
C	-1.987986	0.618445	0.505457
H	3.339818	3.547793	-0.497840
H	3.197538	1.804366	1.268947
H	1.248290	4.496849	-1.496620
H	-2.192971	3.143346	-0.728934
H	-0.909151	5.943317	-0.448185
H	-1.813920	5.097412	0.841366
H	-2.660763	5.601645	-0.658917
H	-2.267532	4.330130	-2.856516
H	-1.004428	3.051092	-2.937252
H	-0.543790	4.785481	-2.757314
H	-0.031531	0.183562	2.358020
H	0.579672	2.010089	3.981871
H	2.318128	1.641146	3.752657
H	1.234939	0.419909	4.505761
H	1.748803	-0.941339	0.975445
H	1.782068	-1.397847	2.703511
H	3.006414	-0.251867	2.059341
H	-2.100998	3.346968	2.360980
H	-4.534439	1.936983	2.141385
H	-6.044433	-0.870065	-2.480469
H	-7.056394	-2.612344	-1.012609
H	-6.323522	-2.844850	1.359313
H	-3.092113	1.187772	-1.542737

H	-5.980244	2.261082	-1.837991
H	-4.465156	3.179073	-2.150804
H	-4.860550	2.643034	-0.487810
H	-3.600484	-0.257848	-3.509550
H	-3.570289	1.491045	-3.868006
H	-5.145188	0.643284	-3.765932
H	-3.451637	-0.883242	2.821682
H	-5.574323	0.412982	3.387098
H	-5.127322	-0.719603	4.704629
H	-6.456595	-1.130626	3.568731
H	-5.225203	-3.385416	3.193572
H	-3.811766	-2.883908	4.165445
H	-3.577801	-3.367181	2.453932
Cl	-0.644292	0.495435	-2.352754
N	0.155746	-2.324820	-1.282747
C	-0.267974	-3.610153	-1.301325
C	1.406037	-2.025153	-1.692744
C	0.556150	-4.648038	-1.753143
C	2.314513	-3.014800	-2.111733
C	1.869264	-4.348757	-2.149965
H	-1.283846	-3.788670	-0.918718
H	0.173317	-5.679054	-1.771150
H	1.678942	-0.956625	-1.681902
H	2.550092	-5.150057	-2.482359
C	3.755050	-2.629256	-2.401941
H	4.271031	-3.460817	-2.927477
H	3.805763	-1.737926	-3.051742
N	4.471345	-2.358764	-1.160187
H	4.583604	-3.151311	-0.505622
C	4.772748	-1.196818	-0.527975
C	5.266247	-1.484522	0.891314
C	4.696412	0.124250	-0.936400
C	5.704720	-0.373418	1.765392
C	5.260893	1.214688	-0.132574
C	5.697813	0.907792	1.284558
Cl	4.021541	0.632782	-2.474319
O	5.361424	2.371192	-0.562659
O	5.265811	-2.658934	1.277373
C	6.097203	2.079835	2.131698
H	7.111894	1.939980	2.562290
H	6.076762	3.011409	1.536811
H	5.402392	2.186549	2.993984
C	6.099120	-0.715157	3.176860
H	5.370697	-0.284976	3.898722

H	6.126108	-1.810699	3.323956
H	7.091931	-0.289619	3.433020
100			
<b>IPrCl2Py5isomer</b> SCF Done: -3468.53786224 A.U.			
Pd	-0.472268	-0.617219	-0.077757
N	-2.374977	1.741950	-0.316350
C	0.319385	4.885431	-1.144412
N	-3.388282	-0.106131	0.210698
C	-0.121022	4.670347	0.169646
C	-0.981314	3.599073	0.483419
Cl	0.198350	0.260006	2.000394
C	-1.384370	2.760307	-0.587695
C	-0.929260	2.926964	-1.917949
C	-0.069198	4.015077	-2.171766
C	-1.383946	2.010668	-3.047942
C	-2.505463	2.686258	-3.865122
C	-0.216348	1.556833	-3.941877
C	-1.474387	3.389467	1.914004
C	-2.671486	4.313466	2.227382
C	-0.355528	3.581851	2.954029
C	-3.738992	2.034630	-0.244005
C	-4.375025	0.872507	0.098799
C	-3.637513	-1.473096	0.615209
C	-4.105763	-2.397862	-0.350977
C	-4.331835	-3.720091	0.083558
C	-4.099077	-4.095739	1.413510
C	-3.648394	-3.151978	2.348320
C	-3.411472	-1.814229	1.974850
C	-4.412296	-1.986196	-1.788551
C	-5.908761	-1.631865	-1.938567
C	-4.006200	-3.055256	-2.819021
C	-3.006906	-0.765826	3.008569
C	-4.264748	-0.094893	3.603410
C	-2.095869	-1.319267	4.115282
C	-2.147726	0.419333	-0.049069
H	0.988429	5.732022	-1.366606
H	0.211767	5.346571	0.971459
H	0.301754	4.178899	-3.194775
H	-1.801215	1.088094	-2.597935
H	-2.145212	3.621927	-4.344659
H	-3.371747	2.948969	-3.222004
H	-2.868055	2.007995	-4.666036
H	-0.569748	0.790320	-4.660823
H	0.590828	1.094417	-3.338995

H	0.217786	2.395292	-4.527173
H	-1.810292	2.334921	1.998453
H	-3.521691	4.143261	1.537181
H	-2.376607	5.381259	2.141990
H	-3.036502	4.141265	3.261773
H	0.528586	2.967314	2.698887
H	-0.710628	3.264978	3.956204
H	-0.042245	4.644364	3.036875
H	-4.117122	3.040017	-0.447343
H	-5.429481	0.647326	0.277851
H	-4.690222	-4.469744	-0.637672
H	-4.275235	-5.136950	1.727813
H	-3.481399	-3.459065	3.391464
H	-3.806685	-1.082264	-2.008103
H	-6.544854	-2.516062	-1.719258
H	-6.130029	-1.299699	-2.974750
H	-6.219561	-0.821039	-1.249425
H	-2.953483	-3.363846	-2.669561
H	-4.099340	-2.644321	-3.845507
H	-4.658234	-3.953388	-2.765733
H	-2.415266	0.014882	2.489120
H	-4.887247	0.378231	2.816582
H	-3.978222	0.694747	4.329661
H	-4.896826	-0.838995	4.133837
H	-2.628435	-2.026409	4.786623
H	-1.718047	-0.485844	4.741497
H	-1.214263	-1.830306	3.680206
Cl	-1.018715	-1.418326	-2.211795
N	1.231158	-1.856076	-0.089769
C	1.527343	-2.604625	0.996303
C	2.051817	-1.888722	-1.163446
C	2.662096	-3.427220	1.036109
C	3.241901	-2.637330	-1.184536
C	3.539169	-3.427980	-0.056532
H	0.843762	-2.507288	1.852459
H	2.863635	-4.031035	1.933072
H	1.753506	-1.266033	-2.019408
H	4.475480	-4.009101	-0.018285
C	4.281633	-2.389552	-2.268362
H	4.711897	-3.341146	-2.639902
H	3.835364	-1.853966	-3.126881
N	5.401889	-1.596062	-1.705253
H	6.168092	-2.176810	-1.344453
C	5.108875	-0.571258	-0.827974

C	4.037799	0.419818	-1.230627
C	5.758305	-0.371983	0.368419
C	3.468199	1.314394	-0.189658
C	5.296867	0.607286	1.377736
C	4.063453	1.407512	1.041283
Cl	7.050280	-1.456424	0.854821
O	5.851655	0.720549	2.473730
O	3.641556	0.439313	-2.400802
C	3.497649	2.270156	2.129171
H	3.300444	3.303144	1.773080
H	2.514846	1.848272	2.438689
H	4.173183	2.298716	3.003826
C	2.249650	2.105003	-0.555868
H	1.932109	1.899031	-1.592957
H	1.409679	1.861068	0.128616
H	2.430858	3.195578	-0.459307

112

**IPrCl2PySisomer--DMF SCF Done: -3716.87476745 A.U.**

Pd	-1.684562	0.703523	-0.300703
N	-1.699891	-1.845066	1.211215
C	2.166164	-1.493432	2.896254
N	-3.536571	-1.595372	0.064000
C	2.020163	-1.756244	1.525951
C	0.750044	-1.853115	0.926016
Cl	-1.647534	-0.087094	-2.505156
C	-0.377756	-1.673376	1.772259
C	-0.265256	-1.380828	3.155811
C	1.034512	-1.299838	3.697597
C	-1.480552	-1.190305	4.062120
C	-1.753996	-2.464684	4.891833
C	-1.334269	0.027209	4.996037
C	0.605358	-2.172581	-0.559376
C	0.220969	-3.652074	-0.779296
C	1.841553	-1.796841	-1.391368
C	-2.505211	-2.953623	1.484680
C	-3.661822	-2.790337	0.773897
C	-4.540461	-1.111711	-0.856418
C	-5.356129	-0.021019	-0.470058
C	-6.356118	0.387387	-1.376787
C	-6.529424	-0.259812	-2.607067
C	-5.693922	-1.327544	-2.965615
C	-4.673047	-1.774583	-2.104672
C	-5.202896	0.698539	0.866896
C	-6.389027	0.385294	1.801501

C	-5.006617	2.213556	0.666341
C	-3.769069	-2.936732	-2.514669
C	-4.476417	-4.291747	-2.289884
C	-3.285147	-2.825281	-3.973288
C	-2.333254	-0.994168	0.338414
H	3.177826	-1.438598	3.325739
H	2.922093	-1.889539	0.914859
H	1.157637	-1.080749	4.769362
H	-2.355538	-0.993816	3.408093
H	-0.899552	-2.681878	5.567896
H	-1.905504	-3.360112	4.256240
H	-2.660925	-2.336958	5.519766
H	-2.296413	0.227121	5.512101
H	-1.056313	0.930582	4.419953
H	-0.570775	-0.145143	5.784610
H	-0.224701	-1.554466	-0.957951
H	-0.716940	-3.919299	-0.250717
H	1.022498	-4.331344	-0.416418
H	0.060927	-3.848957	-1.860078
H	2.149582	-0.747371	-1.209831
H	1.604165	-1.893380	-2.470025
H	2.713028	-2.454809	-1.179318
H	-2.170010	-3.752073	2.151059
H	-4.562724	-3.404739	0.702687
H	-7.011895	1.230252	-1.107616
H	-7.318236	0.076054	-3.299086
H	-5.826385	-1.816381	-3.942764
H	-4.280699	0.334503	1.361095
H	-7.349288	0.744685	1.372705
H	-6.250198	0.881013	2.785545
H	-6.488179	-0.706567	1.976929
H	-4.170916	2.397663	-0.036975
H	-4.746676	2.694239	1.631269
H	-5.922526	2.702046	0.268774
H	-2.864418	-2.895489	-1.871806
H	-4.797979	-4.431988	-1.238395
H	-3.803701	-5.134799	-2.554494
H	-5.384012	-4.367027	-2.926279
H	-4.112499	-2.986469	-4.697112
H	-2.517394	-3.600738	-4.177278
H	-2.834934	-1.831449	-4.159754
Cl	-1.739335	1.549250	1.903973
N	0.646379	1.615047	-0.575617
C	1.081839	1.906605	-1.816857



C	1.532544	1.495040	0.425887
C	2.440614	2.104786	-2.098884
C	2.922769	1.677619	0.244912
C	3.372022	1.993909	-1.052313
H	0.300591	1.956981	-2.594102
H	2.767832	2.341633	-3.122839
H	1.101119	1.239725	1.411985
H	4.442352	2.155664	-1.253550
C	3.865600	1.525690	1.433599
H	3.664024	2.325192	2.178129
H	3.666550	0.567196	1.947771
N	5.284434	1.600572	1.082992
H	5.605443	2.542011	0.825615
C	5.966693	0.629155	0.396241
C	5.726512	-0.824971	0.733132
C	6.959645	0.915873	-0.524211
C	6.313488	-1.875358	-0.145317
C	7.665701	-0.106585	-1.307621
C	7.261062	-1.545648	-1.076963
Cl	7.319207	2.590173	-0.915325
O	8.517615	0.179759	-2.155232
O	5.073366	-1.125357	1.737165
O	-1.993465	2.929021	-1.117948
N	-2.288206	5.003769	-0.173060
C	-1.826464	5.996083	0.782282
H	-1.643192	6.974988	0.286394
H	-2.578980	6.149705	1.587230
H	-0.882955	5.652865	1.250612
C	-3.546602	5.256560	-0.862053
H	-3.732178	4.427868	-1.570319
H	-4.386259	5.306104	-0.134883
H	-3.499110	6.218312	-1.417164
C	-1.623019	3.832952	-0.350644
H	-0.697451	3.737363	0.268575
C	5.878434	-3.295342	0.101634
H	5.148343	-3.346158	0.930901
H	5.414948	-3.727386	-0.811382
H	6.743804	-3.944213	0.355950
C	7.946413	-2.577683	-1.925152
H	7.207002	-3.155113	-2.521360
H	8.667767	-2.096199	-2.611239
H	8.485179	-3.317022	-1.293383

100

IPrCl2Py6 SCF Done: -3468.53369824 A.U.

Pd	0.590620	-0.074539	-0.792433
N	3.219104	-0.798119	0.504106
C	1.948781	-4.637974	1.731416
N	3.118083	1.307436	-0.033220
C	1.591557	-3.505778	2.480616
C	2.012944	-2.217332	2.098630
Cl	-0.474017	1.014500	1.001808
C	2.796002	-2.119117	0.914071
C	3.188630	-3.241968	0.147194
C	2.746078	-4.507307	0.587381
C	4.101759	-3.118531	-1.068902
C	5.559125	-3.452217	-0.679120
C	3.641551	-3.991655	-2.250778
C	1.697380	-0.991610	2.956038
C	2.900930	-0.621878	3.851624
C	0.422940	-1.131566	3.799985
C	4.484008	-0.257898	0.746054
C	4.422206	1.065862	0.400619
C	2.565166	2.626732	-0.252359
C	2.381176	3.092698	-1.574380
C	1.836620	4.384847	-1.730174
C	1.491110	5.164712	-0.618304
C	1.678347	4.667829	0.680495
C	2.214901	3.384392	0.896961
C	2.772980	2.265398	-2.793368
C	4.042373	2.842643	-3.453857
C	1.612137	2.139154	-3.798144
C	2.442413	2.863685	2.315863
C	3.748378	3.443569	2.902678
C	1.258180	3.132029	3.262568
C	2.377582	0.156319	-0.001194
H	1.605234	-5.635231	2.049704
H	0.976400	-3.627379	3.384067
H	3.028756	-5.404429	0.015943
H	4.055850	-2.063863	-1.410363
H	5.644637	-4.506298	-0.338173
H	5.930491	-2.809642	0.145509
H	6.238035	-3.318130	-1.547499
H	4.250800	-3.764020	-3.149944
H	2.581614	-3.786680	-2.496924
H	3.761438	-5.075770	-2.039445
H	1.505534	-0.143357	2.267913
H	3.817160	-0.424002	3.260476
H	3.125986	-1.440454	4.568206

H	2.677110	0.295459	4.436115
H	-0.435922	-1.444209	3.177789
H	0.166582	-0.150914	4.249765
H	0.543198	-1.858835	4.631709
H	5.298498	-0.864447	1.150565
H	5.173118	1.859783	0.427594
H	1.682102	4.783147	-2.744966
H	1.065916	6.170605	-0.763881
H	1.392545	5.285233	1.545577
H	3.006509	1.236012	-2.454296
H	3.868422	3.873704	-3.830166
H	4.354378	2.214361	-4.314554
H	4.887932	2.886767	-2.735653
H	0.708233	1.733769	-3.299618
H	1.884969	1.433712	-4.608621
H	1.355411	3.114967	-4.263221
H	2.558180	1.762808	2.253730
H	4.626532	3.226808	2.261573
H	3.947329	3.018865	3.909293
H	3.675076	4.547372	3.004628
H	1.135080	4.214520	3.478688
H	1.431899	2.624262	4.234730
H	0.316068	2.742995	2.830916
Cl	1.647943	-1.175440	-2.577395
N	-1.276637	-0.296176	-1.751075
C	-2.199430	0.693477	-1.694740
C	-1.620031	-1.478118	-2.315151
C	-3.517628	0.501621	-2.118768
C	-2.924804	-1.744706	-2.744717
C	-3.919441	-0.761345	-2.599932
H	-1.871299	1.637130	-1.234516
H	-4.247374	1.314409	-1.982296
H	-0.817070	-2.228165	-2.379162
H	-3.178636	-2.754495	-3.099366
C	-5.399269	-1.093354	-2.734997
H	-5.832715	-0.594267	-3.627517
H	-5.521269	-2.186983	-2.867214
N	-6.164756	-0.621067	-1.567490
H	-6.838573	0.129126	-1.750612
C	-5.617991	-0.540982	-0.309907
C	-4.635335	-1.609190	0.116817
C	-5.950561	0.423751	0.615949
C	-3.730710	-1.324535	1.259661
C	-5.221790	0.595145	1.888440

C	-4.031379	-0.307925	2.127384
Cl	-7.143589	1.646379	0.209713
O	-5.514274	1.484239	2.692580
O	-4.589401	-2.670790	-0.512354
C	-3.187039	-0.001531	3.327621
H	-3.014840	-0.909197	3.944273
H	-2.186145	0.347892	2.990715
H	-3.657758	0.783644	3.947583
C	-2.517243	-2.200424	1.401128
H	-2.550112	-3.038925	0.681007
H	-1.606374	-1.591459	1.204486
H	-2.419961	-2.613485	2.426808
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<b>IPrCl2Py6del2</b> SCF Done: -3468.53465286 A.U.			
Pd	-0.991771	-0.286004	-0.924019
N	-1.971079	1.160645	1.432018
C	0.948374	4.141275	0.742301
N	-3.396661	-0.411495	0.947895
C	1.338343	2.906642	1.279135
C	0.386221	1.899175	1.545077
Cl	-0.474686	-2.204824	0.345050
C	-0.965741	2.185895	1.240481
C	-1.391993	3.423723	0.690093
C	-0.401694	4.397456	0.458729
C	-2.861865	3.713382	0.386590
C	-3.519107	4.465942	1.565146
C	-3.075763	4.485667	-0.927602
C	0.818749	0.581906	2.180623
C	1.102660	0.788898	3.683872
C	2.031455	-0.029834	1.462014
C	-2.910098	1.140394	2.462901
C	-3.813600	0.158538	2.153707
C	-4.168327	-1.373197	0.193412
C	-4.884089	-0.896601	-0.939305
C	-5.653644	-1.837970	-1.650401
C	-5.716012	-3.180136	-1.244974
C	-5.004946	-3.612928	-0.118267
C	-4.206596	-2.720083	0.627013
C	-4.874951	0.579700	-1.332833
C	-5.911726	1.370879	-0.505045
C	-5.063203	0.821412	-2.837819
C	-3.459727	-3.198445	1.869337
C	-4.421592	-3.309624	3.072338
C	-2.720250	-4.529102	1.635896

C	-2.251601	0.189577	0.504319
H	1.708052	4.912676	0.538657
H	2.403294	2.720220	1.491333
H	-0.691580	5.368806	0.030497
H	-3.376251	2.736899	0.271862
H	-3.042009	5.459193	1.707077
H	-3.423800	3.912922	2.520920
H	-4.600395	4.629214	1.371792
H	-4.159934	4.535492	-1.161750
H	-2.561643	3.978759	-1.766412
H	-2.710005	5.532286	-0.859039
H	-0.011278	-0.146411	2.084794
H	0.214061	1.192144	4.213204
H	1.937491	1.506216	3.838066
H	1.380999	-0.172900	4.165324
H	1.817003	-0.201679	0.389820
H	2.297780	-1.008815	1.909610
H	2.915099	0.632691	1.536522
H	-2.846731	1.827904	3.310240
H	-4.716729	-0.183795	2.665612
H	-6.218450	-1.512547	-2.536219
H	-6.327088	-3.896817	-1.816724
H	-5.061049	-4.668455	0.188718
H	-3.872499	0.986424	-1.092938
H	-6.943310	1.012977	-0.710893
H	-5.863616	2.451078	-0.758814
H	-5.729187	1.275471	0.584925
H	-4.337966	0.227672	-3.429075
H	-4.877726	1.890540	-3.066222
H	-6.092074	0.579105	-3.181937
H	-2.684579	-2.438668	2.099987
H	-4.930581	-2.348498	3.290889
H	-3.872957	-3.619639	3.986687
H	-5.213521	-4.064363	2.877474
H	-3.423606	-5.377695	1.495891
H	-2.085718	-4.769726	2.514189
H	-2.061833	-4.456769	0.748404
Cl	-1.592627	1.557691	-2.240775
N	0.719872	-0.631676	-2.121968
C	1.232824	-1.863477	-2.356390
C	1.498989	0.453710	-2.345040
C	2.555730	-2.048604	-2.772074
C	2.836555	0.342371	-2.741904
C	3.398333	-0.930469	-2.940718

H	0.565309	-2.712298	-2.146952
H	2.932768	-3.072552	-2.923320
H	1.021787	1.430586	-2.170276
H	3.445652	1.251809	-2.847434
C	4.891808	-1.112394	-3.178002
H	5.074135	-1.872462	-3.964447
H	5.354618	-0.163845	-3.508924
N	5.545265	-1.597921	-1.956439
H	5.475531	-2.617260	-1.797786
C	5.517990	-0.972431	-0.741377
C	5.405728	-1.969710	0.405024
C	5.575106	0.373809	-0.441532
C	5.325474	-1.484689	1.801168
C	5.404192	0.875782	0.933865
C	5.311758	-0.139142	2.053073
Cl	5.864342	1.608781	-1.651876
O	5.321881	2.082989	1.186364
O	5.362161	-3.172737	0.120307
C	5.185740	-2.515998	2.887358
H	4.200353	-2.414302	3.392755
H	5.260129	-3.538306	2.472847
H	5.960826	-2.385559	3.671889
C	5.145943	0.406531	3.440377
H	4.152239	0.117266	3.848059
H	5.907665	-0.012439	4.131506
H	5.216491	1.509751	3.436391
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<b>IPrCl2Py6del3</b> SCF Done: -3468.53632644 A.U.			
Pd	0.568455	-0.090158	-0.770333
N	2.623845	-0.928731	1.243959
C	2.002945	-5.072659	0.699351
N	2.778476	1.196455	0.805552
C	1.055100	-4.318796	1.403708
C	1.224748	-2.931566	1.597982
Cl	-0.703689	1.155039	0.792175
C	2.391542	-2.344408	1.059272
C	3.358443	-3.071783	0.315023
C	3.139900	-4.453381	0.158136
C	4.598821	-2.405315	-0.280037
C	5.828361	-2.619126	0.629780
C	4.906437	-2.871234	-1.715363
C	0.182794	-2.129084	2.369418
C	0.223965	-2.475676	3.872308
C	-1.226954	-2.321286	1.784200

C	3.578445	-0.405729	2.117325
C	3.684681	0.929577	1.833854
C	2.702700	2.446826	0.084032
C	3.291373	2.493607	-1.210531
C	3.222282	3.719936	-1.900278
C	2.612782	4.844702	-1.323145
C	2.053960	4.766295	-0.040854
C	2.078319	3.562072	0.692894
C	4.028836	1.293300	-1.803991
C	5.475455	1.228435	-1.265797
C	4.002990	1.243950	-3.338744
C	1.482451	3.498081	2.096808
C	2.467727	4.075145	3.136846
C	0.120475	4.212648	2.188902
C	2.105713	0.057282	0.448262
H	1.850196	-6.154873	0.560259
H	0.159825	-4.812337	1.812773
H	3.866109	-5.052734	-0.411768
H	4.397675	-1.315724	-0.336035
H	6.076334	-3.699548	0.702925
H	5.657410	-2.246871	1.659606
H	6.715148	-2.091077	0.219808
H	5.727642	-2.257267	-2.141753
H	4.016022	-2.758583	-2.363045
H	5.242730	-3.929418	-1.745563
H	0.422168	-1.051156	2.265461
H	1.230951	-2.294767	4.303493
H	-0.031116	-3.542795	4.047140
H	-0.508996	-1.857554	4.432323
H	-1.248828	-2.040319	0.712268
H	-1.955112	-1.679976	2.313014
H	-1.586245	-3.367014	1.880586
H	4.090268	-1.036713	2.848447
H	4.322921	1.711516	2.253236
H	3.659893	3.796776	-2.906264
H	2.574101	5.793758	-1.881464
H	1.577757	5.654867	0.400520
H	3.505333	0.373958	-1.473440
H	6.055861	2.124459	-1.573755
H	5.993468	0.328886	-1.660331
H	5.499976	1.169883	-0.158347
H	2.965667	1.317059	-3.722005
H	4.414030	0.273352	-3.682638
H	4.614551	2.049120	-3.800264

H	1.300075	2.427964	2.327384
H	3.443879	3.548996	3.127668
H	2.048615	3.994709	4.162060
H	2.670131	5.148626	2.933852
H	0.222757	5.316479	2.114698
H	-0.361112	3.993212	3.164453
H	-0.554812	3.862969	1.384007
Cl	1.713535	-1.419903	-2.308201
N	-1.171829	-0.248106	-1.922308
C	-1.865627	0.866694	-2.251402
C	-1.748552	-1.457352	-2.088627
C	-3.185877	0.807625	-2.697847
C	-3.085376	-1.590747	-2.491420
C	-3.842510	-0.439681	-2.767176
H	-1.349112	1.825148	-2.095462
H	-3.726511	1.746556	-2.891396
H	-1.118849	-2.327177	-1.844986
H	-3.547595	-2.588880	-2.512199
C	-5.359343	-0.478410	-2.913050
H	-5.682594	-0.045092	-3.881783
H	-5.724334	-1.523428	-2.872515
N	-5.976456	0.332587	-1.845528
H	-6.067405	1.329666	-2.097366
C	-5.470527	0.275272	-0.561549
C	-5.049070	1.624914	-0.012970
C	-5.227561	-0.849225	0.189638
C	-4.354888	1.707851	1.292885
C	-4.592116	-0.781533	1.525912
C	-4.114414	0.565534	2.011210
Cl	-5.702812	-2.444296	-0.345902
O	-4.441380	-1.789417	2.221274
O	-5.252861	2.621773	-0.720900
C	-3.336604	0.574473	3.292101
H	-3.614041	1.431542	3.938594
H	-3.476947	-0.373716	3.843553
H	-2.254745	0.683442	3.047670
C	-3.856291	3.058292	1.726731
H	-4.194494	3.847051	1.029708
H	-4.199668	3.310660	2.752071
H	-2.745013	3.051944	1.745387
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<b>IPrCl2Py6del5</b> SCF Done: -3468.53463160 A.U.			
Pd	-0.988451	-0.316316	-0.907241
N	-1.972134	1.202948	1.405887



C	0.943197	4.165772	0.628896
N	-3.399064	-0.378405	0.956599
C	1.335083	2.946743	1.198892
C	0.384644	1.946411	1.495826
Cl	-0.482880	-2.197802	0.420799
C	-0.968082	2.223520	1.186359
C	-1.396417	3.445356	0.602956
C	-0.407739	4.413165	0.342243
C	-2.867273	3.726537	0.296046
C	-3.518910	4.516954	1.452835
C	-3.085537	4.456809	-1.041238
C	0.820461	0.647844	2.167330
C	1.108703	0.897781	3.663199
C	2.031513	0.017231	1.462475
C	-2.916626	1.212456	2.432042
C	-3.820579	0.224268	2.144789
C	-4.171070	-1.353627	0.219916
C	-4.877130	-0.899490	-0.928164
C	-5.647889	-1.852640	-1.622039
C	-5.720280	-3.184745	-1.186303
C	-5.017799	-3.595473	-0.046060
C	-4.218871	-2.690206	0.683523
C	-4.857156	0.567086	-1.356841
C	-5.895035	1.382801	-0.554692
C	-5.034904	0.773650	-2.868317
C	-3.481376	-3.144700	1.940319
C	-4.449895	-3.221613	3.140652
C	-2.749619	-4.485254	1.741671
C	-2.250124	0.208106	0.503324
H	1.701943	4.931377	0.401401
H	2.400808	2.766868	1.412247
H	-0.699798	5.371925	-0.112066
H	-3.383882	2.747939	0.214959
H	-3.042482	5.514939	1.559231
H	-3.417273	3.996127	2.425974
H	-4.601507	4.672394	1.260337
H	-4.170903	4.505394	-1.270155
H	-2.579014	3.920324	-1.866084
H	-2.713418	5.502882	-1.008895
H	-0.008911	-0.084340	2.095629
H	0.219514	1.309547	4.184895
H	1.938953	1.624993	3.794139
H	1.395762	-0.048507	4.169622
H	1.813349	-0.184071	0.396229

H	2.299443	-0.949012	1.935976
H	2.916501	0.680513	1.515361
H	-2.856384	1.922848	3.260559
H	-4.726993	-0.102449	2.661034
H	-6.205637	-1.544339	-2.518389
H	-6.332161	-3.910983	-1.744987
H	-5.081153	-4.643532	0.284198
H	-3.853833	0.974073	-1.120861
H	-6.926838	1.023305	-0.756529
H	-5.841952	2.455998	-0.835512
H	-5.718132	1.314311	0.538205
H	-4.309698	0.161672	-3.440710
H	-4.841550	1.835888	-3.121195
H	-6.063130	0.529272	-3.212851
H	-2.701795	-2.385377	2.157129
H	-4.952717	-2.252130	3.335163
H	-3.907960	-3.515162	4.064383
H	-5.246517	-3.974663	2.958756
H	-3.457656	-5.332210	1.616105
H	-2.122389	-4.710168	2.629317
H	-2.084713	-4.437319	0.857329
Cl	-1.559359	1.500972	-2.271858
N	0.714207	-0.723756	-2.096315
C	1.197767	-1.972346	-2.302191
C	1.519040	0.337700	-2.341919
C	2.517203	-2.198105	-2.708362
C	2.855075	0.185924	-2.730793
C	3.387212	-1.104675	-2.897131
H	0.509748	-2.800431	-2.077095
H	2.870014	-3.233795	-2.836500
H	1.064376	1.329287	-2.190837
H	3.485502	1.078063	-2.857462
C	4.877683	-1.327378	-3.114194
H	5.050923	-2.140930	-3.847185
H	5.360394	-0.410899	-3.501978
N	5.513150	-1.742890	-1.857032
H	5.410630	-2.745603	-1.625935
C	5.502647	-1.031436	-0.690008
C	5.361885	-1.940298	0.525020
C	5.598893	0.330619	-0.487529
C	5.303642	-1.354307	1.882919
C	5.436488	0.935011	0.847270
C	5.323726	0.005902	2.036736
Cl	5.930775	1.466381	-1.781400

O	5.378632	2.158597	1.011467
O	5.280276	-3.158598	0.326947
C	5.177924	0.652727	3.382321
H	5.951171	0.285382	4.090184
H	5.250112	1.752527	3.296620
H	4.191809	0.393879	3.826729
C	5.142920	-2.299714	3.041689
H	4.162347	-2.136468	3.540690
H	5.189868	-3.351140	2.702863
H	5.924108	-2.131494	3.812752
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IPrCl2Py6 SCF Done: -3468.52916550 A.U.			
Pd	0.968606	-0.033218	-0.492666
N	3.468733	-0.878916	0.930431
C	2.262617	-4.920909	1.192179
N	3.497181	1.254138	0.511225
C	1.750319	-3.978793	2.095679
C	2.137389	-2.625045	2.031603
Cl	-0.007814	1.013957	1.370606
C	3.055020	-2.262566	1.013073
C	3.592833	-3.188812	0.083663
C	3.175737	-4.530009	0.202631
C	4.614342	-2.781145	-0.976256
C	6.052616	-3.020135	-0.464467
C	4.401074	-3.498605	-2.321763
C	1.647250	-1.616280	3.065959
C	2.582204	-1.630260	4.295323
C	0.179111	-1.826183	3.470341
C	4.664519	-0.382842	1.450601
C	4.688437	0.958316	1.175302
C	3.143655	2.564786	0.012134
C	3.356339	2.830193	-1.365212
C	3.002608	4.110966	-1.834683
C	2.472491	5.077900	-0.968119
C	2.287761	4.786586	0.390762
C	2.615935	3.520331	0.916449
C	4.013908	1.806152	-2.285892
C	5.547391	1.991826	-2.269891
C	3.460852	1.829950	-3.719755
C	2.451335	3.225971	2.405830
C	3.690921	3.708894	3.191668
C	1.169132	3.835603	3.000657
C	2.737219	0.125232	0.353826
H	1.945763	-5.974012	1.260155

H	1.037454	-4.299048	2.870046
H	3.567844	-5.280049	-0.500470
H	4.476621	-1.695759	-1.165565
H	6.218807	-4.099016	-0.257375
H	6.264281	-2.465985	0.471683
H	6.796884	-2.698954	-1.223515
H	5.056215	-3.050374	-3.097202
H	3.351299	-3.396014	-2.658192
H	4.657607	-4.578015	-2.262134
H	1.696515	-0.606331	2.611993
H	3.631742	-1.406549	4.011399
H	2.571279	-2.624740	4.791133
H	2.261265	-0.870549	5.038995
H	-0.475061	-1.856721	2.576422
H	-0.160886	-0.979278	4.100045
H	0.031574	-2.758984	4.056030
H	5.374904	-1.030155	1.971221
H	5.436387	1.728027	1.382315
H	3.148499	4.354321	-2.897628
H	2.201277	6.072557	-1.356980
H	1.871708	5.555508	1.058778
H	3.788814	0.795450	-1.890340
H	5.829850	2.993860	-2.658631
H	6.039712	1.224872	-2.904415
H	5.960044	1.898991	-1.243834
H	2.356741	1.736922	-3.717685
H	3.864098	0.968771	-4.290061
H	3.743813	2.755051	-4.266915
H	2.364061	2.124466	2.514792
H	4.627400	3.242498	2.825732
H	3.590307	3.466256	4.270655
H	3.809262	4.809672	3.097723
H	1.227079	4.943239	3.066690
H	1.012820	3.455201	4.031297
H	0.285669	3.556252	2.394826
Cl	1.940759	-1.062488	-2.365615
N	-0.942927	-0.236482	-1.378944
C	-1.864620	0.749290	-1.277203
C	-1.276087	-1.375178	-2.032804
C	-3.145825	0.631380	-1.827847
C	-2.543996	-1.569277	-2.590606
C	-3.510032	-0.550688	-2.498172
H	-1.555500	1.639146	-0.707919
H	-3.861162	1.459773	-1.712637

H	-0.482891	-2.134491	-2.107061
H	-2.776101	-2.527354	-3.080575
C	-4.897086	-0.729253	-3.101837
H	-4.886491	-0.360347	-4.150162
H	-5.141020	-1.809311	-3.148790
N	-5.942152	0.004762	-2.406278
H	-6.205475	0.931850	-2.773499
C	-6.251935	-0.068690	-1.079457
C	-6.904784	1.214922	-0.591649
C	-6.039353	-1.081856	-0.167225
C	-7.354391	1.352248	0.815693
C	-6.441470	-0.951613	1.246100
C	-7.109711	0.334129	1.698781
Cl	-5.331262	-2.627444	-0.589364
O	-6.263456	-1.856121	2.066240
O	-7.032159	2.144188	-1.400114
C	-7.456612	0.346458	3.157872
H	-7.956610	1.277726	3.477767
H	-8.104177	-0.521349	3.402149
H	-6.537096	0.201783	3.763379
C	-8.018905	2.665893	1.129496
H	-7.314082	3.505856	0.953090
H	-8.870963	2.839077	0.439602
H	-8.384737	2.723470	2.169901

100

**IPrCl2Py6del2Isomer** SCF Done: -3468.53829571 A.U.

Pd	-0.677514	-0.736526	-0.340033
N	-2.362629	1.755259	-0.423913
C	0.737113	4.417458	-1.502290
N	-3.470653	0.070921	0.391033
C	0.271067	4.380921	-0.179517
C	-0.749927	3.491573	0.208581
Cl	0.546618	0.443378	1.283020
C	-1.278859	2.637189	-0.795553
C	-0.810555	2.627842	-2.130015
C	0.203559	3.549362	-2.463728
C	-1.381587	1.690522	-3.188058
C	-2.255679	2.468884	-4.192637
C	-0.272513	0.887088	-3.892664
C	-1.295257	3.512651	1.637254
C	-2.279743	4.690297	1.817682
C	-0.195556	3.569502	2.713569
C	-3.670404	2.196538	-0.212866
C	-4.363916	1.140090	0.312434

C	-3.761118	-1.185257	1.046701
C	-4.565915	-2.142923	0.383581
C	-4.839346	-3.341188	1.075611
C	-4.326053	-3.570399	2.358686
C	-3.533020	-2.599374	2.988821
C	-3.233548	-1.378655	2.352722
C	-5.162674	-1.892537	-0.998726
C	-6.629456	-1.422671	-0.877450
C	-5.064627	-3.122622	-1.920460
C	-2.436129	-0.289898	3.068933
C	-3.385141	0.706694	3.770247
C	-1.379656	-0.836043	4.040579
C	-2.236111	0.436149	-0.077605
H	1.534151	5.124618	-1.782245
H	0.710323	5.056502	0.570073
H	0.589028	3.573664	-3.494557
H	-2.029907	0.946526	-2.683910
H	-1.661075	3.228467	-4.744480
H	-3.083906	3.000084	-3.678383
H	-2.701133	1.777551	-4.938569
H	-0.720626	0.109907	-4.544055
H	0.365704	0.372834	-3.147127
H	0.378582	1.532818	-4.519647
H	-1.854547	2.568099	1.799794
H	-3.106574	4.662910	1.079987
H	-1.754610	5.661089	1.692112
H	-2.728097	4.672847	2.833288
H	0.515390	2.729800	2.598880
H	-0.653755	3.496547	3.722105
H	0.370930	4.524265	2.682022
H	-3.975666	3.217752	-0.454744
H	-5.400798	1.046267	0.645298
H	-5.459599	-4.111381	0.592783
H	-4.546314	-4.517779	2.876183
H	-3.142140	-2.792774	3.998670
H	-4.565591	-1.086415	-1.473237
H	-7.256390	-2.210307	-0.407262
H	-7.054447	-1.200909	-1.879037
H	-6.729156	-0.509239	-0.256259
H	-4.023925	-3.498187	-1.962004
H	-5.373871	-2.848792	-2.950592
H	-5.731562	-3.946176	-1.586611
H	-1.865963	0.275828	2.306192
H	-4.099325	1.164992	3.055402

H	-2.803721	1.529231	4.238172
H	-3.975237	0.203752	4.566131
H	-1.830632	-1.313624	4.936910
H	-0.734487	-0.005943	4.392636
H	-0.723898	-1.574250	3.536667
Cl	-1.856534	-1.787421	-2.072787
N	1.007203	-1.976191	-0.666762
C	1.816062	-2.310864	0.367292
C	1.420380	-2.244647	-1.927901
C	3.102745	-2.818039	0.168360
C	2.703178	-2.733121	-2.201812
C	3.597715	-2.967936	-1.142833
H	1.437355	-2.087727	1.374938
H	3.750446	-2.991818	1.041509
H	0.700136	-2.008959	-2.726554
H	3.030904	-2.825554	-3.247792
C	5.092213	-3.141827	-1.374070
H	5.415697	-4.170709	-1.108946
H	5.322831	-2.979591	-2.445567
N	5.870885	-2.218786	-0.527450
H	6.420642	-2.661947	0.215626
C	5.402767	-0.979235	-0.158247
C	4.604867	-0.181110	-1.165588
C	5.659819	-0.395593	1.063725
C	3.810150	0.976616	-0.687340
C	5.031001	0.867389	1.501937
C	4.045681	1.507786	0.553517
Cl	6.613588	-1.262852	2.256680
O	5.242860	1.348358	2.618630
O	4.616746	-0.524272	-2.352615
C	2.781071	1.542142	-1.620958
H	2.929268	2.628239	-1.790405
H	2.797333	1.023998	-2.597275
H	1.770434	1.434516	-1.167815
C	3.323693	2.728616	1.038333
H	3.554935	3.607041	0.396615
H	2.226668	2.569102	0.968203
H	3.601184	2.960921	2.082924
100			
<b>IPrCl2Py6del2Isomer180</b> SCF Done: -3468.52931718 A.U.			
Pd	-1.011019	-0.397902	-0.314021
N	-3.210362	1.640783	-0.279257
C	-0.666694	4.933665	-1.017289
N	-3.935072	-0.298820	0.386668

C	-1.194152	4.725701	0.265912
C	-2.033486	3.628944	0.539029
Cl	-0.105384	0.845102	1.457745
C	-2.332202	2.759221	-0.542933
C	-1.805394	2.930636	-1.843722
C	-0.966540	4.044130	-2.057535
C	-2.130313	1.975601	-2.986523
C	-3.122672	2.622243	-3.974773
C	-0.856246	1.478540	-3.694861
C	-2.609402	3.418752	1.939851
C	-3.842935	4.321328	2.165963
C	-1.575249	3.642050	3.059008
C	-4.588209	1.766098	-0.098004
C	-5.042602	0.549158	0.333332
C	-3.961741	-1.635616	0.936346
C	-4.542494	-2.683894	0.181840
C	-4.568246	-3.963835	0.774025
C	-4.031467	-4.184018	2.048921
C	-3.464555	-3.123033	2.771466
C	-3.421344	-1.819950	2.238609
C	-5.163177	-2.456832	-1.194285
C	-6.698473	-2.327013	-1.080557
C	-4.789934	-3.559685	-2.203035
C	-2.881189	-0.648121	3.056670
C	-4.031728	0.087161	3.778286
C	-1.767324	-1.042051	4.037900
C	-2.800756	0.362189	-0.006556
H	-0.005859	5.794982	-1.204701
H	-0.936056	5.422382	1.077945
H	-0.538404	4.211086	-3.058055
H	-2.618258	1.076153	-2.561642
H	-2.690712	3.532380	-4.444014
H	-4.061950	2.921653	-3.464051
H	-3.384505	1.911092	-4.786389
H	-1.106624	0.646893	-4.384240
H	-0.126098	1.096814	-2.952582
H	-0.364497	2.281425	-4.284544
H	-2.936589	2.360585	2.012863
H	-4.632616	4.153208	1.406843
H	-3.555611	5.393303	2.114805
H	-4.287377	4.133970	3.166293
H	-0.665862	3.037727	2.879398
H	-2.007839	3.340275	4.036118
H	-1.284577	4.710495	3.147801



H	-5.106883	2.708408	-0.291645
H	-6.041094	0.205307	0.614927
H	-5.009939	-4.804287	0.217531
H	-4.054782	-5.194636	2.487209
H	-3.052275	-3.309956	3.774001
H	-4.749269	-1.506050	-1.589846
H	-7.144954	-3.270060	-0.698370
H	-7.149190	-2.114134	-2.072878
H	-7.002488	-1.515899	-0.387927
H	-3.691856	-3.695558	-2.245025
H	-5.141749	-3.279688	-3.217729
H	-5.263751	-4.532163	-1.948947
H	-2.412429	0.071248	2.356524
H	-4.798349	0.449343	3.062826
H	-3.640688	0.970159	4.326962
H	-4.535567	-0.580494	4.509776
H	-2.144662	-1.651699	4.887220
H	-1.304565	-0.127176	4.459771
H	-0.967300	-1.608850	3.520551
Cl	-1.943032	-1.569115	-2.130022
N	0.902216	-1.230291	-0.722878
C	1.760492	-1.522186	0.282634
C	1.295854	-1.463336	-1.998295
C	3.032896	-2.056256	0.047965
C	2.558026	-1.979769	-2.307616
C	3.456861	-2.293544	-1.272006
H	1.408564	-1.284446	1.298045
H	3.694743	-2.268276	0.901332
H	0.554598	-1.233321	-2.778424
H	2.838430	-2.118005	-3.363150
C	4.833154	-2.870032	-1.576873
H	4.763545	-3.979095	-1.596710
H	5.148198	-2.554337	-2.591328
N	5.848460	-2.529113	-0.594270
H	6.046172	-3.209783	0.154720
C	6.237051	-1.282527	-0.200429
C	6.861712	-1.316780	1.188674
C	6.126865	-0.066889	-0.846910
C	7.388610	-0.073862	1.795635
C	6.612541	1.187061	-0.241281
C	7.248746	1.116179	1.132748
Cl	5.461080	0.109937	-2.458615
O	6.527898	2.272434	-0.822649
O	6.894640	-2.404257	1.779810

C	8.030124	-0.179611	3.153620
H	7.466712	0.413243	3.906306
H	8.065528	-1.231674	3.492364
H	9.063165	0.228614	3.138442
C	7.725376	2.413230	1.716855
H	7.220656	2.618340	2.686014
H	8.814834	2.372930	1.934957
H	7.525959	3.248750	1.020823
100			
<b>IPrCl2Py6del6Isomer</b> SCF Done: -3468.53369962 A.U.			
Pd	0.590358	-0.073654	-0.792274
N	3.218939	-0.798245	0.503946
C	1.950907	-4.639632	1.728963
N	3.117768	1.307591	-0.032265
C	1.593002	-3.508090	2.478819
C	2.013480	-2.219139	2.097511
Cl	-0.474468	1.013635	1.002918
C	2.796307	-2.119710	0.912917
C	3.189424	-3.241859	0.145251
C	2.747838	-4.507755	0.584812
C	4.101933	-3.117157	-1.071192
C	5.559646	-3.450548	-0.682523
C	3.641371	-3.989629	-2.253427
C	1.696975	-0.994104	2.955553
C	2.900474	-0.623463	3.850870
C	0.423112	-1.135835	3.800090
C	4.483857	-0.258104	0.745968
C	4.421926	1.065853	0.401304
C	2.564766	2.627003	-0.250562
C	2.380993	3.093921	-1.572281
C	1.836273	4.386096	-1.727255
C	1.490452	5.165106	-0.614885
C	1.677473	4.667296	0.683593
C	2.214109	3.383757	0.899244
C	2.773261	2.267562	-2.791748
C	4.043006	2.845258	-3.451205
C	1.612919	2.142234	-3.797195
C	2.441135	2.861901	2.317816
C	3.747326	3.440585	2.905290
C	1.256938	3.130316	3.264550
C	2.377285	0.156422	-0.000682
H	1.608156	-5.637306	2.046800
H	0.978016	-3.630600	3.382266
H	3.031005	-5.404343	0.012778

H	4.055378	-2.062271	-1.411893
H	5.645826	-4.504856	-0.342451
H	5.931240	-2.808422	0.142345
H	6.237973	-3.315507	-1.551212
H	4.250125	-3.761248	-3.152740
H	2.581272	-3.784758	-2.498965
H	3.761617	-5.073849	-2.042838
H	1.503963	-0.145766	2.267848
H	3.816242	-0.424117	3.259509
H	3.126728	-1.442212	4.566870
H	2.675797	0.293255	4.436004
H	-0.435621	-1.450170	3.178549
H	0.165444	-0.155458	4.249722
H	0.544982	-1.862637	4.632000
H	5.298409	-0.864820	1.150101
H	5.172823	1.859774	0.428657
H	1.681888	4.785108	-2.741788
H	1.065167	6.171055	-0.759817
H	1.391398	5.284024	1.549063
H	3.006551	1.237895	-2.453370
H	3.869239	3.876623	-3.826763
H	4.355330	2.217626	-4.312258
H	4.888253	2.888770	-2.732601
H	0.708688	1.736651	-3.299443
H	1.886087	1.437404	-4.608090
H	1.356598	3.118433	-4.261696
H	2.556157	1.760982	2.254888
H	4.625482	3.223867	2.264187
H	3.945890	3.014956	3.911593
H	3.674568	4.544339	3.008138
H	1.134629	4.212707	3.481617
H	1.430103	2.621558	4.236293
H	0.314606	2.742360	2.832428
Cl	1.647960	-1.173082	-2.577978
N	-1.276774	-0.294011	-1.751496
C	-2.199586	0.695547	-1.693831
C	-1.620097	-1.475136	-2.317338
C	-3.517749	0.504266	-2.118217
C	-2.924842	-1.741136	-2.747376
C	-3.919518	-0.758030	-2.601166
H	-1.871551	1.638518	-1.232143
H	-4.247544	1.316804	-1.980530
H	-0.817127	-2.225079	-2.382397
H	-3.178638	-2.750431	-3.103454

C	-5.399378	-1.089895	-2.736515
H	-5.832945	-0.589567	-3.628278
H	-5.521343	-2.183352	-2.870260
N	-6.164649	-0.619239	-1.568270
H	-6.838883	0.130856	-1.750188
C	-5.617837	-0.540968	-0.310624
C	-4.634791	-1.609528	0.114330
C	-5.950607	0.422196	0.616800
C	-3.729942	-1.326210	1.257302
C	-5.221669	0.591876	1.889423
C	-4.030840	-0.311089	2.126697
Cl	-7.144160	1.645009	0.212649
O	-5.514291	1.479644	2.694974
O	-4.588871	-2.670318	-0.516200
C	-3.186371	-0.006432	3.327288
H	-3.015239	-0.914806	3.943230
H	-2.185088	0.342308	2.990887
H	-3.656529	0.778579	3.947882
C	-2.516121	-2.201853	1.397264
H	-2.548589	-3.039068	0.675625
H	-1.605495	-1.592120	1.201884
H	-2.418864	-2.616801	2.422189

112

**IPrCl2Py6isomer+DMF** SCF Done: -3716.90028255 A.U.

Pd	-1.187099	-0.525247	-0.588777
N	-1.003023	1.841610	1.028218
C	2.714289	2.335283	-0.924194
N	-3.038485	1.112704	1.271673
C	2.620063	1.473643	0.175059
C	1.407549	1.316623	0.877366
Cl	-1.233565	-1.885667	1.327277
C	0.294101	2.060212	0.418054
C	0.361987	2.965832	-0.675788
C	1.599829	3.082479	-1.337187
C	-0.843563	3.805811	-1.092101
C	-0.895167	5.115104	-0.272260
C	-0.893270	4.119218	-2.596652
C	1.343030	0.411473	2.099597
C	1.961266	1.134225	3.317467
C	2.025897	-0.943883	1.856571
C	-1.575655	2.598433	2.047873
C	-2.859910	2.145598	2.198397
C	-4.306336	0.475338	1.004465
C	-5.025345	0.891026	-0.152011

C	-6.273211	0.278357	-0.379984
C	-6.775685	-0.696921	0.495139
C	-6.042320	-1.079764	1.624927
C	-4.786324	-0.502378	1.908712
C	-4.474231	1.961421	-1.095877
C	-4.650034	3.380189	-0.509154
C	-5.052105	1.903121	-2.518356
C	-4.020815	-0.893471	3.170150
C	-4.615478	-0.171897	4.399639
C	-3.981039	-2.416146	3.396488
C	-1.890742	0.900816	0.562253
H	3.667361	2.422012	-1.467876
H	3.496499	0.892259	0.490564
H	1.689024	3.758690	-2.199904
H	-1.750738	3.213030	-0.853856
H	-0.004817	5.743561	-0.487530
H	-0.915626	4.927196	0.819242
H	-1.801629	5.701868	-0.531552
H	-1.870156	4.580485	-2.851346
H	-0.783086	3.194323	-3.194558
H	-0.105291	4.843006	-2.896464
H	0.275970	0.202216	2.317641
H	1.465297	2.109014	3.510162
H	3.044357	1.326415	3.159707
H	1.861025	0.510218	4.230146
H	1.601820	-1.447691	0.968945
H	1.871689	-1.612079	2.726962
H	3.118116	-0.832839	1.715211
H	-1.017691	3.381133	2.568736
H	-3.668507	2.463819	2.861695
H	-6.860318	0.560768	-1.265640
H	-7.751715	-1.164746	0.289958
H	-6.445463	-1.848292	2.301626
H	-3.386923	1.766216	-1.209709
H	-5.726314	3.624342	-0.381327
H	-4.205749	4.133623	-1.193243
H	-4.152743	3.495094	0.474069
H	-4.962896	0.890720	-2.958329
H	-4.484099	2.595353	-3.172275
H	-6.119461	2.210857	-2.554295
H	-2.968709	-0.567453	3.035693
H	-4.614299	0.930733	4.277515
H	-4.034640	-0.413691	5.314409
H	-5.668228	-0.483647	4.570586

H	-4.986694	-2.834463	3.615234
H	-3.331753	-2.650461	4.265248
H	-3.558851	-2.934169	2.513701
Cl	-1.505611	0.681973	-2.586153
N	0.355209	-1.726325	-1.451370
C	0.678387	-2.974824	-1.038471
C	1.317252	-0.958999	-2.025028
C	1.989375	-3.463759	-1.123198
C	2.644352	-1.381315	-2.136908
C	3.012295	-2.650387	-1.646516
H	-0.136786	-3.571377	-0.607460
H	2.203280	-4.478244	-0.751311
H	0.997069	0.035335	-2.373975
H	3.388524	-0.709627	-2.586743
C	4.474480	-3.066713	-1.585482
H	4.558684	-4.171745	-1.559487
H	5.029971	-2.690100	-2.460990
N	5.118639	-2.567842	-0.358767
H	4.909369	-3.116219	0.485006
C	5.485836	-1.289095	-0.052087
C	5.808082	-0.289819	-1.144091
C	5.671762	-0.882469	1.264231
C	6.132126	1.116656	-0.769623
C	5.947410	0.500296	1.655903
C	6.185996	1.498179	0.543508
Cl	5.444115	-2.032722	2.568306
O	5.959556	0.866624	2.837498
O	5.803032	-0.637281	-2.330617
O	-1.755960	-4.452050	-1.959840
N	-3.448742	-2.881195	-1.816118
C	-4.109556	-1.739328	-2.417818
H	-5.164958	-1.976674	-2.683829
H	-4.112522	-0.887470	-1.709238
H	-3.559077	-1.416322	-3.322122
C	-3.955309	-3.348227	-0.536370
H	-3.307981	-4.172653	-0.184893
H	-3.927719	-2.523114	0.204994
H	-5.004907	-3.705404	-0.633111
C	-2.367578	-3.477651	-2.402275
H	-2.080986	-2.960335	-3.360353
C	6.409439	2.069948	-1.902754
H	6.091540	1.637237	-2.869510
H	5.902362	3.044505	-1.750083
H	7.498465	2.286462	-1.973184

C	6.461868	2.911672	0.963033
H	7.393664	3.298414	0.499483
H	5.635087	3.576542	0.627411
H	6.538574	2.979342	2.064026
112			
<b>IPrCl2Py6isomer--DMF SCF Done: -3716.88510177 A.U.</b>			
Pd	-1.729913	-0.922452	-0.344559
N	-0.693733	1.608135	0.813211
C	2.972613	1.929788	-1.269609
N	-2.780135	1.284337	1.344295
C	2.929285	1.266352	-0.039013
C	1.714820	1.093005	0.657418
Cl	-1.014668	-1.911003	1.657355
C	0.549866	1.638120	0.072270
C	0.554764	2.307817	-1.183559
C	1.794127	2.432615	-1.841608
C	-0.713833	2.901563	-1.789508
C	-0.943218	4.348021	-1.301423
C	-0.748815	2.825773	-3.324308
C	1.706249	0.345636	1.983715
C	2.463713	1.137922	3.070010
C	2.289441	-1.068502	1.810283
C	-1.038059	2.604018	1.730510
C	-2.349858	2.401181	2.063349
C	-4.164851	0.873678	1.262674
C	-4.978239	1.488328	0.273082
C	-6.331737	1.099206	0.219333
C	-6.847562	0.145061	1.109134
C	-6.019299	-0.436580	2.078420
C	-4.657576	-0.082840	2.181817
C	-4.441660	2.569242	-0.661882
C	-4.703679	3.970674	-0.067293
C	-4.996431	2.469283	-2.092915
C	-3.782314	-0.655306	3.288808
C	-4.040931	0.105845	4.607114
C	-3.957073	-2.172823	3.464745
C	-1.753752	0.764477	0.592851
H	3.929911	2.039626	-1.800206
H	3.850518	0.860562	0.399590
H	1.837233	2.936858	-2.818073
H	-1.562728	2.278937	-1.442985
H	-0.112682	5.012339	-1.623213
H	-1.019991	4.405305	-0.197205
H	-1.888447	4.751115	-1.722856

H	-1.756631	3.114809	-3.686717
H	-0.559788	1.791432	-3.673841
H	-0.015820	3.512417	-3.799739
H	0.651461	0.219241	2.302884
H	2.050641	2.161391	3.194203
H	3.543943	1.233343	2.826802
H	2.392166	0.617704	4.047854
H	1.724945	-1.632964	1.045687
H	2.222825	-1.630978	2.763535
H	3.356651	-1.033102	1.517003
H	-0.311913	3.356451	2.050952
H	-3.020519	2.939451	2.738609
H	-6.991638	1.550770	-0.536460
H	-7.908061	-0.147043	1.045615
H	-6.434434	-1.179872	2.775988
H	-3.345119	2.429258	-0.738615
H	-5.794327	4.156952	0.033645
H	-4.279439	4.758495	-0.724617
H	-4.246934	4.086529	0.936076
H	-4.844637	1.450148	-2.498800
H	-4.455758	3.178676	-2.753444
H	-6.075090	2.731135	-2.143775
H	-2.724312	-0.499192	2.997098
H	-3.854157	1.194197	4.492265
H	-3.375507	-0.270764	5.412160
H	-5.092828	-0.019518	4.943557
H	-4.972274	-2.443578	3.826810
H	-3.225639	-2.551169	4.207623
H	-3.755267	-2.700428	2.511597
Cl	-2.541094	0.003165	-2.350798
N	0.328829	-1.958631	-1.494673
C	0.790146	-3.124978	-1.004769
C	1.206141	-1.112284	-2.062433
C	2.147815	-3.479986	-1.048941
C	2.581954	-1.380495	-2.154404
C	3.075416	-2.590822	-1.628131
H	0.029409	-3.776955	-0.544699
H	2.477856	-4.442666	-0.624560
H	0.782354	-0.168914	-2.447337
H	3.262578	-0.653487	-2.620140
C	4.566237	-2.897129	-1.614386
H	4.723319	-3.995512	-1.605380
H	5.063478	-2.477263	-2.504047
N	5.224605	-2.375136	-0.408024



H	5.053525	-2.921127	0.445751
C	5.688650	-1.125439	-0.130347
C	5.931207	-0.114707	-1.234271
C	6.001194	-0.745984	1.172721
C	6.436920	1.241507	-0.873644
C	6.425423	0.598064	1.553612
C	6.649098	1.589149	0.432897
Cl	5.802621	-1.897826	2.482006
O	6.588211	0.941884	2.731912
O	5.707762	-0.405115	-2.415112
O	-2.315668	-3.094282	-1.099299
N	-4.425119	-2.748444	-1.976633
C	-5.210409	-2.611682	-3.192210
H	-6.228933	-3.032984	-3.053329
H	-5.299043	-1.538715	-3.472595
H	-4.712862	-3.147190	-4.025237
C	-4.946207	-2.110866	-0.773669
H	-4.369712	-2.451059	0.105504
H	-4.846252	-1.007022	-0.844009
H	-6.015252	-2.374673	-0.645051
C	-3.140308	-3.174370	-2.027033
H	-2.870905	-3.644461	-3.009081
C	6.683307	2.202681	-2.007085
H	6.388411	1.755036	-2.974243
H	6.120193	3.148908	-1.860694
H	7.757994	2.481743	-2.061337
C	7.110454	2.959363	0.832616
H	8.082262	3.208470	0.354113
H	6.385810	3.731384	0.493221
H	7.217035	3.023816	1.931411

112

**IPrCl2Py6isomer--DMFisomer** SCF Done: -3716.86727586 A.U.

Pd	1.760248	0.533580	-0.284656
N	2.837546	-2.206350	0.064035
C	-0.543182	-4.208778	-1.503366
N	4.188086	-0.714739	0.900469
C	-0.585628	-3.667529	-0.210359
C	0.517017	-2.975524	0.327916
Cl	1.245432	1.055245	1.940499
C	1.672427	-2.860380	-0.490887
C	1.744961	-3.389008	-1.804562
C	0.606059	-4.064269	-2.291805
C	3.005980	-3.285990	-2.659378
C	3.834502	-4.586966	-2.567178

C	2.703286	-2.952110	-4.132503
C	0.477222	-2.408242	1.742713
C	1.103656	-3.397695	2.748892
C	-0.926395	-1.966460	2.184022
C	3.951234	-2.894040	0.551392
C	4.804757	-1.955843	1.064867
C	4.736690	0.533067	1.380845
C	5.339796	1.411091	0.446757
C	5.879256	2.612442	0.948163
C	5.819910	2.916126	2.316213
C	5.211486	2.026750	3.212946
C	4.645522	0.815450	2.767342
C	5.456910	1.048403	-1.029828
C	6.792289	0.321564	-1.296462
C	5.270882	2.254978	-1.965057
C	3.992480	-0.150385	3.755280
C	5.055759	-1.042549	4.434631
C	3.142720	0.565152	4.821766
C	2.977409	-0.854563	0.269827
H	-1.419807	-4.743262	-1.903551
H	-1.500148	-3.771186	0.391107
H	0.624690	-4.484926	-3.308466
H	3.607094	-2.445747	-2.254109
H	3.257740	-5.448321	-2.967301
H	4.117375	-4.833913	-1.524330
H	4.769590	-4.498137	-3.159492
H	3.647714	-2.728047	-4.670563
H	2.047401	-2.063368	-4.208986
H	2.221665	-3.802716	-4.660670
H	1.091442	-1.486568	1.755426
H	2.150381	-3.647548	2.478038
H	0.526163	-4.346284	2.792260
H	1.117142	-2.954114	3.766740
H	-1.391421	-1.305782	1.425536
H	-0.851900	-1.387130	3.126163
H	-1.606314	-2.826526	2.368286
H	4.022670	-3.983078	0.493297
H	5.790338	-2.048285	1.527947
H	6.358840	3.319248	0.254194
H	6.249604	3.860114	2.688194
H	5.161199	2.283748	4.281665
H	4.637424	0.345579	-1.277642
H	7.658385	0.977416	-1.062295
H	6.866570	0.016784	-2.361752

H	6.883157	-0.592623	-0.673342
H	4.359636	2.824708	-1.694704
H	5.150221	1.904620	-3.010211
H	6.137034	2.951208	-1.938685
H	3.301255	-0.797566	3.174830
H	5.657450	-1.617143	3.702650
H	4.575000	-1.769632	5.122572
H	5.760152	-0.423027	5.030049
H	3.771957	1.123715	5.547340
H	2.561455	-0.180661	5.403099
H	2.430284	1.266783	4.347414
Cl	2.302307	0.084846	-2.537601
N	-0.676140	0.424720	-0.823468
C	-1.565060	1.082281	-0.055224
C	-1.095833	-0.640732	-1.527843
C	-2.910140	0.696639	0.045359
C	-2.422830	-1.099654	-1.489050
C	-3.359395	-0.427566	-0.681930
H	-1.157838	1.929195	0.522260
H	-3.596815	1.260484	0.696688
H	-0.326544	-1.148095	-2.136688
H	-2.712273	-1.985589	-2.075593
C	-4.783080	-0.930523	-0.554969
H	-5.011459	-1.668404	-1.355881
H	-4.896781	-1.489235	0.397566
N	-5.723263	0.185540	-0.579624
H	-5.368670	1.062557	-0.979987
C	-7.013345	0.259780	-0.155056
C	-7.727241	-0.989326	0.313113
C	-7.722060	1.454729	-0.178674
C	-9.121282	-0.870044	0.825218
C	-9.103254	1.588541	0.277073
C	-9.776710	0.331902	0.791094
Cl	-6.925005	2.914619	-0.743568
O	-9.714780	2.664168	0.265063
O	-7.155565	-2.083691	0.255341
O	1.174062	2.807482	-0.785601
N	2.134858	4.588218	-1.877126
C	2.781001	5.090354	-3.077601
H	2.227723	5.959589	-3.497068
H	3.823394	5.413552	-2.860051
H	2.816974	4.290845	-3.843745
C	2.016205	5.487069	-0.737025
H	1.562691	4.928538	0.103449

H	3.019615	5.856057	-0.431962
H	1.379506	6.363257	-0.988440
C	1.713607	3.296328	-1.790500
H	1.918330	2.681162	-2.703090
C	-9.769889	-2.128597	1.338886
H	-9.069932	-2.982844	1.280697
H	-10.098382	-2.004937	2.393165
H	-10.679967	-2.378701	0.751757
C	-11.193429	0.482523	1.263294
H	-11.284612	0.208947	2.337245
H	-11.534763	1.525644	1.127306
H	-11.872459	-0.200844	0.708683
79			
<b>IPrCl2PEPPSI</b> SCF Done: -2915.31856266 A.U.			
Pd	0.541378	-0.673426	-0.017381
N	-0.851361	1.853478	0.754193
C	2.689836	4.159071	0.796602
N	-2.294509	0.308166	0.244517
C	2.427855	3.273719	1.850590
C	1.258878	2.484358	1.866013
Cl	-0.091217	-1.771375	1.964465
C	0.367461	2.631659	0.778151
C	0.610362	3.503622	-0.316367
C	1.790530	4.270335	-0.274642
C	-0.365809	3.637902	-1.485109
C	-1.305363	4.847541	-1.282888
C	0.338217	3.734009	-2.851371
C	0.974272	1.544993	3.033041
C	0.551965	2.348855	4.280673
C	2.164416	0.613009	3.327038
C	-2.114610	2.374722	1.035165
C	-3.023949	1.406493	0.703351
C	-2.884025	-0.864678	-0.361752
C	-2.849643	-0.956355	-1.780559
C	-3.438886	-2.096093	-2.362101
C	-4.043094	-3.084647	-1.570263
C	-4.073213	-2.953843	-0.175827
C	-3.489470	-1.841266	0.465489
C	-2.266356	0.160606	-2.644237
C	-3.313594	1.273143	-2.871531
C	-1.675616	-0.328717	-3.974730
C	-3.565333	-1.693811	1.982665
C	-4.949407	-1.152590	2.404500
C	-3.249369	-3.007046	2.722647

C	-0.950921	0.569003	0.289710
H	3.609557	4.765630	0.804909
H	3.143718	3.190772	2.683139
H	2.016597	4.957483	-1.103908
H	-0.985900	2.717655	-1.508107
H	-0.723375	5.793469	-1.257691
H	-1.876927	4.783041	-0.335857
H	-2.036318	4.916972	-2.115955
H	-0.412614	3.665711	-3.666338
H	1.063979	2.908173	-2.978429
H	0.868225	4.702198	-2.977429
H	0.127436	0.886750	2.753786
H	-0.340795	2.975622	4.073255
H	1.366092	3.025589	4.618698
H	0.305370	1.665412	5.120311
H	2.460231	0.059696	2.412798
H	1.877815	-0.138794	4.089695
H	3.047429	1.169852	3.707518
H	-2.240029	3.381157	1.442581
H	-4.116317	1.394195	0.738179
H	-3.429166	-2.209546	-3.456053
H	-4.498160	-3.966813	-2.048490
H	-4.553243	-3.734700	0.433481
H	-1.416377	0.608348	-2.092203
H	-4.189292	0.886399	-3.435584
H	-2.868855	2.108521	-3.452889
H	-3.682942	1.692067	-1.913118
H	-0.950799	-1.150415	-3.808668
H	-1.126604	0.501886	-4.462882
H	-2.457746	-0.675829	-4.684158
H	-2.786587	-0.962180	2.282080
H	-5.186541	-0.182790	1.921460
H	-4.994708	-1.004635	3.504127
H	-5.753228	-1.865974	2.122457
H	-4.044760	-3.769057	2.577170
H	-3.172087	-2.818228	3.813475
H	-2.283339	-3.424487	2.378483
Cl	1.195161	0.435426	-1.973796
N	2.177672	-2.003434	-0.227493
C	2.038148	-3.322393	0.045951
C	3.380564	-1.522473	-0.611097
C	3.111823	-4.215759	-0.066987
C	4.499410	-2.364999	-0.723359
C	4.372835	-3.738129	-0.454019

H	1.041281	-3.639657	0.386443
H	2.957129	-5.282166	0.154324
H	3.432740	-0.451255	-0.858154
H	5.242937	-4.404740	-0.547154
Cl	6.033271	-1.684441	-1.200244
91			
<b>IPrCl2PEPPSI+DMF</b> SCF Done: -3163.67876690 A.U.			
Pd	-0.492231	0.009181	0.322439
N	1.923857	-1.714869	0.278260
C	-0.307680	-5.278185	-0.160562
N	2.509469	0.378329	0.169689
C	-0.256659	-4.641877	1.086917
C	0.473576	-3.448453	1.266749
Cl	-0.039812	0.793664	2.495534
C	1.151199	-2.929583	0.139017
C	1.109837	-3.540680	-1.142799
C	0.368306	-4.731546	-1.261928
C	1.854974	-2.959857	-2.344651
C	3.237561	-3.628140	-2.513065
C	1.059168	-3.059641	-3.659332
C	0.541164	-2.781786	2.636239
C	1.456570	-3.585804	3.582869
C	-0.858537	-2.562626	3.239650
C	3.316146	-1.683818	0.354195
C	3.684962	-0.368455	0.273482
C	2.505679	1.800808	-0.100852
C	2.245613	2.217007	-1.432973
C	2.333806	3.595316	-1.701457
C	2.660975	4.512014	-0.692865
C	2.900204	4.068819	0.614300
C	2.826420	2.699811	0.944119
C	1.909883	1.216738	-2.536210
C	3.191645	0.611983	-3.149305
C	0.984874	1.789751	-3.620463
C	3.131606	2.231207	2.364634
C	4.653743	2.225785	2.624624
C	2.401712	3.073592	3.428068
C	1.415497	-0.444647	0.190357
H	-0.886142	-6.208401	-0.279280
H	-0.794527	-5.076056	1.944003
H	0.308841	-5.232797	-2.239676
H	2.012399	-1.879851	-2.144410
H	3.122132	-4.711527	-2.730841
H	3.864151	-3.535194	-1.604378

H	3.793040	-3.165847	-3.356215
H	1.570134	-2.474788	-4.452680
H	0.036982	-2.654232	-3.534843
H	0.988788	-4.107268	-4.022785
H	0.985625	-1.773981	2.512758
H	2.477888	-3.693230	3.160754
H	1.057298	-4.607934	3.758971
H	1.542712	-3.078681	4.566944
H	-1.500963	-2.000561	2.531880
H	-0.781903	-1.958609	4.166154
H	-1.360002	-3.521192	3.493594
H	3.904282	-2.599149	0.457366
H	4.667050	0.111214	0.264490
H	2.129645	3.958491	-2.719118
H	2.723113	5.586924	-0.927685
H	3.150275	4.798206	1.400112
H	1.336605	0.389415	-2.074188
H	3.808329	1.397109	-3.637491
H	2.930561	-0.147887	-3.916249
H	3.819724	0.112571	-2.383115
H	0.106548	2.276153	-3.152723
H	0.620783	0.966220	-4.267964
H	1.501850	2.527097	-4.272607
H	2.747445	1.194764	2.461998
H	5.199981	1.588099	1.899724
H	4.877433	1.848314	3.644922
H	5.071639	3.252033	2.541186
H	2.795881	4.111184	3.478846
H	2.537797	2.619970	4.432020
H	1.316060	3.111435	3.213771
Cl	-0.933883	-0.833120	-1.834871
N	-2.568176	0.359095	0.628069
C	-3.000636	1.418942	1.350347
C	-3.466239	-0.515919	0.124107
C	-4.363278	1.646330	1.586018
C	-4.845170	-0.347628	0.333229
C	-5.314208	0.752402	1.071001
H	-2.213092	2.066747	1.762961
H	-4.673854	2.522486	2.174256
H	-3.064781	-1.341755	-0.483962
H	-6.392947	0.892399	1.235199
Cl	-5.957478	-1.508539	-0.345618
O	-0.633474	2.891155	-0.854848
N	-2.889095	3.247384	-1.228467

C	-4.051025	4.071158	-0.963239
H	-4.428925	4.554210	-1.892686
H	-4.877827	3.461962	-0.532242
H	-3.790538	4.868109	-0.237014
C	-3.041285	2.140790	-2.162814
H	-2.136137	1.503131	-2.134427
H	-3.918402	1.522048	-1.877290
H	-3.199122	2.512382	-3.200165
C	-1.669511	3.518125	-0.659498
H	-1.723219	4.399454	0.042654

91

**IPrCl<sub>2</sub>PEPPSI--DMF** SCF Done: -3163.66768661 A.U.

Pd	0.122935	0.732836	0.216490
N	-0.628888	-1.905595	-0.866171
C	-4.684046	-1.131352	0.050886
N	1.538910	-1.679051	-0.793528
C	-3.802797	-1.548772	1.058039
C	-2.454698	-1.838640	0.771016
Cl	0.894167	0.132940	2.358744
C	-2.029037	-1.677289	-0.575826
C	-2.899598	-1.276188	-1.619146
C	-4.239412	-1.007138	-1.271175
C	-2.442002	-1.197224	-3.072594
C	-2.765170	-2.520291	-3.803291
C	-3.047140	-0.003844	-3.833650
C	-1.512918	-2.362815	1.852032
C	-1.420179	-3.903428	1.788102
C	-1.873303	-1.888969	3.267720
C	-0.081844	-3.054509	-1.439607
C	1.280536	-2.908831	-1.402918
C	2.842391	-1.179544	-0.417510
C	3.455527	-0.193063	-1.227479
C	4.709687	0.295022	-0.807428
C	5.315550	-0.177349	0.365151
C	4.679027	-1.151445	1.148251
C	3.423819	-1.675046	0.779090
C	2.836739	0.278567	-2.538687
C	3.495658	-0.462651	-3.721946
C	2.897511	1.805732	-2.711004
C	2.752348	-2.760625	1.618904
C	3.247494	-4.160420	1.189854
C	2.949865	-2.571246	3.133500
C	0.365961	-1.042860	-0.480528
H	-5.726537	-0.881115	0.300802



H	-4.167191	-1.644487	2.090781
H	-4.941122	-0.669392	-2.047566
H	-1.342101	-1.050299	-3.062540
H	-3.862598	-2.691435	-3.833552
H	-2.310090	-3.399617	-3.303483
H	-2.393723	-2.492350	-4.849472
H	-2.571721	0.088777	-4.832066
H	-2.873324	0.941789	-3.284674
H	-4.138460	-0.127062	-4.001399
H	-0.504196	-1.952810	1.647445
H	-1.085544	-4.255301	0.790861
H	-2.406519	-4.369441	1.999687
H	-0.692851	-4.278948	2.538918
H	-1.999354	-0.788765	3.296290
H	-1.053509	-2.148358	3.967609
H	-2.802817	-2.365274	3.648120
H	-0.711437	-3.864908	-1.815735
H	2.087017	-3.555862	-1.757662
H	5.219162	1.056905	-1.416878
H	6.297120	0.217767	0.673414
H	5.161342	-1.508060	2.070425
H	1.760083	0.016225	-2.527725
H	4.580970	-0.231557	-3.786058
H	3.023650	-0.163938	-4.681507
H	3.393333	-1.563355	-3.616987
H	2.382239	2.308872	-1.870597
H	2.371142	2.100817	-3.641084
H	3.941164	2.182121	-2.780887
H	1.660894	-2.697730	1.424924
H	3.072521	-4.357467	0.113943
H	2.728381	-4.952970	1.768899
H	4.338529	-4.260024	1.374008
H	3.998397	-2.768581	3.444136
H	2.307577	-3.286567	3.688033
H	2.669440	-1.545718	3.440676
Cl	-0.480140	1.403416	-1.953789
N	-1.851920	1.852553	1.169993
C	-2.038402	1.894926	2.504016
C	-2.914593	1.952118	0.352562
C	-3.311618	2.028575	3.081205
C	-4.219614	2.092059	0.856712
C	-4.435027	2.125477	2.243685
H	-1.125991	1.785864	3.114448
H	-3.423475	2.051645	4.176235

H	-2.711190	1.901118	-0.730772
H	-5.454184	2.222365	2.646688
Cl	-5.567915	2.209194	-0.257014
O	1.175889	2.925715	0.550769
N	3.371898	3.607368	0.448687
C	4.746531	3.384330	0.856627
H	5.407502	3.268154	-0.030776
H	5.128856	4.234382	1.465289
H	4.809849	2.454510	1.454969
C	3.090836	4.748515	-0.409617
H	2.011151	4.746333	-0.650782
H	3.355507	5.702130	0.098128
H	3.676412	4.675004	-1.351818
C	2.371725	2.770763	0.845643
H	2.720828	1.903873	1.463229
87			
<b>IPrCl2PEPPSI+K3PO4</b> SCF Done: -5357.64394850 A.U.			
Pd	-0.473144	-0.417974	-0.279047
N	-2.613212	1.542083	0.289030
C	-5.438181	-1.586789	0.598654
N	-0.721676	2.602728	0.122859
C	-4.930168	-1.228407	-0.658317
C	-4.006499	-0.172201	-0.795493
Cl	0.048097	0.333888	-2.470187
C	-3.601564	0.491542	0.389115
C	-4.102151	0.159635	1.674525
C	-5.038310	-0.890371	1.747896
C	-3.676916	0.914648	2.933075
C	-4.704189	2.017015	3.277995
C	-3.462076	-0.000896	4.152875
C	-3.543917	0.281810	-2.177089
C	-4.608897	1.210537	-2.800299
C	-3.192346	-0.888466	-3.110319
C	-2.907625	2.899826	0.391983
C	-1.718171	3.567329	0.300436
C	0.674260	2.964968	0.003404
C	1.570327	2.640520	1.063262
C	2.907773	3.069019	0.918095
C	3.316383	3.825260	-0.192251
C	2.406841	4.138267	-1.213724
C	1.066992	3.693606	-1.152129
C	1.120881	1.863707	2.302214
C	0.093469	2.644024	3.153708
C	2.294563	1.413372	3.186391

C	0.108186	4.023174	-2.299034
C	-0.278434	5.518562	-2.284114
C	0.682556	3.633034	-3.675907
C	-1.263392	1.343174	0.108111
H	-6.157364	-2.417155	0.683064
H	-5.263084	-1.771950	-1.555627
H	-5.445013	-1.181964	2.727892
H	-2.700650	1.397019	2.716248
H	-5.691882	1.566722	3.514469
H	-4.859172	2.728877	2.442799
H	-4.373139	2.599479	4.163633
H	-3.017140	0.581600	4.986628
H	-2.776869	-0.833586	3.903554
H	-4.417869	-0.425419	4.527444
H	-2.613823	0.871761	-2.057892
H	-4.812374	2.085822	-2.148010
H	-5.569473	0.672380	-2.950042
H	-4.268591	1.589030	-3.787356
H	-2.435994	-1.548481	-2.641106
H	-2.750988	-0.502495	-4.050957
H	-4.081725	-1.497830	-3.378351
H	-3.932346	3.256548	0.520559
H	-1.475971	4.631107	0.359218
H	3.657493	2.771413	1.660681
H	4.365810	4.152523	-0.267338
H	2.741098	4.726427	-2.083250
H	0.635365	0.941744	1.919496
H	0.541245	3.577134	3.559004
H	-0.230759	2.019947	4.012833
H	-0.820051	2.924676	2.594199
H	3.066164	0.879375	2.595030
H	1.916523	0.738166	3.984868
H	2.772984	2.273115	3.704904
H	-0.810952	3.417849	-2.157741
H	-0.718844	5.828815	-1.314747
H	-1.017470	5.743097	-3.081831
H	0.613440	6.157900	-2.457890
H	1.594105	4.215692	-3.928269
H	-0.065229	3.831801	-4.471914
H	0.922187	2.552153	-3.705394
Cl	-1.135396	-1.253168	1.851855
N	0.019556	-2.394250	-0.833395
C	1.245812	-2.812215	-1.223923
C	-1.027547	-3.251712	-0.833451

C	1.456148	-4.140441	-1.631435
C	-0.873599	-4.584576	-1.242777
C	0.389233	-5.049444	-1.652759
H	2.105274	-2.112030	-1.155088
H	2.474849	-4.439367	-1.919886
H	-1.998290	-2.864827	-0.486476
H	0.518024	-6.095013	-1.970808
Cl	-2.263397	-5.647178	-1.225040
O	2.203303	-0.523387	0.592382
P	3.740542	-0.919144	0.518878
O	4.107095	-1.965566	1.671101
K	3.087713	0.701783	-1.778732
O	4.044779	-1.584449	-0.911684
O	4.673446	0.363728	0.635993
K	1.744901	-2.130478	2.502608
K	6.442150	-1.582878	0.585581

**Table S4.** Basic details about X-ray experiments for PEPPSI-BQ complexes

	PEPPSI-o-BQ ( <b>7a</b> )	PEPPSI-m-BQ ( <b>7b</b> )	PEPPSI-p-BQ ( <b>7c</b> )
Crystal data			
Chemical formula	C <sub>43</sub> H <sub>47</sub> Cl <sub>3</sub> N <sub>4</sub> O <sub>2</sub> Pd ·0.5(CH <sub>2</sub> Cl <sub>2</sub> )	2(C <sub>41</sub> H <sub>49</sub> Cl <sub>3</sub> N <sub>4</sub> O <sub>2</sub> Pd) ·CH <sub>2</sub> Cl <sub>2</sub>	C <sub>41</sub> H <sub>49</sub> Cl <sub>3</sub> N <sub>4</sub> O <sub>2</sub> Pd ·CH <sub>2</sub> Cl <sub>2</sub>
<i>M<sub>r</sub></i>	907.06	1768.09	927.51
Crystal system, space group	Tetragonal, <i>I</i> <sub>4</sub> /a	Monoclinic, <i>Pc</i>	Monoclinic, <i>P</i> <sub>2</sub> <sub>1</sub> / <i>n</i>
Temperature (K)	100	100	100
<i>a</i> (Å)	40.0508 (7)	15.6908 (11)	13.4813 (2)
<i>b</i> (Å)		13.6342 (5)	18.6879 (3)
<i>c</i> (Å)	13.6975 (3)	20.8321 (7)	17.6589 (3)
β (°)		101.582 (5)	97.6005 (13)
<i>V</i> (Å <sup>3</sup> )	21971.8 (9)	4365.9 (4)	4409.85 (12)
<i>Z</i>	16	2	4
Radiation type	Mo <i>K</i> α	Mo <i>K</i> β	Ag <i>K</i> α, λ = 0.56087 Å
μ (mm <sup>-1</sup> )	0.56	0.71	0.40
Crystal size (mm)	0.21 × 0.12 × 0.06	-	0.31 × 0.21 × 0.16
Data collection			
Diffractometer	SuperNova, Single source at offset, Eos	SuperNova, Single source at offset/far, Eos	SuperNova, Single source at offset, Eos
Absorption correction	Analytical	Multi-scan	Multi-scan
<i>T<sub>min</sub></i> , <i>T<sub>max</sub></i>	0.923, 0.969	0.488, 1.000	0.871, 1.000
No. of measured, independent and observed [ <i>I</i> > 2σ( <i>I</i> )] reflections	96168, 13117, 9525	136524, 21733, 17616	98345, 11703, 10282
<i>R<sub>int</sub></i>	0.095	0.121	0.055
(sin θ/λ) <sub>max</sub> (Å <sup>-1</sup> )	0.670	0.689	0.701
Refinement			
<i>R</i> [ <i>F</i> <sup>2</sup> > 2σ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.087, 0.233, 1.14	0.115, 0.260, 1.04	0.070, 0.161, 1.20
No. of reflections	13117	21733	11703
No. of parameters	513	501	586
No. of restraints	336	2	430
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained
Δ <sub>max</sub> , Δ <sub>min</sub> (e Å <sup>-3</sup> )	1.08, -1.04	2.79, -2.47	0.85, -1.54
Absolute structure parameter		0.306 (16)	

**Table S5.** Basic details about X-ray experiments for PEPPSI-NQ complexes

	PEPPSI-o-NQ ( <b>7d</b> )	PEPPSI-m-NQ ( <b>7e</b> )		PEPPSI-p-NQ ( <b>7f</b> )
Crystal data				
Chemical formula	C <sub>43</sub> H <sub>47</sub> Cl <sub>3</sub> N <sub>4</sub> O <sub>2</sub> Pd·0.5(CH <sub>2</sub> Cl <sub>2</sub> )	C <sub>43</sub> H <sub>47</sub> Cl <sub>3</sub> N <sub>4</sub> O <sub>2</sub> Pd		C <sub>43</sub> H <sub>47</sub> Cl <sub>3</sub> N <sub>4</sub> O <sub>2</sub> Pd·CH <sub>2</sub> Cl <sub>2</sub>
<i>M<sub>r</sub></i>	907.06	864.59		949.52
Crystal system, space group	Tetragonal, <i>I</i> 4 <sub>1</sub> / <i>a</i>	Tetragonal, <i>I</i> 4 <sub>1</sub> / <i>a</i>		Monoclinic, <i>P</i> 2 <sub>1</sub> / <i>c</i>
Temperature (K)	100	100		100
<i>a</i> (Å)	40.0508 (7)	40.3260 (6)		10.79029 (16)
<i>b</i> (Å)				27.3220 (3)
<i>c</i> (Å)	13.6975 (3)	13.4661 (2)		16.1751 (2)
$\beta$ (°)				93.8745 (13)
<i>V</i> (Å <sup>3</sup> )	21971.8 (9)	21898.4 (7)		4757.73 (11)
<i>Z</i>	16	16		4
Radiation type	Mo <i>K</i> $\alpha$	Cu <i>K</i> $\alpha$		Mo <i>K</i> $\alpha$
$\mu$ (mm <sup>-1</sup> )	0.56	4.32		0.71
Crystal size (mm)	0.21 × 0.12 × 0.06	0.13 × 0.06 × 0.06		0.25 × 0.12 × 0.08
Data collection				
Diffractometer	SuperNova, Single source at offset, Eos	SuperNova, Dual, Cu at home/near, Atlas		SuperNova, Single source at offset/far, Eos
Absorption correction	Analytical	Gaussian		Gaussian
<i>T<sub>min</sub></i> , <i>T<sub>max</sub></i>	0.923, 0.969	0.705, 0.862		0.679, 1.000
No. of measured, independent and observed [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )] reflections	96168, 13117, 9525	81391, 10808, 8351		199136, 21617, 19112
<i>R<sub>int</sub></i>	0.095	0.079		0.058
( <i>sin</i> $\theta$ / $\lambda$ ) <sub>max</sub> (Å <sup>-1</sup> )	0.670	0.621		0.823
Refinement				
<i>R</i> [ <i>F</i> <sup>2</sup> > 2 $\sigma$ ( <i>F</i> <sup>2</sup> )], <i>wR</i> [ <i>F</i> <sup>2</sup> ], <i>S</i>	0.087, 0.233, 1.14	0.067, 0.179, 1.03		0.040, 0.077, 1.09
No. of reflections	13117	10808		21617
No. of parameters	513	476		517
No. of restraints	336	73		1
H-atom treatment	H-atom parameters constrained	mixture treatment		mixture treatment
$\Delta$ <sub>max</sub> , $\Delta$ <sub>min</sub> (e Å <sup>-3</sup> )	1.08, -1.04	0.82, -0.92		1.11, -1.05

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