Supplementary Material (ESI) for New Journal of Chemistry

SUPPORTING INFORMATION

Table S1: Atomic cartesian coordinates of the optimized compounds

$[Pc]^{2-}$ D_{4h}

Bonding energy -14.90219777 a.u.
-405.50959927 eV

Atom	X	Y	Z (Angstrom)
1.N	1.977544	0.000000	0.000000
2.N	0.000000	1.977544	0.000000
3.N	-1.977544	0.000000	0.000000
4.N	0.000000	-1.977544	0.000000
5.C	2.767694	1.100698	0.000000
6.C	2.767694	-1.100698	0.000000
7.C	4.194119	0.708347	0.000000
8.C	4.194119	-0.708347	0.000000
9.C	5.394936	1.420292	0.000000
10.C	5.394936	-1.420292	0.000000
11.C	6.600508	0.704242	0.000000
12.C	6.600508	-0.704242	0.000000
13.H	5.382442	2.512290	0.000000
14.H	5.382442	-2.512290	0.000000
15.H	7.553852	1.241739	0.000000
16.H	7.553852	-1.241739	0.000000
17.C	-1.100698	2.767694	0.000000
18.C	1.100698	2.767694	0.000000
19.C	-0.708347	4.194119	0.000000
20.C	0.708347	4.194119	0.000000
21.C	-1.420292	5.394936	0.000000
22.C	1.420292	5.394936	0.000000
23.C	-0.704242	6.600508	0.000000
24.C	0.704242	6.600508	0.000000
25.H	-2.512290	5.382442	0.000000
26.H	2.512290	5.382442	0.000000
27.H	-1.241739	7.553852	0.000000
28.H	1.241739	7.553852	0.000000
29.C	-2.767694	-1.100698	0.000000
30.C	-2.767694	1.100698	0.000000
31.C	-4.194119	-0.708347	0.000000
32.C	-4.194119	0.708347	0.000000
33.C	-5.394936	-1.420292	0.000000
34.C	-5.394936	1.420292	0.000000
35.C	-6.600508	-0.704242	0.000000
36.C	-6.600508	0.704242	0.000000
37.H	-5.382442	-2.512290	0.000000
38.H	-5.382442	2.512290	0.000000
39.H	-7.553852	-1.241739	0.000000
40.H	-7.553852	1.241739	0.000000
41.C	1.100698	-2.767694	0.000000
42.C	-1.100698	-2.767694	0.000000
43.C	0.708347	-4.194119	0.000000
44.C	-0.708347	-4.194119	0.000000
45.C	1.420292	-5.394936	0.000000
46.C	-1.420292	-5.394936	0.000000
47.C	0.704242	-6.600508	0.000000
48.C	-0.704242	-6.600508	0.000000

49.H	2.512290	-5.382442	0.000000
50.H	-2.512290	-5.382442	0.000000
51.H	1.241739	-7.553852	0.000000
52.H	-1.241739	-7.553852	0.000000
53.N	2.394087	2.394087	0.000000
54.N	-2.394087	2.394087	0.000000
55.N	-2.394087	-2.394087	0.000000
56.N	2.394087	-2.394087	0.000000

$[(np\text{-}Cl_8)Pc]^{2-}$ D_{4h}

Bonding energy -14.45464413 a.u.
-393.33104013 eV

Atom	X	Y	Z (Angstrom)
1.N	1.395730	1.395730	0.000000
2.N	-1.395730	1.395730	0.000000
3.N	-1.395730	-1.395730	0.000000
4.N	1.395730	-1.395730	0.000000
5.C	1.174772	2.731504	0.000000
6.C	2.731504	1.174772	0.000000
7.C	2.459883	3.459219	0.000000
8.C	3.459219	2.459883	0.000000
9.C	2.798136	4.810165	0.000000
10.C	4.810165	2.798136	0.000000
11.C	4.153270	5.149555	0.000000
12.C	5.149555	4.153270	0.000000
13.H	2.032312	5.584670	0.000000
14.H	5.584670	2.032312	0.000000
15.CL	4.592989	6.869150	0.000000
16.CL	6.869150	4.592989	0.000000
17.C	-2.731504	1.174772	0.000000
18.C	-1.174772	2.731504	0.000000
19.C	-3.459219	2.459883	0.000000
20.C	-2.459883	3.459219	0.000000
21.C	-4.810165	2.798136	0.000000
22.C	-2.798136	4.810165	0.000000
23.C	-5.149555	4.153270	0.000000
24.C	-4.153270	5.149555	0.000000
25.H	-5.584670	2.032312	0.000000
26.H	-2.032312	5.584670	0.000000
27.CL	-6.869150	4.592989	0.000000
28.CL	-4.592989	6.869150	0.000000
29.C	-1.174772	-2.731504	0.000000
30.C	-2.731504	-1.174772	0.000000
31.C	-2.459883	-3.459219	0.000000
32.C	-3.459219	-2.459883	0.000000
33.C	-2.798136	-4.810165	0.000000
34.C	-4.810165	-2.798136	0.000000
35.C	-4.153270	-5.149555	0.000000
36.C	-5.149555	-4.153270	0.000000
37.H	-2.032312	-5.584670	0.000000
38.H	-5.584670	-2.032312	0.000000
39.CL	-4.592989	-6.869150	0.000000
40.CL	-6.869150	-4.592989	0.000000
41.C	2.731504	-1.174772	0.000000
42.C	1.174772	-2.731504	0.000000
43.C	3.459219	-2.459883	0.000000
44.C	2.459883	-3.459219	0.000000
45.C	4.810165	-2.798136	0.000000

46.C	2.798136	-4.810165	0.000000
47.C	5.149555	-4.153270	0.000000
48.C	4.153270	-5.149555	0.000000
49.H	5.584670	-2.032312	0.000000
50.H	2.032312	-5.584670	0.000000
51.CL	6.869150	-4.592989	0.000000
52.CL	4.592989	-6.869150	0.000000
53.N	0.000000	3.383220	0.000000
54.N	-3.383220	0.000000	0.000000
55.N	0.000000	-3.383220	0.000000
56.N	3.383220	0.000000	0.000000

$[(p\text{-}Cl_8)Pc]^{2-}$ D_{4h}

Bonding energy -14.40841632 a.u.
-392.07311689 eV

Atom	X	Y	Z (Angstrom)
1.N	1.409163	1.409163	0.000000
2.N	-1.409163	1.409163	0.000000
3.N	-1.409163	-1.409163	0.000000
4.N	1.409163	-1.409163	0.000000
5.C	1.180802	2.741684	0.000000
6.C	2.741684	1.180802	0.000000
7.C	2.472301	3.482615	0.000000
8.C	3.482615	2.472301	0.000000
9.C	2.855291	4.825388	0.000000
10.C	4.825388	2.855291	0.000000
11.C	4.203015	5.189199	0.000000
12.C	5.189199	4.203015	0.000000
13.CL	1.688838	6.154334	0.000000
14.CL	6.154334	1.688838	0.000000
15.H	4.474132	6.245036	0.000000
16.H	6.245036	4.474132	0.000000
17.C	-2.741684	1.180802	0.000000
18.C	-1.180802	2.741684	0.000000
19.C	-3.482615	2.472301	0.000000
20.C	-2.472301	3.482615	0.000000
21.C	-4.825388	2.855291	0.000000
22.C	-2.855291	4.825388	0.000000
23.C	-5.189199	4.203015	0.000000
24.C	-4.203015	5.189199	0.000000
25.CL	-6.154334	1.688838	0.000000
26.CL	-1.688838	6.154334	0.000000
27.H	-6.245036	4.474132	0.000000
28.H	-4.474132	6.245036	0.000000
29.C	-1.180802	-2.741684	0.000000
30.C	-2.741684	-1.180802	0.000000
31.C	-2.472301	-3.482615	0.000000
32.C	-3.482615	-2.472301	0.000000
33.C	-2.855291	-4.825388	0.000000
34.C	-4.825388	-2.855291	0.000000
35.C	-4.203015	-5.189199	0.000000
36.C	-5.189199	-4.203015	0.000000
37.CL	-1.688838	-6.154334	0.000000
38.CL	-6.154334	-1.688838	0.000000
39.H	-4.474132	-6.245036	0.000000
40.H	-6.245036	-4.474132	0.000000
41.C	2.741684	-1.180802	0.000000

42.C	1.180802	-2.741684	0.000000
43.C	3.482615	-2.472301	0.000000
44.C	2.472301	-3.482615	0.000000
45.C	4.825388	-2.855291	0.000000
46.C	2.855291	-4.825388	0.000000
47.C	5.189199	-4.203015	0.000000
48.C	4.203015	-5.189199	0.000000
49.CL	6.154334	-1.688838	0.000000
50.CL	1.688838	-6.154334	0.000000
51.H	6.245036	-4.474132	0.000000
52.H	4.474132	-6.245036	0.000000
53.N	0.000000	3.380489	0.000000
54.N	-3.380489	0.000000	0.000000
55.N	0.000000	-3.380489	0.000000
56.N	3.380489	0.000000	0.000000

$[Cl_{16}Pc]^{2-}$ D_{4h}

Bonding energy -13.89475519 a.u.
-378.09568060 eV

Atom	X	Y	Z (Angstrom)
1.N	1.410369	1.410369	0.000000
2.N	-1.410369	1.410369	0.000000
3.N	-1.410369	-1.410369	0.000000
4.N	1.410369	-1.410369	0.000000
5.C	1.180173	2.741193	0.000000
6.C	2.741193	1.180173	0.000000
7.C	2.476378	3.479502	0.000000
8.C	3.479502	2.476378	0.000000
9.C	2.837313	4.829337	0.000000
10.C	4.829337	2.837313	0.000000
11.C	4.195832	5.191036	0.000000
12.C	5.191036	4.195832	0.000000
13.CL	1.631036	6.086375	0.000000
14.CL	6.086375	1.631036	0.000000
15.CL	4.666311	6.881456	0.000000
16.CL	6.881456	4.666311	0.000000
17.C	-2.741193	1.180173	0.000000
18.C	-1.180173	2.741193	0.000000
19.C	-3.479502	2.476378	0.000000
20.C	-2.476378	3.479502	0.000000
21.C	-4.829337	2.837313	0.000000
22.C	-2.837313	4.829337	0.000000
23.C	-5.191036	4.195832	0.000000
24.C	-4.195832	5.191036	0.000000
25.CL	-6.086375	1.631036	0.000000
26.CL	-1.631036	6.086375	0.000000
27.CL	-6.881456	4.666311	0.000000
28.CL	-4.666311	6.881456	0.000000
29.C	-1.180173	-2.741193	0.000000
30.C	-2.741193	-1.180173	0.000000
31.C	-2.476378	-3.479502	0.000000
32.C	-3.479502	-2.476378	0.000000
33.C	-2.837313	-4.829337	0.000000
34.C	-4.829337	-2.837313	0.000000
35.C	-4.195832	-5.191036	0.000000
36.C	-5.191036	-4.195832	0.000000

37.CL	-1.631036	-6.086375	0.000000
38.CL	-6.086375	-1.631036	0.000000
39.CL	-4.666311	-6.881456	0.000000
40.CL	-6.881456	-4.666311	0.000000
41.C	2.741193	-1.180173	0.000000
42.C	1.180173	-2.741193	0.000000
43.C	3.479502	-2.476378	0.000000
44.C	2.476378	-3.479502	0.000000
45.C	4.829337	-2.837313	0.000000
46.C	2.837313	-4.829337	0.000000
47.C	5.191036	-4.195832	0.000000
48.C	4.195832	-5.191036	0.000000
49.CL	6.086375	-1.631036	0.000000
50.CL	1.631036	-6.086375	0.000000
51.CL	6.881456	-4.666311	0.000000
52.CL	4.666311	-6.881456	0.000000
53.N	0.000000	3.376646	0.000000
54.N	-3.376646	0.000000	0.000000
55.N	0.000000	-3.376646	0.000000
56.N	3.376646	0.000000	0.000000

$[LuPc_2]^+$ C_{4v}

Bonding energy -29.89732876 a.u.
-813.54804127 eV

Atom	X	Y	Z (Angstrom)
1.N	1.393593	1.393593	1.385292
2.N	-1.393593	1.393593	1.385292
3.N	-1.393593	-1.393593	1.385292
4.N	1.393593	-1.393593	1.385292
5.C	1.171620	2.738347	1.566823
6.C	2.738347	1.171620	1.566823
7.C	2.446327	3.438296	1.765806
8.C	3.438296	2.446327	1.765806
9.C	2.767810	4.788777	1.901094
10.C	4.788777	2.767810	1.901094
11.C	4.127944	5.122622	2.011330
12.C	5.122622	4.127944	2.011330
13.H	1.989347	5.555096	1.907493
14.H	5.555096	1.989347	1.907493
15.H	4.419965	6.171372	2.098015
16.H	6.171372	4.419965	2.098015
17.C	-2.738347	1.171620	1.566823
18.C	-1.171620	2.738347	1.566823
19.C	-3.438296	2.446327	1.765806
20.C	-2.446327	3.438296	1.765806
21.C	-4.788777	2.767810	1.901094
22.C	-2.767810	4.788777	1.901094
23.C	-5.122622	4.127944	2.011330
24.C	-4.127944	5.122622	2.011330
25.H	-5.555096	1.989347	1.907493
26.H	-1.989347	5.555096	1.907493
27.H	-6.171372	4.419965	2.098015
28.H	-4.419965	6.171372	2.098015
29.C	-1.171620	-2.738347	1.566823
30.C	-2.738347	-1.171620	1.566823
31.C	-2.446327	-3.438296	1.765806
32.C	-3.438296	-2.446327	1.765806

33.C	-2.767810	-4.788777	1.901094
34.C	-4.788777	-2.767810	1.901094
35.C	-4.127944	-5.122622	2.011330
36.C	-5.122622	-4.127944	2.011330
37.H	-1.989347	-5.555096	1.907493
38.H	-5.555096	-1.989347	1.907493
39.H	-4.419965	-6.171372	2.098015
40.H	-6.171372	-4.419965	2.098015
41.C	2.738347	-1.171620	1.566823
42.C	1.171620	-2.738347	1.566823
43.C	3.438296	-2.446327	1.765806
44.C	2.446327	-3.438296	1.765806
45.C	4.788777	-2.767810	1.901094
46.C	2.767810	-4.788777	1.901094
47.C	5.122622	-4.127944	2.011330
48.C	4.127944	-5.122622	2.011330
49.H	5.555096	-1.989347	1.907493
50.H	1.989347	-5.555096	1.907493
51.H	6.171372	-4.419965	2.098015
52.H	4.419965	-6.171372	2.098015
53.N	0.000000	3.373268	1.617785
54.N	-3.373268	0.000000	1.617785
55.N	0.000000	-3.373268	1.617785
56.N	3.373268	0.000000	1.617785
57.LU	0.000000	0.000000	0.025306
58.N	1.974545	0.000000	-1.345016
59.N	0.000000	1.974545	-1.345016
60.N	-1.974545	0.000000	-1.345016
61.N	0.000000	-1.974545	-1.345016
62.C	2.767854	1.111040	-1.528895
63.C	2.767854	-1.111040	-1.528895
64.C	4.168055	0.703612	-1.737070
65.C	4.168055	-0.703612	-1.737070
66.C	5.348852	1.430195	-1.885478
67.C	5.348852	-1.430195	-1.885478
68.C	6.545403	0.703234	-2.004449
69.C	6.545403	-0.703234	-2.004449
70.H	5.340079	2.522422	-1.894076
71.H	5.340079	-2.522422	-1.894076
72.H	7.492813	1.238183	-2.098372
73.H	7.492813	-1.238183	-2.098372
74.C	-1.111040	2.767854	-1.528895
75.C	1.111040	2.767854	-1.528895
76.C	-0.703612	4.168055	-1.737070
77.C	0.703612	4.168055	-1.737070
78.C	-1.430195	5.348852	-1.885478
79.C	1.430195	5.348852	-1.885478
80.C	-0.703234	6.545403	-2.004449
81.C	0.703234	6.545403	-2.004449
82.H	-2.522422	5.340079	-1.894076
83.H	2.522422	5.340079	-1.894076
84.H	-1.238183	7.492813	-2.098372
85.H	1.238183	7.492813	-2.098372
86.C	-2.767854	-1.111040	-1.528895
87.C	-2.767854	1.111040	-1.528895
88.C	-4.168055	-0.703612	-1.737070
89.C	-4.168055	0.703612	-1.737070
90.C	-5.348852	-1.430195	-1.885478
91.C	-5.348852	1.430195	-1.885478

92.C	-6.545403	-0.703234	-2.004449
93.C	-6.545403	0.703234	-2.004449
94.H	-5.340079	-2.522422	-1.894076
95.H	-5.340079	2.522422	-1.894076
96.H	-7.492813	-1.238183	-2.098372
97.H	-7.492813	1.238183	-2.098372
98.C	1.111040	-2.767854	-1.528895
99.C	-1.111040	-2.767854	-1.528895
100.C	0.703612	-4.168055	-1.737070
101.C	-0.703612	-4.168055	-1.737070
102.C	1.430195	-5.348852	-1.885478
103.C	-1.430195	-5.348852	-1.885478
104.C	0.703234	-6.545403	-2.004449
105.C	-0.703234	-6.545403	-2.004449
106.H	2.522422	-5.340079	-1.894076
107.H	-2.522422	-5.340079	-1.894076
108.H	1.238183	-7.492813	-2.098372
109.H	-1.238183	-7.492813	-2.098372
110.N	2.389572	2.389572	-1.579427
111.N	-2.389572	2.389572	-1.579427
112.N	-2.389572	-2.389572	-1.579427
113.N	2.389572	-2.389572	-1.579427

[$LuPc_2$] C_{4v}

Bonding energy -30.10834543 a.u.
-819.29009936 eV

1.N	1.975181	0.000000	1.410492
2.N	0.000000	1.975181	1.410492
3.N	-1.975181	0.000000	1.410492
4.N	0.000000	-1.975181	1.410492
5.C	2.767145	1.109505	1.587919
6.C	2.767145	-1.109505	1.587919
7.C	4.164817	0.702681	1.769287
8.C	4.164817	-0.702681	1.769287
9.C	5.353710	1.427692	1.870799
10.C	5.353710	-1.427692	1.870799
11.C	6.552113	0.704306	1.946038
12.C	6.552113	-0.704306	1.946038
13.H	5.344262	2.520101	1.866926
14.H	5.344262	-2.520101	1.866926
15.H	7.503327	1.239144	1.998228
16.H	7.503327	-1.239144	1.998228
17.C	-1.109505	2.767145	1.587919
18.C	1.109505	2.767145	1.587919
19.C	-0.702681	4.164817	1.769287
20.C	0.702681	4.164817	1.769287
21.C	-1.427692	5.353710	1.870799
22.C	1.427692	5.353710	1.870799
23.C	-0.704306	6.552113	1.946038
24.C	0.704306	6.552113	1.946038
25.H	-2.520101	5.344262	1.866926
26.H	2.520101	5.344262	1.866926
27.H	-1.239144	7.503327	1.998228
28.H	1.239144	7.503327	1.998228
29.C	-2.767145	-1.109505	1.587919
30.C	-2.767145	1.109505	1.587919
31.C	-4.164817	-0.702681	1.769287

32.C	-4.164817	0.702681	1.769287
33.C	-5.353710	-1.427692	1.870799
34.C	-5.353710	1.427692	1.870799
35.C	-6.552113	-0.704306	1.946038
36.C	-6.552113	0.704306	1.946038
37.H	-5.344262	-2.520101	1.866926
38.H	-5.344262	2.520101	1.866926
39.H	-7.503327	-1.239144	1.998228
40.H	-7.503327	1.239144	1.998228
41.C	1.109505	-2.767145	1.587919
42.C	-1.109505	-2.767145	1.587919
43.C	0.702681	-4.164817	1.769287
44.C	-0.702681	-4.164817	1.769287
45.C	1.427692	-5.353710	1.870799
46.C	-1.427692	-5.353710	1.870799
47.C	0.704306	-6.552113	1.946038
48.C	-0.704306	-6.552113	1.946038
49.H	2.520101	-5.344262	1.866926
50.H	-2.520101	-5.344262	1.866926
51.H	1.239144	-7.503327	1.998228
52.H	-1.239144	-7.503327	1.998228
53.N	2.386855	2.386855	1.637944
54.N	-2.386855	2.386855	1.637944
55.N	-2.386855	-2.386855	1.637944
56.N	2.386855	-2.386855	1.637944
57.LU	0.000000	0.000000	0.019654
58.N	1.398600	-1.398600	-1.371041
59.N	1.398600	1.398600	-1.371041
60.N	-1.398600	1.398600	-1.371041
61.N	-1.398600	-1.398600	-1.371041
62.C	2.744784	-1.171994	-1.550414
63.C	1.171994	-2.744784	-1.550414
64.C	3.446199	-2.450197	-1.738682
65.C	2.450197	-3.446199	-1.738682
66.C	4.798513	-2.777950	-1.850856
67.C	2.777950	-4.798513	-1.850856
68.C	5.132830	-4.136715	-1.934194
69.C	4.136715	-5.132830	-1.934194
70.H	5.563821	-1.998491	-1.848758
71.H	1.998491	-5.563821	-1.848758
72.H	6.183149	-4.430911	-1.993351
73.H	4.430911	-6.183149	-1.993351
74.C	1.171994	2.744784	-1.550414
75.C	2.744784	1.171994	-1.550414
76.C	2.450197	3.446199	-1.738682
77.C	3.446199	2.450197	-1.738682
78.C	2.777950	4.798513	-1.850856
79.C	4.798513	2.777950	-1.850856
80.C	4.136715	5.132830	-1.934194
81.C	5.132830	4.136715	-1.934194
82.H	1.998491	5.563821	-1.848758
83.H	5.563821	1.998491	-1.848758
84.H	4.430911	6.183149	-1.993351
85.H	6.183149	4.430911	-1.993351
86.C	-2.744784	1.171994	-1.550414
87.C	-1.171994	2.744784	-1.550414
88.C	-3.446199	2.450197	-1.738682
89.C	-2.450197	3.446199	-1.738682
90.C	-4.798513	2.777950	-1.850856

91.C	-2.777950	4.798513	-1.850856
92.C	-5.132830	4.136715	-1.934194
93.C	-4.136715	5.132830	-1.934194
94.H	-5.563821	1.998491	-1.848758
95.H	-1.998491	5.563821	-1.848758
96.H	-6.183149	4.430911	-1.993351
97.H	-4.430911	6.183149	-1.993351
98.C	-1.171994	-2.744784	-1.550414
99.C	-2.744784	-1.171994	-1.550414
100.C	-2.450197	-3.446199	-1.738682
101.C	-3.446199	-2.450197	-1.738682
102.C	-2.777950	-4.798513	-1.850856
103.C	-4.798513	-2.777950	-1.850856
104.C	-4.136715	-5.132830	-1.934194
105.C	-5.132830	-4.136715	-1.934194
106.H	-1.998491	-5.563821	-1.848758
107.H	-5.563821	-1.998491	-1.848758
108.H	-4.430911	-6.183149	-1.993351
109.H	-6.183149	-4.430911	-1.993351
110.N	3.379982	0.000000	-1.600947
111.N	0.000000	3.379982	-1.600947
112.N	-3.379982	0.000000	-1.600947
113.N	0.000000	-3.379982	-1.600947

$[LuPc_2]^-$ C_{4v}

Bonding energy -30.23258640 a.u.
-822.67086952 eV

Atom	X	Y	Z (Angstrom)
1.N	1.398598	1.398598	1.406244
2.N	-1.398598	1.398598	1.406244
3.N	-1.398598	-1.398598	1.406244
4.N	1.398598	-1.398598	1.406244
5.C	1.171620	2.740318	1.602319
6.C	2.740318	1.171620	1.602319
7.C	2.441543	3.435783	1.802211
8.C	3.435783	2.441543	1.802211
9.C	2.771319	4.791027	1.921043
10.C	4.791027	2.771319	1.921043
11.C	4.126966	5.126705	2.019502
12.C	5.126705	4.126966	2.019502
13.H	1.990324	5.555414	1.908858
14.H	5.555414	1.990324	1.908858
15.H	4.420579	6.177742	2.085729
16.H	6.177742	4.420579	2.085729
17.C	-2.740318	1.171620	1.602319
18.C	-1.171620	2.740318	1.602319
19.C	-3.435783	2.441543	1.802211
20.C	-2.441543	3.435783	1.802211
21.C	-4.791027	2.771319	1.921043
22.C	-2.771319	4.791027	1.921043
23.C	-5.126705	4.126966	2.019502
24.C	-4.126966	5.126705	2.019502
25.H	-5.555414	1.990324	1.908858
26.H	-1.990324	5.555414	1.908858
27.H	-6.177742	4.420579	2.085729
28.H	-4.420579	6.177742	2.085729
29.C	-1.171620	-2.740318	1.602319
30.C	-2.740318	-1.171620	1.602319

31.C	-2.441543	-3.435783	1.802211
32.C	-3.435783	-2.441543	1.802211
33.C	-2.771319	-4.791027	1.921043
34.C	-4.791027	-2.771319	1.921043
35.C	-4.126966	-5.126705	2.019502
36.C	-5.126705	-4.126966	2.019502
37.H	-1.990324	-5.555414	1.908858
38.H	-5.555414	-1.990324	1.908858
39.H	-4.420579	-6.177742	2.085729
40.H	-6.177742	-4.420579	2.085729
41.C	2.740318	-1.171620	1.602319
42.C	1.171620	-2.740318	1.602319
43.C	3.435783	-2.441543	1.802211
44.C	2.441543	-3.435783	1.802211
45.C	4.791027	-2.771319	1.921043
46.C	2.771319	-4.791027	1.921043
47.C	5.126705	-4.126966	2.019502
48.C	4.126966	-5.126705	2.019502
49.H	5.555414	-1.990324	1.908858
50.H	1.990324	-5.555414	1.908858
51.H	6.177742	-4.420579	2.085729
52.H	4.420579	-6.177742	2.085729
53.N	0.000000	3.374771	1.657601
54.N	-3.374771	0.000000	1.657601
55.N	0.000000	-3.374771	1.657601
56.N	3.374771	0.000000	1.657601
57.LU	0.000000	0.000000	0.019558
58.N	1.983714	0.000000	-1.364016
59.N	0.000000	1.983714	-1.364016
60.N	-1.983714	0.000000	-1.364016
61.N	0.000000	-1.983714	-1.364016
62.C	2.771131	1.113347	-1.562093
63.C	2.771131	-1.113347	-1.562093
64.C	4.165613	0.705600	-1.768750
65.C	4.165613	-0.705600	-1.768750
66.C	5.355942	1.429114	-1.902866
67.C	5.355942	-1.429114	-1.902866
68.C	6.550552	0.706709	-2.013773
69.C	6.550552	-0.706709	-2.013773
70.H	5.345001	2.521834	-1.893166
71.H	5.345001	-2.521834	-1.893166
72.H	7.500574	1.242094	-2.091569
73.H	7.500574	-1.242094	-2.091569
74.C	-1.113347	2.771131	-1.562093
75.C	1.113347	2.771131	-1.562093
76.C	-0.705600	4.165613	-1.768750
77.C	0.705600	4.165613	-1.768750
78.C	-1.429114	5.355942	-1.902866
79.C	1.429114	5.355942	-1.902866
80.C	-0.706709	6.550552	-2.013773
81.C	0.706709	6.550552	-2.013773
82.H	-2.521834	5.345001	-1.893166
83.H	2.521834	5.345001	-1.893166
84.H	-1.242094	7.500574	-2.091569
85.H	1.242094	7.500574	-2.091569
86.C	-2.771131	-1.113347	-1.562093
87.C	-2.771131	1.113347	-1.562093
88.C	-4.165613	-0.705600	-1.768750
89.C	-4.165613	0.705600	-1.768750

90.C	-5.355942	-1.429114	-1.902866
91.C	-5.355942	1.429114	-1.902866
92.C	-6.550552	-0.706709	-2.013773
93.C	-6.550552	0.706709	-2.013773
94.H	-5.345001	-2.521834	-1.893166
95.H	-5.345001	2.521834	-1.893166
96.H	-7.500574	-1.242094	-2.091569
97.H	-7.500574	1.242094	-2.091569
98.C	1.113347	-2.771131	-1.562093
99.C	-1.113347	-2.771131	-1.562093
100.C	0.705600	-4.165613	-1.768750
101.C	-0.705600	-4.165613	-1.768750
102.C	1.429114	-5.355942	-1.902866
103.C	-1.429114	-5.355942	-1.902866
104.C	0.706709	-6.550552	-2.013773
105.C	-0.706709	-6.550552	-2.013773
106.H	2.521834	-5.345001	-1.893166
107.H	-2.521834	-5.345001	-1.893166
108.H	1.242094	-7.500574	-2.091569
109.H	-1.242094	-7.500574	-2.091569
110.N	2.390947	2.390947	-1.617372
111.N	-2.390947	2.390947	-1.617372
112.N	-2.390947	-2.390947	-1.617372
113.N	2.390947	-2.390947	-1.617372

$PcLu[Pc(p\text{-}Cl_8)]^+$ C_{4v}

Bonding energy -29.37773770 a.u.
-799.40924322 eV

Atom	X	Y	Z (Angstrom)
1.N	1.391921	1.391921	1.285888
2.N	-1.391921	1.391921	1.285888
3.N	-1.391921	-1.391921	1.285888
4.N	1.391921	-1.391921	1.285888
5.C	1.169713	2.736587	1.463947
6.C	2.736587	1.169713	1.463947
7.C	2.443961	3.434140	1.652429
8.C	3.434140	2.443961	1.652429
9.C	2.765428	4.784546	1.758096
10.C	4.784546	2.765428	1.758096
11.C	4.125321	5.128878	1.832867
12.C	5.128878	4.125321	1.832867
13.H	1.999083	5.561602	1.760945
14.H	5.561602	1.999083	1.760945
15.CL	4.556787	6.813819	1.906927
16.CL	6.813819	4.556787	1.906927
17.C	-2.736587	1.169713	1.463947
18.C	-1.169713	2.736587	1.463947
19.C	-3.434140	2.443961	1.652429
20.C	-2.443961	3.434140	1.652429
21.C	-4.784546	2.765428	1.758096
22.C	-2.765428	4.784546	1.758096
23.C	-5.128878	4.125321	1.832867
24.C	-4.125321	5.128878	1.832867
25.H	-5.561602	1.999083	1.760945
26.H	-1.999083	5.561602	1.760945
27.CL	-6.813819	4.556787	1.906927
28.CL	-4.556787	6.813819	1.906927
29.C	-1.169713	-2.736587	1.463947

30.C	-2.736587	-1.169713	1.463947
31.C	-2.443961	-3.434140	1.652429
32.C	-3.434140	-2.443961	1.652429
33.C	-2.765428	-4.784546	1.758096
34.C	-4.784546	-2.765428	1.758096
35.C	-4.125321	-5.128878	1.832867
36.C	-5.128878	-4.125321	1.832867
37.H	-1.999083	-5.561602	1.760945
38.H	-5.561602	-1.999083	1.760945
39.CL	-4.556787	-6.813819	1.906927
40.CL	-6.813819	-4.556787	1.906927
41.C	2.736587	-1.169713	1.463947
42.C	1.169713	-2.736587	1.463947
43.C	3.434140	-2.443961	1.652429
44.C	2.443961	-3.434140	1.652429
45.C	4.784546	-2.765428	1.758096
46.C	2.765428	-4.784546	1.758096
47.C	5.128878	-4.125321	1.832867
48.C	4.125321	-5.128878	1.832867
49.H	5.561602	-1.999083	1.760945
50.H	1.999083	-5.561602	1.760945
51.CL	6.813819	-4.556787	1.906927
52.CL	4.556787	-6.813819	1.906927
53.N	0.000000	3.373470	1.515075
54.N	-3.373470	0.000000	1.515075
55.N	0.000000	-3.373470	1.515075
56.N	3.373470	0.000000	1.515075
57.LU	0.000000	0.000000	-0.082301
58.N	1.974356	0.000000	-1.429574
59.N	0.000000	1.974356	-1.429574
60.N	-1.974356	0.000000	-1.429574
61.N	0.000000	-1.974356	-1.429574
62.C	2.768516	1.111377	-1.616728
63.C	2.768516	-1.111377	-1.616728
64.C	4.168803	0.703484	-1.825440
65.C	4.168803	-0.703484	-1.825440
66.C	5.350686	1.430385	-1.970321
67.C	5.350686	-1.430385	-1.970321
68.C	6.548440	0.703174	-2.084387
69.C	6.548440	-0.703174	-2.084387
70.H	5.343435	2.522542	-1.979211
71.H	5.343435	-2.522542	-1.979211
72.H	7.496057	1.238337	-2.173385
73.H	7.496057	-1.238337	-2.173385
74.C	-1.111377	2.768516	-1.616728
75.C	1.111377	2.768516	-1.616728
76.C	-0.703484	4.168803	-1.825440
77.C	0.703484	4.168803	-1.825440
78.C	-1.430385	5.350686	-1.970321
79.C	1.430385	5.350686	-1.970321
80.C	-0.703174	6.548440	-2.084387
81.C	0.703174	6.548440	-2.084387
82.H	-2.522542	5.343435	-1.979211
83.H	2.522542	5.343435	-1.979211
84.H	-1.238337	7.496057	-2.173385
85.H	1.238337	7.496057	-2.173385
86.C	-2.768516	-1.111377	-1.616728
87.C	-2.768516	1.111377	-1.616728
88.C	-4.168803	-0.703484	-1.825440

89.C	-4.168803	0.703484	-1.825440
90.C	-5.350686	-1.430385	-1.970321
91.C	-5.350686	1.430385	-1.970321
92.C	-6.548440	-0.703174	-2.084387
93.C	-6.548440	0.703174	-2.084387
94.H	-5.343435	-2.522542	-1.979211
95.H	-5.343435	2.522542	-1.979211
96.H	-7.496057	-1.238337	-2.173385
97.H	-7.496057	1.238337	-2.173385
98.C	1.111377	-2.768516	-1.616728
99.C	-1.111377	-2.768516	-1.616728
100.C	0.703484	-4.168803	-1.825440
101.C	-0.703484	-4.168803	-1.825440
102.C	1.430385	-5.350686	-1.970321
103.C	-1.430385	-5.350686	-1.970321
104.C	0.703174	-6.548440	-2.084387
105.C	-0.703174	-6.548440	-2.084387
106.H	2.522542	-5.343435	-1.979211
107.H	-2.522542	-5.343435	-1.979211
108.H	1.238337	-7.496057	-2.173385
109.H	-1.238337	-7.496057	-2.173385
110.N	2.389994	2.389994	-1.665520
111.N	-2.389994	2.389994	-1.665520
112.N	-2.389994	-2.389994	-1.665520
113.N	2.389994	-2.389994	-1.665520

PcLu[Pc(p-Cl_8)] C_{4v}

Bonding energy -29.60271944 a.u.
-805.53131041 eV

Atom	X	Y	Z (Angstrom)
1.N	1.393770	1.393770	1.324757
2.N	-1.393770	1.393770	1.324757
3.N	-1.393770	-1.393770	1.324757
4.N	1.393770	-1.393770	1.324757
5.C	1.169487	2.737708	1.502897
6.C	2.737708	1.169487	1.502897
7.C	2.443786	3.434775	1.679416
8.C	3.434775	2.443786	1.679416
9.C	2.769620	4.788359	1.756766
10.C	4.788359	2.769620	1.756766
11.C	4.127293	5.131161	1.802324
12.C	5.131161	4.127293	1.802324
13.H	2.002636	5.564724	1.749741
14.H	5.564724	2.002636	1.749741
15.CL	4.562844	6.824627	1.831805
16.CL	6.824627	4.562844	1.831805
17.C	-2.737708	1.169487	1.502897
18.C	-1.169487	2.737708	1.502897
19.C	-3.434775	2.443786	1.679416
20.C	-2.443786	3.434775	1.679416
21.C	-4.788359	2.769620	1.756766
22.C	-2.769620	4.788359	1.756766
23.C	-5.131161	4.127293	1.802324
24.C	-4.127293	5.131161	1.802324
25.H	-5.564724	2.002636	1.749741
26.H	-2.002636	5.564724	1.749741
27.CL	-6.824627	4.562844	1.831805
28.CL	-4.562844	6.824627	1.831805

29.C	-1.169487	-2.737708	1.502897
30.C	-2.737708	-1.169487	1.502897
31.C	-2.443786	-3.434775	1.679416
32.C	-3.434775	-2.443786	1.679416
33.C	-2.769620	-4.788359	1.756766
34.C	-4.788359	-2.769620	1.756766
35.C	-4.127293	-5.131161	1.802324
36.C	-5.131161	-4.127293	1.802324
37.H	-2.002636	-5.564724	1.749741
38.H	-5.564724	-2.002636	1.749741
39.CL	-4.562844	-6.824627	1.831805
40.CL	-6.824627	-4.562844	1.831805
41.C	2.737708	-1.169487	1.502897
42.C	1.169487	-2.737708	1.502897
43.C	3.434775	-2.443786	1.679416
44.C	2.443786	-3.434775	1.679416
45.C	4.788359	-2.769620	1.756766
46.C	2.769620	-4.788359	1.756766
47.C	5.131161	-4.127293	1.802324
48.C	4.127293	-5.131161	1.802324
49.H	5.564724	-2.002636	1.749741
50.H	2.002636	-5.564724	1.749741
51.CL	6.824627	-4.562844	1.831805
52.CL	4.562844	-6.824627	1.831805
53.N	0.000000	3.374477	1.554569
54.N	-3.374477	0.000000	1.554569
55.N	0.000000	-3.374477	1.554569
56.N	3.374477	0.000000	1.554569
57.LU	0.000000	0.000000	-0.068172
58.N	1.977409	0.000000	-1.429743
59.N	0.000000	1.977409	-1.429743
60.N	-1.977409	0.000000	-1.429743
61.N	0.000000	-1.977409	-1.429743
62.C	2.769708	1.112353	-1.618988
63.C	2.769708	-1.112353	-1.618988
64.C	4.169587	0.703977	-1.816743
65.C	4.169587	-0.703977	-1.816743
66.C	5.357876	1.429530	-1.935140
67.C	5.357876	-1.429530	-1.935140
68.C	6.555900	0.704601	-2.021045
69.C	6.555900	-0.704601	-2.021045
70.H	5.349799	2.521903	-1.936049
71.H	5.349799	-2.521903	-1.936049
72.H	7.506104	1.239893	-2.081519
73.H	7.506104	-1.239893	-2.081519
74.C	-1.112353	2.769708	-1.618988
75.C	1.112353	2.769708	-1.618988
76.C	-0.703977	4.169587	-1.816743
77.C	0.703977	4.169587	-1.816743
78.C	-1.429530	5.357876	-1.935140
79.C	1.429530	5.357876	-1.935140
80.C	-0.704601	6.555900	-2.021045
81.C	0.704601	6.555900	-2.021045
82.H	-2.521903	5.349799	-1.936049
83.H	2.521903	5.349799	-1.936049
84.H	-1.239893	7.506104	-2.081519
85.H	1.239893	7.506104	-2.081519
86.C	-2.769708	-1.112353	-1.618988
87.C	-2.769708	1.112353	-1.618988

88.C	-4.169587	-0.703977	-1.816743
89.C	-4.169587	0.703977	-1.816743
90.C	-5.357876	-1.429530	-1.935140
91.C	-5.357876	1.429530	-1.935140
92.C	-6.555900	-0.704601	-2.021045
93.C	-6.555900	0.704601	-2.021045
94.H	-5.349799	-2.521903	-1.936049
95.H	-5.349799	2.521903	-1.936049
96.H	-7.506104	-1.239893	-2.081519
97.H	-7.506104	1.239893	-2.081519
98.C	1.112353	-2.769708	-1.618988
99.C	-1.112353	-2.769708	-1.618988
100.C	0.703977	-4.169587	-1.816743
101.C	-0.703977	-4.169587	-1.816743
102.C	1.429530	-5.357876	-1.935140
103.C	-1.429530	-5.357876	-1.935140
104.C	0.704601	-6.555900	-2.021045
105.C	-0.704601	-6.555900	-2.021045
106.H	2.521903	-5.349799	-1.936049
107.H	-2.521903	-5.349799	-1.936049
108.H	1.239893	-7.506104	-2.081519
109.H	-1.239893	-7.506104	-2.081519
110.N	2.390607	2.390607	-1.669037
111.N	-2.390607	2.390607	-1.669037
112.N	-2.390607	-2.390607	-1.669037
113.N	2.390607	-2.390607	-1.669037

$PcLu[Pc(p\text{-}Cl_8)]^-$ C_{4v}

Bonding energy -29.74021516 a.u.
-809.27276076 eV

Atom	X	Y	Z (Angstrom)
1.N	1.395669	1.395669	1.347820
2.N	-1.395669	1.395669	1.347820
3.N	-1.395669	-1.395669	1.347820
4.N	1.395669	-1.395669	1.347820
5.C	1.169435	2.738148	1.529290
6.C	2.738148	1.169435	1.529290
7.C	2.442223	3.434415	1.701524
8.C	3.434415	2.442223	1.701524
9.C	2.771305	4.790006	1.764350
10.C	4.790006	2.771305	1.764350
11.C	4.127331	5.131398	1.797826
12.C	5.131398	4.127331	1.797826
13.H	2.003726	5.565659	1.746872
14.H	5.565659	2.003726	1.746872
15.CL	4.565671	6.831920	1.804724
16.CL	6.831920	4.565671	1.804724
17.C	-2.738148	1.169435	1.529290
18.C	-1.169435	2.738148	1.529290
19.C	-3.434415	2.442223	1.701524
20.C	-2.442223	3.434415	1.701524
21.C	-4.790006	2.771305	1.764350
22.C	-2.771305	4.790006	1.764350
23.C	-5.131398	4.127331	1.797826
24.C	-4.127331	5.131398	1.797826
25.H	-5.565659	2.003726	1.746872
26.H	-2.003726	5.565659	1.746872

27.CL	-6.831920	4.565671	1.804724
28.CL	-4.565671	6.831920	1.804724
29.C	-1.169435	-2.738148	1.529290
30.C	-2.738148	-1.169435	1.529290
31.C	-2.442223	-3.434415	1.701524
32.C	-3.434415	-2.442223	1.701524
33.C	-2.771305	-4.790006	1.764350
34.C	-4.790006	-2.771305	1.764350
35.C	-4.127331	-5.131398	1.797826
36.C	-5.131398	-4.127331	1.797826
37.H	-2.003726	-5.565659	1.746872
38.H	-5.565659	-2.003726	1.746872
39.CL	-4.565671	-6.831920	1.804724
40.CL	-6.831920	-4.565671	1.804724
41.C	2.738148	-1.169435	1.529290
42.C	1.169435	-2.738148	1.529290
43.C	3.434415	-2.442223	1.701524
44.C	2.442223	-3.434415	1.701524
45.C	4.790006	-2.771305	1.764350
46.C	2.771305	-4.790006	1.764350
47.C	5.131398	-4.127331	1.797826
48.C	4.127331	-5.131398	1.797826
49.H	5.565659	-2.003726	1.746872
50.H	2.003726	-5.565659	1.746872
51.CL	6.831920	-4.565671	1.804724
52.CL	4.565671	-6.831920	1.804724
53.N	0.000000	3.374870	1.583047
54.N	-3.374870	0.000000	1.583047
55.N	0.000000	-3.374870	1.583047
56.N	3.374870	0.000000	1.583047
57.LU	0.000000	0.000000	-0.085117
58.N	1.981672	0.000000	-1.448891
59.N	0.000000	1.981672	-1.448891
60.N	-1.981672	0.000000	-1.448891
61.N	0.000000	-1.981672	-1.448891
62.C	2.773146	1.114474	-1.635420
63.C	2.773146	-1.114474	-1.635420
64.C	4.170537	0.705475	-1.820308
65.C	4.170537	-0.705475	-1.820308
66.C	5.365709	1.428839	-1.916566
67.C	5.365709	-1.428839	-1.916566
68.C	6.563688	0.706507	-1.978526
69.C	6.563688	-0.706507	-1.978526
70.H	5.356696	2.521532	-1.910411
71.H	5.356696	-2.521532	-1.910411
72.H	7.515596	1.242324	-2.014025
73.H	7.515596	-1.242324	-2.014025
74.C	-1.114474	2.773146	-1.635420
75.C	1.114474	2.773146	-1.635420
76.C	-0.705475	4.170537	-1.820308
77.C	0.705475	4.170537	-1.820308
78.C	-1.428839	5.365709	-1.916566
79.C	1.428839	5.365709	-1.916566
80.C	-0.706507	6.563688	-1.978526
81.C	0.706507	6.563688	-1.978526
82.H	-2.521532	5.356696	-1.910411
83.H	2.521532	5.356696	-1.910411
84.H	-1.242324	7.515596	-2.014025
85.H	1.242324	7.515596	-2.014025

86.C	-2.773146	-1.114474	-1.635420
87.C	-2.773146	1.114474	-1.635420
88.C	-4.170537	-0.705475	-1.820308
89.C	-4.170537	0.705475	-1.820308
90.C	-5.365709	-1.428839	-1.916566
91.C	-5.365709	1.428839	-1.916566
92.C	-6.563688	-0.706507	-1.978526
93.C	-6.563688	0.706507	-1.978526
94.H	-5.356696	-2.521532	-1.910411
95.H	-5.356696	2.521532	-1.910411
96.H	-7.515596	-1.242324	-2.014025
97.H	-7.515596	1.242324	-2.014025
98.C	1.114474	-2.773146	-1.635420
99.C	-1.114474	-2.773146	-1.635420
100.C	0.705475	-4.170537	-1.820308
101.C	-0.705475	-4.170537	-1.820308
102.C	1.428839	-5.365709	-1.916566
103.C	-1.428839	-5.365709	-1.916566
104.C	0.706507	-6.563688	-1.978526
105.C	-0.706507	-6.563688	-1.978526
106.H	2.521532	-5.356696	-1.910411
107.H	-2.521532	-5.356696	-1.910411
108.H	1.242324	-7.515596	-2.014025
109.H	-1.242324	-7.515596	-2.014025
110.N	2.392573	2.392573	-1.684797
111.N	-2.392573	2.392573	-1.684797
112.N	-2.392573	-2.392573	-1.684797
113.N	2.392573	-2.392573	-1.684797

$PcLu[Pc(np\text{-}Cl_8)]^+$ C_{4v}

Bonding energy -29.35113133 a.u.
-798.68524681 eV

Atom	X	Y	Z (Angstrom)
1.N	1.407062	1.407062	1.347689
2.N	-1.407062	1.407062	1.347689
3.N	-1.407062	-1.407062	1.347689
4.N	1.407062	-1.407062	1.347689
5.C	1.176104	2.747405	1.540556
6.C	2.747405	1.176104	1.540556
7.C	2.451420	3.451318	1.760896
8.C	3.451318	2.451420	1.760896
9.C	2.798400	4.799031	1.931352
10.C	4.799031	2.798400	1.931352
11.C	4.154362	5.138082	2.084823
12.C	5.138082	4.154362	2.084823
13.CL	1.650187	6.100317	1.946920
14.CL	6.100317	1.650187	1.946920
15.H	4.426897	6.187623	2.205674
16.H	6.187623	4.426897	2.205674
17.C	-2.747405	1.176104	1.540556
18.C	-1.176104	2.747405	1.540556
19.C	-3.451318	2.451420	1.760896
20.C	-2.451420	3.451318	1.760896
21.C	-4.799031	2.798400	1.931352
22.C	-2.798400	4.799031	1.931352
23.C	-5.138082	4.154362	2.084823
24.C	-4.154362	5.138082	2.084823
25.CL	-6.100317	1.650187	1.946920

26.CL	-1.650187	6.100317	1.946920
27.H	-6.187623	4.426897	2.205674
28.H	-4.426897	6.187623	2.205674
29.C	-1.176104	-2.747405	1.540556
30.C	-2.747405	-1.176104	1.540556
31.C	-2.451420	-3.451318	1.760896
32.C	-3.451318	-2.451420	1.760896
33.C	-2.798400	-4.799031	1.931352
34.C	-4.799031	-2.798400	1.931352
35.C	-4.154362	-5.138082	2.084823
36.C	-5.138082	-4.154362	2.084823
37.CL	-1.650187	-6.100317	1.946920
38.CL	-6.100317	-1.650187	1.946920
39.H	-4.426897	-6.187623	2.205674
40.H	-6.187623	-4.426897	2.205674
41.C	2.747405	-1.176104	1.540556
42.C	1.176104	-2.747405	1.540556
43.C	3.451318	-2.451420	1.760896
44.C	2.451420	-3.451318	1.760896
45.C	4.799031	-2.798400	1.931352
46.C	2.798400	-4.799031	1.931352
47.C	5.138082	-4.154362	2.084823
48.C	4.154362	-5.138082	2.084823
49.CL	6.100317	-1.650187	1.946920
50.CL	1.650187	-6.100317	1.946920
51.H	6.187623	-4.426897	2.205674
52.H	4.426897	-6.187623	2.205674
53.N	0.000000	3.370857	1.594146
54.N	-3.370857	0.000000	1.594146
55.N	0.000000	-3.370857	1.594146
56.N	3.370857	0.000000	1.594146
57.Lu	0.000000	0.000000	-0.006195
58.N	1.981356	0.000000	-1.352770
59.N	0.000000	1.981356	-1.352770
60.N	-1.981356	0.000000	-1.352770
61.N	0.000000	-1.981356	-1.352770
62.C	2.767121	1.110317	-1.580414
63.C	2.767121	-1.110317	-1.580414
64.C	4.152950	0.703007	-1.868682
65.C	4.152950	-0.703007	-1.868682
66.C	5.315347	1.429852	-2.126913
67.C	5.315347	-1.429852	-2.126913
68.C	6.495058	0.703212	-2.358981
69.C	6.495058	-0.703212	-2.358981
70.H	5.306221	2.522039	-2.138011
71.H	5.306221	-2.522039	-2.138011
72.H	7.428970	1.238233	-2.543013
73.H	7.428970	-1.238233	-2.543013
74.C	-1.110317	2.767121	-1.580414
75.C	1.110317	2.767121	-1.580414
76.C	-0.703007	4.152950	-1.868682
77.C	0.703007	4.152950	-1.868682
78.C	-1.429852	5.315347	-2.126913
79.C	1.429852	5.315347	-2.126913
80.C	-0.703212	6.495058	-2.358981
81.C	0.703212	6.495058	-2.358981
82.H	-2.522039	5.306221	-2.138011
83.H	2.522039	5.306221	-2.138011
84.H	-1.238233	7.428970	-2.543013

85.H	1.238233	7.428970	-2.543013
86.C	-2.767121	-1.110317	-1.580414
87.C	-2.767121	1.110317	-1.580414
88.C	-4.152950	-0.703007	-1.868682
89.C	-4.152950	0.703007	-1.868682
90.C	-5.315347	-1.429852	-2.126913
91.C	-5.315347	1.429852	-2.126913
92.C	-6.495058	-0.703212	-2.358981
93.C	-6.495058	0.703212	-2.358981
94.H	-5.306221	-2.522039	-2.138011
95.H	-5.306221	2.522039	-2.138011
96.H	-7.428970	-1.238233	-2.543013
97.H	-7.428970	1.238233	-2.543013
98.C	1.110317	-2.767121	-1.580414
99.C	-1.110317	-2.767121	-1.580414
100.C	0.703007	-4.152950	-1.868682
101.C	-0.703007	-4.152950	-1.868682
102.C	1.429852	-5.315347	-2.126913
103.C	-1.429852	-5.315347	-2.126913
104.C	0.703212	-6.495058	-2.358981
105.C	-0.703212	-6.495058	-2.358981
106.H	2.522039	-5.306221	-2.138011
107.H	-2.522039	-5.306221	-2.138011
108.H	1.238233	-7.428970	-2.543013
109.H	-1.238233	-7.428970	-2.543013
110.N	2.388110	2.388110	-1.633692
111.N	-2.388110	2.388110	-1.633692
112.N	-2.388110	-2.388110	-1.633692
113.N	2.388110	-2.388110	-1.633692

PcLu[Pc(np-Cl_8)] C_{4v}

Bonding energy -29.57099831 a.u.
-804.66813432 eV

Atom	X	Y	Z (Angstrom)
1.N	1.408640	1.408640	1.360465
2.N	-1.408640	1.408640	1.360465
3.N	-1.408640	-1.408640	1.360465
4.N	1.408640	-1.408640	1.360465
5.C	1.175364	2.747932	1.560563
6.C	2.747932	1.175364	1.560563
7.C	2.449018	3.449992	1.782690
8.C	3.449992	2.449018	1.782690
9.C	2.800950	4.798354	1.946952
10.C	4.798354	2.800950	1.946952
11.C	4.152182	5.138446	2.093824
12.C	5.138446	4.152182	2.093824
13.CL	1.648352	6.104603	1.953352
14.CL	6.104603	1.648352	1.953352
15.H	4.425445	6.187508	2.206436
16.H	6.187508	4.425445	2.206436
17.C	-2.747932	1.175364	1.560563
18.C	-1.175364	2.747932	1.560563
19.C	-3.449992	2.449018	1.782690
20.C	-2.449018	3.449992	1.782690
21.C	-4.798354	2.800950	1.946952
22.C	-2.800950	4.798354	1.946952
23.C	-5.138446	4.152182	2.093824

24.C	-4.152182	5.138446	2.093824
25.CL	-6.104603	1.648352	1.953352
26.CL	-1.648352	6.104603	1.953352
27.H	-6.187508	4.425445	2.206436
28.H	-4.425445	6.187508	2.206436
29.C	-1.175364	-2.747932	1.560563
30.C	-2.747932	-1.175364	1.560563
31.C	-2.449018	-3.449992	1.782690
32.C	-3.449992	-2.449018	1.782690
33.C	-2.800950	-4.798354	1.946952
34.C	-4.798354	-2.800950	1.946952
35.C	-4.152182	-5.138446	2.093824
36.C	-5.138446	-4.152182	2.093824
37.CL	-1.648352	-6.104603	1.953352
38.CL	-6.104603	-1.648352	1.953352
39.H	-4.425445	-6.187508	2.206436
40.H	-6.187508	-4.425445	2.206436
41.C	2.747932	-1.175364	1.560563
42.C	1.175364	-2.747932	1.560563
43.C	3.449992	-2.449018	1.782690
44.C	2.449018	-3.449992	1.782690
45.C	4.798354	-2.800950	1.946952
46.C	2.800950	-4.798354	1.946952
47.C	5.138446	-4.152182	2.093824
48.C	4.152182	-5.138446	2.093824
49.CL	6.104603	-1.648352	1.953352
50.CL	1.648352	-6.104603	1.953352
51.H	6.187508	-4.425445	2.206436
52.H	4.425445	-6.187508	2.206436
53.N	0.000000	3.370851	1.616784
54.N	-3.370851	0.000000	1.616784
55.N	0.000000	-3.370851	1.616784
56.N	3.370851	0.000000	1.616784
57.Lu	0.000000	0.000000	-0.011122
58.N	1.985048	0.000000	-1.371044
59.N	0.000000	1.985048	-1.371044
60.N	-1.985048	0.000000	-1.371044
61.N	0.000000	-1.985048	-1.371044
62.C	2.768069	1.111198	-1.604467
63.C	2.768069	-1.111198	-1.604467
64.C	4.151706	0.703449	-1.892747
65.C	4.151706	-0.703449	-1.892747
66.C	5.318987	1.428968	-2.141976
67.C	5.318987	-1.428968	-2.141976
68.C	6.498526	0.704465	-2.365879
69.C	6.498526	-0.704465	-2.365879
70.H	5.308925	2.521289	-2.146374
71.H	5.308925	-2.521289	-2.146374
72.H	7.434905	1.239534	-2.539215
73.H	7.434905	-1.239534	-2.539215
74.C	-1.111198	2.768069	-1.604467
75.C	1.111198	2.768069	-1.604467
76.C	-0.703449	4.151706	-1.892747
77.C	0.703449	4.151706	-1.892747
78.C	-1.428968	5.318987	-2.141976
79.C	1.428968	5.318987	-2.141976
80.C	-0.704465	6.498526	-2.365879
81.C	0.704465	6.498526	-2.365879
82.H	-2.521289	5.308925	-2.146374

83.H	2.521289	5.308925	-2.146374
84.H	-1.239534	7.434905	-2.539215
85.H	1.239534	7.434905	-2.539215
86.C	-2.768069	-1.111198	-1.604467
87.C	-2.768069	1.111198	-1.604467
88.C	-4.151706	-0.703449	-1.892747
89.C	-4.151706	0.703449	-1.892747
90.C	-5.318987	-1.428968	-2.141976
91.C	-5.318987	1.428968	-2.141976
92.C	-6.498526	-0.704465	-2.365879
93.C	-6.498526	0.704465	-2.365879
94.H	-5.308925	-2.521289	-2.146374
95.H	-5.308925	2.521289	-2.146374
96.H	-7.434905	-1.239534	-2.539215
97.H	-7.434905	1.239534	-2.539215
98.C	1.111198	-2.768069	-1.604467
99.C	-1.111198	-2.768069	-1.604467
100.C	0.703449	-4.151706	-1.892747
101.C	-0.703449	-4.151706	-1.892747
102.C	1.428968	-5.318987	-2.141976
103.C	-1.428968	-5.318987	-2.141976
104.C	0.704465	-6.498526	-2.365879
105.C	-0.704465	-6.498526	-2.365879
106.H	2.521289	-5.308925	-2.146374
107.H	-2.521289	-5.308925	-2.146374
108.H	1.239534	-7.434905	-2.539215
109.H	-1.239534	-7.434905	-2.539215
110.N	2.388215	2.388215	-1.660710
111.N	-2.388215	2.388215	-1.660710
112.N	-2.388215	-2.388215	-1.660710
113.N	2.388215	-2.388215	-1.660710

$PcLu[Pc(np\text{-}Cl_8)]^-$ C_{4v}

Bonding energy -29.70455557 a.u.
-808.30241375 eV

Atom	X	Y	Z (Angstrom)
1.N	1.412145	1.412145	1.371527
2.N	-1.412145	1.412145	1.371527
3.N	-1.412145	-1.412145	1.371527
4.N	1.412145	-1.412145	1.371527
5.C	1.175278	2.747160	1.586885
6.C	2.747160	1.175278	1.586885
7.C	2.444616	3.446780	1.826891
8.C	3.446780	2.444616	1.826891
9.C	2.798921	4.793454	2.007573
10.C	4.793454	2.798921	2.007573
11.C	4.145215	5.133387	2.174143
12.C	5.133387	4.145215	2.174143
13.CL	1.644784	6.104887	2.005172
14.CL	6.104887	1.644784	2.005172
15.H	4.417079	6.181937	2.298489
16.H	6.181937	4.417079	2.298489
17.C	-2.747160	1.175278	1.586885
18.C	-1.175278	2.747160	1.586885
19.C	-3.446780	2.444616	1.826891
20.C	-2.444616	3.446780	1.826891
21.C	-4.793454	2.798921	2.007573

22.C	-2.798921	4.793454	2.007573
23.C	-5.133387	4.145215	2.174143
24.C	-4.145215	5.133387	2.174143
25.CL	-6.104887	1.644784	2.005172
26.CL	-1.644784	6.104887	2.005172
27.H	-6.181937	4.417079	2.298489
28.H	-4.417079	6.181937	2.298489
29.C	-1.175278	-2.747160	1.586885
30.C	-2.747160	-1.175278	1.586885
31.C	-2.444616	-3.446780	1.826891
32.C	-3.446780	-2.444616	1.826891
33.C	-2.798921	-4.793454	2.007573
34.C	-4.793454	-2.798921	2.007573
35.C	-4.145215	-5.133387	2.174143
36.C	-5.133387	-4.145215	2.174143
37.CL	-1.644784	-6.104887	2.005172
38.CL	-6.104887	-1.644784	2.005172
39.H	-4.417079	-6.181937	2.298489
40.H	-6.181937	-4.417079	2.298489
41.C	2.747160	-1.175278	1.586885
42.C	1.175278	-2.747160	1.586885
43.C	3.446780	-2.444616	1.826891
44.C	2.444616	-3.446780	1.826891
45.C	4.793454	-2.798921	2.007573
46.C	2.798921	-4.793454	2.007573
47.C	5.133387	-4.145215	2.174143
48.C	4.145215	-5.133387	2.174143
49.CL	6.104887	-1.644784	2.005172
50.CL	1.644784	-6.104887	2.005172
51.H	6.181937	-4.417079	2.298489
52.H	4.417079	-6.181937	2.298489
53.N	0.000000	3.369273	1.648181
54.N	-3.369273	0.000000	1.648181
55.N	0.000000	-3.369273	1.648181
56.N	3.369273	0.000000	1.648181
57.Lu	0.000000	0.000000	-0.038445
58.N	1.993898	0.000000	-1.391697
59.N	0.000000	1.993898	-1.391697
60.N	-1.993898	0.000000	-1.391697
61.N	0.000000	-1.993898	-1.391697
62.C	2.771203	1.112866	-1.640239
63.C	2.771203	-1.112866	-1.640239
64.C	4.145300	0.704781	-1.950233
65.C	4.145300	-0.704781	-1.950233
66.C	5.311391	1.428501	-2.226813
67.C	5.311391	-1.428501	-2.226813
68.C	6.483262	0.706448	-2.479286
69.C	6.483262	-0.706448	-2.479286
70.H	5.300184	2.521205	-2.228144
71.H	5.300184	-2.521205	-2.228144
72.H	7.416412	1.241616	-2.673546
73.H	7.416412	-1.241616	-2.673546
74.C	-1.112866	2.771203	-1.640239
75.C	1.112866	2.771203	-1.640239
76.C	-0.704781	4.145300	-1.950233
77.C	0.704781	4.145300	-1.950233
78.C	-1.428501	5.311391	-2.226813
79.C	1.428501	5.311391	-2.226813
80.C	-0.706448	6.483262	-2.479286

81.C	0.706448	6.483262	-2.479286
82.H	-2.521205	5.300184	-2.228144
83.H	2.521205	5.300184	-2.228144
84.H	-1.241616	7.416412	-2.673546
85.H	1.241616	7.416412	-2.673546
86.C	-2.771203	-1.112866	-1.640239
87.C	-2.771203	1.112866	-1.640239
88.C	-4.145300	-0.704781	-1.950233
89.C	-4.145300	0.704781	-1.950233
90.C	-5.311391	-1.428501	-2.226813
91.C	-5.311391	1.428501	-2.226813
92.C	-6.483262	-0.706448	-2.479286
93.C	-6.483262	0.706448	-2.479286
94.H	-5.300184	-2.521205	-2.228144
95.H	-5.300184	2.521205	-2.228144
96.H	-7.416412	-1.241616	-2.673546
97.H	-7.416412	1.241616	-2.673546
98.C	1.112866	-2.771203	-1.640239
99.C	-1.112866	-2.771203	-1.640239
100.C	0.704781	-4.145300	-1.950233
101.C	-0.704781	-4.145300	-1.950233
102.C	1.428501	-5.311391	-2.226813
103.C	-1.428501	-5.311391	-2.226813
104.C	0.706448	-6.483262	-2.479286
105.C	-0.706448	-6.483262	-2.479286
106.H	2.521205	-5.300184	-2.228144
107.H	-2.521205	-5.300184	-2.228144
108.H	1.241616	-7.416412	-2.673546
109.H	-1.241616	-7.416412	-2.673546
110.N	2.388725	2.388725	-1.700922
111.N	-2.388725	2.388725	-1.700922
112.N	-2.388725	-2.388725	-1.700922
113.N	2.388725	-2.388725	-1.700922

$PcLu[PcCl_{16}]^{+}$ C_{4v}

Bonding energy -28.79131289 a.u.
-783.45180573 eV

Atom	X	Y	Z (Angstrom)
1.N	1.406397	1.406397	1.336058
2.N	-1.406397	1.406397	1.336058
3.N	-1.406397	-1.406397	1.336058
4.N	1.406397	-1.406397	1.336058
5.C	1.176466	2.748542	1.512209
6.C	2.748542	1.176466	1.512209
7.C	2.457794	3.454134	1.696080
8.C	3.454134	2.457794	1.696080
9.C	2.796309	4.810132	1.807434
10.C	4.810132	2.796309	1.807434
11.C	4.167174	5.165005	1.870078
12.C	5.165005	4.167174	1.870078
13.CL	1.614716	6.065335	1.850184
14.CL	6.065335	1.614716	1.850184
15.CL	4.625076	6.833054	1.939321
16.CL	6.833054	4.625076	1.939321
17.C	-2.748542	1.176466	1.512209
18.C	-1.176466	2.748542	1.512209
19.C	-3.454134	2.457794	1.696080
20.C	-2.457794	3.454134	1.696080

21.C	-4.810132	2.796309	1.807434
22.C	-2.796309	4.810132	1.807434
23.C	-5.165005	4.167174	1.870078
24.C	-4.167174	5.165005	1.870078
25.CL	-6.065335	1.614716	1.850184
26.CL	-1.614716	6.065335	1.850184
27.CL	-6.833054	4.625076	1.939321
28.CL	-4.625076	6.833054	1.939321
29.C	-1.176466	-2.748542	1.512209
30.C	-2.748542	-1.176466	1.512209
31.C	-2.457794	-3.454134	1.696080
32.C	-3.454134	-2.457794	1.696080
33.C	-2.796309	-4.810132	1.807434
34.C	-4.810132	-2.796309	1.807434
35.C	-4.167174	-5.165005	1.870078
36.C	-5.165005	-4.167174	1.870078
37.CL	-1.614716	-6.065335	1.850184
38.CL	-6.065335	-1.614716	1.850184
39.CL	-4.625076	-6.833054	1.939321
40.CL	-6.833054	-4.625076	1.939321
41.C	2.748542	-1.176466	1.512209
42.C	1.176466	-2.748542	1.512209
43.C	3.454134	-2.457794	1.696080
44.C	2.457794	-3.454134	1.696080
45.C	4.810132	-2.796309	1.807434
46.C	2.796309	-4.810132	1.807434
47.C	5.165005	-4.167174	1.870078
48.C	4.167174	-5.165005	1.870078
49.CL	6.065335	-1.614716	1.850184
50.CL	1.614716	-6.065335	1.850184
51.CL	6.833054	-4.625076	1.939321
52.CL	4.625076	-6.833054	1.939321
53.N	0.000000	3.370003	1.564387
54.N	-3.370003	0.000000	1.564387
55.N	0.000000	-3.370003	1.564387
56.N	3.370003	0.000000	1.564387
57.Lu	0.000000	0.000000	-0.031458
58.N	1.979234	0.000000	-1.383488
59.N	0.000000	1.979234	-1.383488
60.N	-1.979234	0.000000	-1.383488
61.N	0.000000	-1.979234	-1.383488
62.C	2.768412	1.110931	-1.598270
63.C	2.768412	-1.110931	-1.598270
64.C	4.160082	0.703320	-1.859969
65.C	4.160082	-0.703320	-1.859969
66.C	5.331508	1.429985	-2.075206
67.C	5.331508	-1.429985	-2.075206
68.C	6.519687	0.702841	-2.261819
69.C	6.519687	-0.702841	-2.261819
70.H	5.324360	2.522181	-2.085388
71.H	5.324360	-2.522181	-2.085388
72.H	7.460121	1.238334	-2.405885
73.H	7.460121	-1.238334	-2.405885
74.C	-1.110931	2.768412	-1.598270
75.C	1.110931	2.768412	-1.598270
76.C	-0.703320	4.160082	-1.859969
77.C	0.703320	4.160082	-1.859969
78.C	-1.429985	5.331508	-2.075206
79.C	1.429985	5.331508	-2.075206

80.C	-0.702841	6.519687	-2.261819
81.C	0.702841	6.519687	-2.261819
82.H	-2.522181	5.324360	-2.085388
83.H	2.522181	5.324360	-2.085388
84.H	-1.238334	7.460121	-2.405885
85.H	1.238334	7.460121	-2.405885
86.C	-2.768412	-1.110931	-1.598270
87.C	-2.768412	1.110931	-1.598270
88.C	-4.160082	-0.703320	-1.859969
89.C	-4.160082	0.703320	-1.859969
90.C	-5.331508	-1.429985	-2.075206
91.C	-5.331508	1.429985	-2.075206
92.C	-6.519687	-0.702841	-2.261819
93.C	-6.519687	0.702841	-2.261819
94.H	-5.324360	-2.522181	-2.085388
95.H	-5.324360	2.522181	-2.085388
96.H	-7.460121	-1.238334	-2.405885
97.H	-7.460121	1.238334	-2.405885
98.C	1.110931	-2.768412	-1.598270
99.C	-1.110931	-2.768412	-1.598270
100.C	0.703320	-4.160082	-1.859969
101.C	-0.703320	-4.160082	-1.859969
102.C	1.429985	-5.331508	-2.075206
103.C	-1.429985	-5.331508	-2.075206
104.C	0.702841	-6.519687	-2.261819
105.C	-0.702841	-6.519687	-2.261819
106.H	2.522181	-5.324360	-2.085388
107.H	-2.522181	-5.324360	-2.085388
108.H	1.238334	-7.460121	-2.405885
109.H	-1.238334	-7.460121	-2.405885
110.N	2.389157	2.389157	-1.648488
111.N	-2.389157	2.389157	-1.648488
112.N	-2.389157	-2.389157	-1.648488
113.N	2.389157	-2.389157	-1.648488

$PcLu[PcCl_{16}]$ C_{4v}

Bonding energy -29.01954545 a.u.
-789.66233238 eV

Atom	X	Y	Z (Angstrom)
1.N	1.409992	1.409992	1.318454
2.N	-1.409992	1.409992	1.318454
3.N	-1.409992	-1.409992	1.318454
4.N	1.409992	-1.409992	1.318454
5.C	1.176319	2.748901	1.511856
6.C	2.748901	1.176319	1.511856
7.C	2.454121	3.451142	1.718959
8.C	3.451142	2.454121	1.718959
9.C	2.793852	4.805968	1.858828
10.C	4.805968	2.793852	1.858828
11.C	4.156627	5.155647	1.977107
12.C	5.155647	4.156627	1.977107
13.CL	1.610275	6.065393	1.860314
14.CL	6.065393	1.610275	1.860314
15.CL	4.616478	6.825852	2.110106
16.CL	6.825852	4.616478	2.110106
17.C	-2.748901	1.176319	1.511856
18.C	-1.176319	2.748901	1.511856
19.C	-3.451142	2.454121	1.718959

20.C	-2.454121	3.451142	1.718959
21.C	-4.805968	2.793852	1.858828
22.C	-2.793852	4.805968	1.858828
23.C	-5.155647	4.156627	1.977107
24.C	-4.156627	5.155647	1.977107
25.CL	-6.065393	1.610275	1.860314
26.CL	-1.610275	6.065393	1.860314
27.CL	-6.825852	4.616478	2.110106
28.CL	-4.616478	6.825852	2.110106
29.C	-1.176319	-2.748901	1.511856
30.C	-2.748901	-1.176319	1.511856
31.C	-2.454121	-3.451142	1.718959
32.C	-3.451142	-2.454121	1.718959
33.C	-2.793852	-4.805968	1.858828
34.C	-4.805968	-2.793852	1.858828
35.C	-4.156627	-5.155647	1.977107
36.C	-5.155647	-4.156627	1.977107
37.CL	-1.610275	-6.065393	1.860314
38.CL	-6.065393	-1.610275	1.860314
39.CL	-4.616478	-6.825852	2.110106
40.CL	-6.825852	-4.616478	2.110106
41.C	2.748901	-1.176319	1.511856
42.C	1.176319	-2.748901	1.511856
43.C	3.451142	-2.454121	1.718959
44.C	2.454121	-3.451142	1.718959
45.C	4.805968	-2.793852	1.858828
46.C	2.793852	-4.805968	1.858828
47.C	5.155647	-4.156627	1.977107
48.C	4.156627	-5.155647	1.977107
49.CL	6.065393	-1.610275	1.860314
50.CL	1.610275	-6.065393	1.860314
51.CL	6.825852	-4.616478	2.110106
52.CL	4.616478	-6.825852	2.110106
53.N	0.000000	3.368914	1.567881
54.N	-3.368914	0.000000	1.567881
55.N	0.000000	-3.368914	1.567881
56.N	3.368914	0.000000	1.567881
57.Lu	0.000000	0.000000	-0.062986
58.N	1.985496	0.000000	-1.417615
59.N	0.000000	1.985496	-1.417615
60.N	-1.985496	0.000000	-1.417615
61.N	0.000000	-1.985496	-1.417615
62.C	2.767544	1.111014	-1.660188
63.C	2.767544	-1.111014	-1.660188
64.C	4.147602	0.703441	-1.963394
65.C	4.147602	-0.703441	-1.963394
66.C	5.309333	1.429410	-2.235898
67.C	5.309333	-1.429410	-2.235898
68.C	6.484126	0.704297	-2.482698
69.C	6.484126	-0.704297	-2.482698
70.H	5.299795	2.521715	-2.244199
71.H	5.299795	-2.521715	-2.244199
72.H	7.417467	1.240099	-2.676749
73.H	7.417467	-1.240099	-2.676749
74.C	-1.111014	2.767544	-1.660188
75.C	1.111014	2.767544	-1.660188
76.C	-0.703441	4.147602	-1.963394
77.C	0.703441	4.147602	-1.963394
78.C	-1.429410	5.309333	-2.235898

79.C	1.429410	5.309333	-2.235898
80.C	-0.704297	6.484126	-2.482698
81.C	0.704297	6.484126	-2.482698
82.H	-2.521715	5.299795	-2.244199
83.H	2.521715	5.299795	-2.244199
84.H	-1.240099	7.417467	-2.676749
85.H	1.240099	7.417467	-2.676749
86.C	-2.767544	-1.111014	-1.660188
87.C	-2.767544	1.111014	-1.660188
88.C	-4.147602	-0.703441	-1.963394
89.C	-4.147602	0.703441	-1.963394
90.C	-5.309333	-1.429410	-2.235898
91.C	-5.309333	1.429410	-2.235898
92.C	-6.484126	-0.704297	-2.482698
93.C	-6.484126	0.704297	-2.482698
94.H	-5.299795	-2.521715	-2.244199
95.H	-5.299795	2.521715	-2.244199
96.H	-7.417467	-1.240099	-2.676749
97.H	-7.417467	1.240099	-2.676749
98.C	1.111014	-2.767544	-1.660188
99.C	-1.111014	-2.767544	-1.660188
100.C	0.703441	-4.147602	-1.963394
101.C	-0.703441	-4.147602	-1.963394
102.C	1.429410	-5.309333	-2.235898
103.C	-1.429410	-5.309333	-2.235898
104.C	0.704297	-6.484126	-2.482698
105.C	-0.704297	-6.484126	-2.482698
106.H	2.521715	-5.299795	-2.244199
107.H	-2.521715	-5.299795	-2.244199
108.H	1.240099	-7.417467	-2.676749
109.H	-1.240099	-7.417467	-2.676749
110.N	2.388001	2.388001	-1.715947
111.N	-2.388001	2.388001	-1.715947
112.N	-2.388001	-2.388001	-1.715947
113.N	2.388001	-2.388001	-1.715947

$PcLu[PcCl_{16}]^-$ C_{4v}

Bonding energy -29.16398519 a.u.
-793.59273932 eV

Atom	X	Y	Z (Angstrom)
1.N	1.412293	1.412293	1.328818
2.N	-1.412293	1.412293	1.328818
3.N	-1.412293	-1.412293	1.328818
4.N	1.412293	-1.412293	1.328818
5.C	1.176054	2.748296	1.530347
6.C	2.748296	1.176054	1.530347
7.C	2.452338	3.450289	1.741461
8.C	3.450289	2.452338	1.741461
9.C	2.795353	4.805814	1.878641
10.C	4.805814	2.795353	1.878641
11.C	4.154942	5.154480	1.994848
12.C	5.154480	4.154942	1.994848
13.CL	1.609001	6.067184	1.873688
14.CL	6.067184	1.609001	1.873688
15.CL	4.618950	6.830100	2.122165
16.CL	6.830100	4.618950	2.122165
17.C	-2.748296	1.176054	1.530347
18.C	-1.176054	2.748296	1.530347

19.C	-3.450289	2.452338	1.741461
20.C	-2.452338	3.450289	1.741461
21.C	-4.805814	2.795353	1.878641
22.C	-2.795353	4.805814	1.878641
23.C	-5.154480	4.154942	1.994848
24.C	-4.154942	5.154480	1.994848
25.CL	-6.067184	1.609001	1.873688
26.CL	-1.609001	6.067184	1.873688
27.CL	-6.830100	4.618950	2.122165
28.CL	-4.618950	6.830100	2.122165
29.C	-1.176054	-2.748296	1.530347
30.C	-2.748296	-1.176054	1.530347
31.C	-2.452338	-3.450289	1.741461
32.C	-3.450289	-2.452338	1.741461
33.C	-2.795353	-4.805814	1.878641
34.C	-4.805814	-2.795353	1.878641
35.C	-4.154942	-5.154480	1.994848
36.C	-5.154480	-4.154942	1.994848
37.CL	-1.609001	-6.067184	1.873688
38.CL	-6.067184	-1.609001	1.873688
39.CL	-4.618950	-6.830100	2.122165
40.CL	-6.830100	-4.618950	2.122165
41.C	2.748296	-1.176054	1.530347
42.C	1.176054	-2.748296	1.530347
43.C	3.450289	-2.452338	1.741461
44.C	2.452338	-3.450289	1.741461
45.C	4.805814	-2.795353	1.878641
46.C	2.795353	-4.805814	1.878641
47.C	5.154480	-4.154942	1.994848
48.C	4.154942	-5.154480	1.994848
49.CL	6.067184	-1.609001	1.873688
50.CL	1.609001	-6.067184	1.873688
51.CL	6.830100	-4.618950	2.122165
52.CL	4.618950	-6.830100	2.122165
53.N	0.000000	3.368136	1.590485
54.N	-3.368136	0.000000	1.590485
55.N	0.000000	-3.368136	1.590485
56.N	3.368136	0.000000	1.590485
57.Lu	0.000000	0.000000	-0.104563
58.N	1.992492	0.000000	-1.441092
59.N	0.000000	1.992492	-1.441092
60.N	-1.992492	0.000000	-1.441092
61.N	0.000000	-1.992492	-1.441092
62.C	2.772153	1.113622	-1.684597
63.C	2.772153	-1.113622	-1.684597
64.C	4.148004	0.704903	-1.984958
65.C	4.148004	-0.704903	-1.984958
66.C	5.316832	1.428696	-2.250230
67.C	5.316832	-1.428696	-2.250230
68.C	6.491222	0.706380	-2.489570
69.C	6.491222	-0.706380	-2.489570
70.H	5.306580	2.521380	-2.253397
71.H	5.306580	-2.521380	-2.253397
72.H	7.425919	1.241595	-2.673710
73.H	7.425919	-1.241595	-2.673710
74.C	-1.113622	2.772153	-1.684597
75.C	1.113622	2.772153	-1.684597
76.C	-0.704903	4.148004	-1.984958
77.C	0.704903	4.148004	-1.984958

78.C	-1.428696	5.316832	-2.250230
79.C	1.428696	5.316832	-2.250230
80.C	-0.706380	6.491222	-2.489570
81.C	0.706380	6.491222	-2.489570
82.H	-2.521380	5.306580	-2.253397
83.H	2.521380	5.306580	-2.253397
84.H	-1.241595	7.425919	-2.673710
85.H	1.241595	7.425919	-2.673710
86.C	-2.772153	-1.113622	-1.684597
87.C	-2.772153	1.113622	-1.684597
88.C	-4.148004	-0.704903	-1.984958
89.C	-4.148004	0.704903	-1.984958
90.C	-5.316832	-1.428696	-2.250230
91.C	-5.316832	1.428696	-2.250230
92.C	-6.491222	-0.706380	-2.489570
93.C	-6.491222	0.706380	-2.489570
94.H	-5.306580	-2.521380	-2.253397
95.H	-5.306580	2.521380	-2.253397
96.H	-7.425919	-1.241595	-2.673710
97.H	-7.425919	1.241595	-2.673710
98.C	1.113622	-2.772153	-1.684597
99.C	-1.113622	-2.772153	-1.684597
100.C	0.704903	-4.148004	-1.984958
101.C	-0.704903	-4.148004	-1.984958
102.C	1.428696	-5.316832	-2.250230
103.C	-1.428696	-5.316832	-2.250230
104.C	0.706380	-6.491222	-2.489570
105.C	-0.706380	-6.491222	-2.489570
106.H	2.521380	-5.306580	-2.253397
107.H	-2.521380	-5.306580	-2.253397
108.H	1.241595	-7.425919	-2.673710
109.H	-1.241595	-7.425919	-2.673710
110.N	2.389773	2.389773	-1.741528
111.N	-2.389773	2.389773	-1.741528
112.N	-2.389773	-2.389773	-1.741528
113.N	2.389773	-2.389773	-1.741528

$\{PcLu[PcCl_{16}]\}_2^+$ D_{4d}

Bonding energy -57.84417035 a.u.
-1574.01996205 eV

Atom	X	Y	Z (Angstrom)
1.N	1.853977	.767942	-2.327777
2.N	-.767942	1.853977	-2.327777
3.N	-1.853977	-.767942	-2.327777
4.N	.767942	-1.853977	-2.327777
5.C	2.147473	2.098928	-2.166174
6.C	3.002659	.034326	-2.166174
7.C	3.606309	2.259109	-2.000479
8.C	4.147477	.952614	-2.000479
9.C	4.443065	3.376711	-1.916103
10.C	5.529416	.754026	-1.916103
11.C	5.837761	3.179960	-1.857105
12.C	6.376492	1.879349	-1.857105
13.CL	3.828886	4.992640	-1.925078
14.CL	6.237761	-.822898	-1.925078

15.CL	6.904459	4.548935	-1.803798
16.CL	8.098773	1.665607	-1.803798
17.C	-2.098928	2.147473	-2.166174
18.C	-.034326	3.002659	-2.166174
19.C	-2.259109	3.606309	-2.000479
20.C	-.952614	4.147477	-2.000479
21.C	-3.376711	4.443065	-1.916103
22.C	-.754026	5.529416	-1.916103
23.C	-3.179960	5.837761	-1.857105
24.C	-1.879349	6.376492	-1.857105
25.CL	-4.992640	3.828886	-1.925078
26.CL	.822898	6.237761	-1.925078
27.CL	-4.548935	6.904459	-1.803798
28.CL	-1.665607	8.098773	-1.803798
29.C	-2.147473	-2.098928	-2.166174
30.C	-3.002659	-.034326	-2.166174
31.C	-3.606309	-2.259109	-2.000479
32.C	-4.147477	-.952614	-2.000479
33.C	-4.443065	-3.376711	-1.916103
34.C	-5.529416	-.754026	-1.916103
35.C	-5.837761	-3.179960	-1.857105
36.C	-6.376492	-1.879349	-1.857105
37.CL	-3.828886	-4.992640	-1.925078
38.CL	-6.237761	.822898	-1.925078
39.CL	-6.904459	-4.548935	-1.803798
40.CL	-8.098773	-1.665607	-1.803798
41.C	2.098928	-2.147473	-2.166174
42.C	.034326	-3.002659	-2.166174
43.C	2.259109	-3.606309	-2.000479
44.C	.952614	-4.147477	-2.000479
45.C	3.376711	-4.443065	-1.916103
46.C	.754026	-5.529416	-1.916103
47.C	3.179960	-5.837761	-1.857105
48.C	1.879349	-6.376492	-1.857105
49.CL	4.992640	-3.828886	-1.925078
50.CL	-.822898	-6.237761	-1.925078
51.CL	4.548935	-6.904459	-1.803798
52.CL	1.665607	-8.098773	-1.803798
53.N	1.292536	3.120459	-2.119459
54.N	-3.120459	1.292536	-2.119459
55.N	-1.292536	-3.120459	-2.119459
56.N	3.120459	-1.292536	-2.119459
57.Lu	.000000	.000000	-3.747085
58.N	.762786	1.841529	-5.153853
59.N	-1.841529	.762786	-5.153853
60.N	-.762786	-1.841529	-5.153853
61.N	1.841529	-.762786	-5.153853
62.C	.034164	2.988159	-5.376464
63.C	2.088790	2.137105	-5.376464
64.C	.941526	4.110914	-5.650862
65.C	2.241096	3.572614	-5.650862
66.C	.719736	5.465753	-5.886154
67.C	3.355941	4.373801	-5.886154
68.C	1.841550	6.279618	-6.094279
69.C	3.138188	5.742533	-6.094279
70.H	-.289979	5.875276	-5.895305
71.H	4.359494	3.949401	-5.895305
72.H	1.707039	7.349293	-6.257245
73.H	3.989676	6.403794	-6.257245

74.C	-2.988159	.034164	-5.376464
75.C	-2.137105	2.088790	-5.376464
76.C	-4.110914	.941526	-5.650862
77.C	-3.572614	2.241096	-5.650862
78.C	-5.465753	.719736	-5.886154
79.C	-4.373801	3.355941	-5.886154
80.C	-6.279618	1.841550	-6.094279
81.C	-5.742533	3.138188	-6.094279
82.H	-5.875276	-.289979	-5.895305
83.H	-3.949401	4.359494	-5.895305
84.H	-7.349293	1.707039	-6.257245
85.H	-6.403794	3.989676	-6.257245
86.C	-.034164	-2.988159	-5.376464
87.C	-2.088790	-2.137105	-5.376464
88.C	-.941526	-4.110914	-5.650862
89.C	-2.241096	-3.572614	-5.650862
90.C	-.719736	-5.465753	-5.886154
91.C	-3.355941	-4.373801	-5.886154
92.C	-1.841550	-6.279618	-6.094279
93.C	-3.138188	-5.742533	-6.094279
94.H	.289979	-5.875276	-5.895305
95.H	-4.359494	-3.949401	-5.895305
96.H	-1.707039	-7.349293	-6.257245
97.H	-3.989676	-6.403794	-6.257245
98.C	2.988159	-.034164	-5.376464
99.C	2.137105	-2.088790	-5.376464
100.C	4.110914	-.941526	-5.650862
101.C	3.572614	-2.241096	-5.650862
102.C	5.465753	-.719736	-5.886154
103.C	4.373801	-3.355941	-5.886154
104.C	6.279618	-1.841550	-6.094279
105.C	5.742533	-3.138188	-6.094279
106.H	5.875276	.289979	-5.895305
107.H	3.949401	-4.359494	-5.895305
108.H	7.349293	-1.707039	-6.257245
109.H	6.403794	-3.989676	-6.257245
110.N	3.121133	1.292816	-5.426134
111.N	-1.292816	3.121133	-5.426134
112.N	-3.121133	-1.292816	-5.426134
113.N	1.292816	-3.121133	-5.426134
114.N	1.853977	-.767942	2.327777
115.N	-.767942	-1.853977	2.327777
116.N	-1.853977	.767942	2.327777
117.N	.767942	1.853977	2.327777
118.C	2.147473	-2.098928	2.166174
119.C	3.002659	-.034326	2.166174
120.C	3.606309	-2.259109	2.000479
121.C	4.147477	-.952614	2.000479
122.C	4.443065	-3.376711	1.916103
123.C	5.529416	-.754026	1.916103
124.C	5.837761	-3.179960	1.857105
125.C	6.376492	-1.879349	1.857105
126.CL	3.828886	-4.992640	1.925078
127.CL	6.237761	.822898	1.925078
128.CL	6.904459	-4.548935	1.803798
129.CL	8.098773	-1.665607	1.803798
130.C	-2.098928	-2.147473	2.166174
131.C	-.034326	-3.002659	2.166174
132.C	-2.259109	-3.606309	2.000479

133.C	-.952614	-4.147477	2.000479
134.C	-3.376711	-4.443065	1.916103
135.C	-.754026	-5.529416	1.916103
136.C	-3.179960	-5.837761	1.857105
137.C	-1.879349	-6.376492	1.857105
138.CL	-4.992640	-3.828886	1.925078
139.CL	.822898	-6.237761	1.925078
140.CL	-4.548935	-6.904459	1.803798
141.CL	-1.665607	-8.098773	1.803798
142.C	-2.147473	2.098928	2.166174
143.C	-3.002659	.034326	2.166174
144.C	-3.606309	2.259109	2.000479
145.C	-4.147477	.952614	2.000479
146.C	-4.443065	3.376711	1.916103
147.C	-5.529416	.754026	1.916103
148.C	-5.837761	3.179960	1.857105
149.C	-6.376492	1.879349	1.857105
150.CL	-3.828886	4.992640	1.925078
151.CL	-6.237761	-.822898	1.925078
152.CL	-6.904459	4.548935	1.803798
153.CL	-8.098773	1.665607	1.803798
154.C	2.098928	2.147473	2.166174
155.C	.034326	3.002659	2.166174
156.C	2.259109	3.606309	2.000479
157.C	.952614	4.147477	2.000479
158.C	3.376711	4.443065	1.916103
159.C	.754026	5.529416	1.916103
160.C	3.179960	5.837761	1.857105
161.C	1.879349	6.376492	1.857105
162.CL	4.992640	3.828886	1.925078
163.CL	-.822898	6.237761	1.925078
164.CL	4.548935	6.904459	1.803798
165.CL	1.665607	8.098773	1.803798
166.N	3.120459	1.292536	2.119459
167.N	1.292536	-3.120459	2.119459
168.N	-3.120459	-1.292536	2.119459
169.N	-1.292536	3.120459	2.119459
170.Lu	.000000	.000000	3.747085
171.N	1.841529	.762786	5.153853
172.N	.762786	-1.841529	5.153853
173.N	-1.841529	-.762786	5.153853
174.N	-.762786	1.841529	5.153853
175.C	2.988159	.034164	5.376464
176.C	2.137105	2.088790	5.376464
177.C	4.110914	.941526	5.650862
178.C	3.572614	2.241096	5.650862
179.C	5.465753	.719736	5.886154
180.C	4.373801	3.355941	5.886154
181.C	6.279618	1.841550	6.094279
182.C	5.742533	3.138188	6.094279
183.H	5.875276	-.289979	5.895305
184.H	3.949401	4.359494	5.895305
185.H	7.349293	1.707039	6.257245
186.H	6.403794	3.989676	6.257245
187.C	.034164	-2.988159	5.376464
188.C	2.088790	-2.137105	5.376464
189.C	.941526	-4.110914	5.650862
190.C	2.241096	-3.572614	5.650862
191.C	.719736	-5.465753	5.886154

192.C	3.355941	-4.373801	5.886154
193.C	1.841550	-6.279618	6.094279
194.C	3.138188	-5.742533	6.094279
195.H	-.289979	-5.875276	5.895305
196.H	4.359494	-3.949401	5.895305
197.H	1.707039	-7.349293	6.257245
198.H	3.989676	-6.403794	6.257245
199.C	-2.988159	-.034164	5.376464
200.C	-2.137105	-2.088790	5.376464
201.C	-4.110914	-.941526	5.650862
202.C	-3.572614	-2.241096	5.650862
203.C	-5.465753	-.719736	5.886154
204.C	-4.373801	-3.355941	5.886154
205.C	-6.279618	-1.841550	6.094279
206.C	-5.742533	-3.138188	6.094279
207.H	-5.875276	.289979	5.895305
208.H	-3.949401	-4.359494	5.895305
209.H	-7.349293	-1.707039	6.257245
210.H	-6.403794	-3.989676	6.257245
211.C	-.034164	2.988159	5.376464
212.C	-2.088790	2.137105	5.376464
213.C	-.941526	4.110914	5.650862
214.C	-2.241096	3.572614	5.650862
215.C	-.719736	5.465753	5.886154
216.C	-3.355941	4.373801	5.886154
217.C	-1.841550	6.279618	6.094279
218.C	-3.138188	5.742533	6.094279
219.H	.289979	5.875276	5.895305
220.H	-4.359494	3.949401	5.895305
221.H	-1.707039	7.349293	6.257245
222.H	-3.989676	6.403794	6.257245
223.N	3.121133	-1.292816	5.426134
224.N	-1.292816	-3.121133	5.426134
225.N	-3.121133	1.292816	5.426134
226.N	1.292816	3.121133	5.426134

$\{PcLu[PcCl_{16}]\}_2$ triplet D_{4d}

Bonding energy -58.06212231 a.u.
-1579.95073650 eV

Atom	X	Y	Z (Angstrom)
1.N	1.855070	.768395	-2.322423
2.N	-.768395	1.855070	-2.322423
3.N	-1.855070	-.768395	-2.322423
4.N	.768395	-1.855070	-2.322423
5.C	2.147284	2.099205	-2.159462
6.C	3.002722	.033997	-2.159462
7.C	3.605905	2.259221	-1.995994
8.C	4.147270	.952249	-1.995994
9.C	4.443819	3.376786	-1.914459
10.C	5.530003	.754506	-1.914459
11.C	5.837103	3.179779	-1.857030
12.C	6.375899	1.879012	-1.857030
13.CL	3.828922	4.993756	-1.925976
14.CL	6.238575	-.823662	-1.925976
15.CL	6.906138	4.550625	-1.805534
16.CL	8.101155	1.665599	-1.805534

17.C	-2.099205	2.147284	-2.159462
18.C	-.033997	3.002722	-2.159462
19.C	-2.259221	3.605905	-1.995994
20.C	-.952249	4.147270	-1.995994
21.C	-3.376786	4.443819	-1.914459
22.C	-.754506	5.530003	-1.914459
23.C	-3.179779	5.837103	-1.857030
24.C	-1.879012	6.375899	-1.857030
25.CL	-4.993756	3.828922	-1.925976
26.CL	.823662	6.238575	-1.925976
27.CL	-4.550625	6.906138	-1.805534
28.CL	-1.665599	8.101155	-1.805534
29.C	-2.147284	-2.099205	-2.159462
30.C	-3.002722	-.033997	-2.159462
31.C	-3.605905	-2.259221	-1.995994
32.C	-4.147270	-.952249	-1.995994
33.C	-4.443819	-3.376786	-1.914459
34.C	-5.530003	-.754506	-1.914459
35.C	-5.837103	-3.179779	-1.857030
36.C	-6.375899	-1.879012	-1.857030
37.CL	-3.828922	-4.993756	-1.925976
38.CL	-6.238575	.823662	-1.925976
39.CL	-6.906138	-4.550625	-1.805534
40.CL	-8.101155	-1.665599	-1.805534
41.C	2.099205	-2.147284	-2.159462
42.C	.033997	-3.002722	-2.159462
43.C	2.259221	-3.605905	-1.995994
44.C	.952249	-4.147270	-1.995994
45.C	3.376786	-4.443819	-1.914459
46.C	.754506	-5.530003	-1.914459
47.C	3.179779	-5.837103	-1.857030
48.C	1.879012	-6.375899	-1.857030
49.CL	4.993756	-3.828922	-1.925976
50.CL	-.823662	-6.238575	-1.925976
51.CL	4.550625	-6.906138	-1.805534
52.CL	1.665599	-8.101155	-1.805534
53.N	1.292602	3.120618	-2.112973
54.N	-3.120618	1.292602	-2.112973
55.N	-1.292602	-3.120618	-2.112973
56.N	3.120618	-1.292602	-2.112973
57.Lu	.000000	.000000	-3.745693
58.N	.763431	1.843087	-5.155602
59.N	-1.843087	.763431	-5.155602
60.N	-.763431	-1.843087	-5.155602
61.N	1.843087	-.763431	-5.155602
62.C	.033924	2.988595	-5.379458
63.C	2.089268	2.137244	-5.379458
64.C	.941095	4.110661	-5.652334
65.C	2.241221	3.572131	-5.652334
66.C	.720465	5.466907	-5.884799
67.C	3.356242	4.375132	-5.884799
68.C	1.841178	6.280277	-6.092144
69.C	3.138917	5.742736	-6.092144
70.H	-.289435	5.876246	-5.890128
71.H	4.359795	3.950472	-5.890128
72.H	1.706678	7.350632	-6.251936
73.H	3.990878	6.404486	-6.251936
74.C	-2.988595	.033924	-5.379458
75.C	-2.137244	2.089268	-5.379458

76.C	-4.110661	.941095	-5.652334
77.C	-3.572131	2.241221	-5.652334
78.C	-5.466907	.720465	-5.884799
79.C	-4.375132	3.356242	-5.884799
80.C	-6.280277	1.841178	-6.092144
81.C	-5.742736	3.138917	-6.092144
82.H	-5.876246	-.289435	-5.890128
83.H	-3.950472	4.359795	-5.890128
84.H	-7.350632	1.706678	-6.251936
85.H	-6.404486	3.990878	-6.251936
86.C	-.033924	-2.988595	-5.379458
87.C	-2.089268	-2.137244	-5.379458
88.C	-.941095	-4.110661	-5.652334
89.C	-2.241221	-3.572131	-5.652334
90.C	-.720465	-5.466907	-5.884799
91.C	-3.356242	-4.375132	-5.884799
92.C	-1.841178	-6.280277	-6.092144
93.C	-3.138917	-5.742736	-6.092144
94.H	.289435	-5.876246	-5.890128
95.H	-4.359795	-3.950472	-5.890128
96.H	-1.706678	-7.350632	-6.251936
97.H	-3.990878	-6.404486	-6.251936
98.C	2.988595	-.033924	-5.379458
99.C	2.137244	-2.089268	-5.379458
100.C	4.110661	-.941095	-5.652334
101.C	3.572131	-2.241221	-5.652334
102.C	5.466907	-.720465	-5.884799
103.C	4.375132	-3.356242	-5.884799
104.C	6.280277	-1.841178	-6.092144
105.C	5.742736	-3.138917	-6.092144
106.H	5.876246	.289435	-5.890128
107.H	3.950472	-4.359795	-5.890128
108.H	7.350632	-1.706678	-6.251936
109.H	6.404486	-3.990878	-6.251936
110.N	3.121160	1.292827	-5.431038
111.N	-1.292827	3.121160	-5.431038
112.N	-3.121160	-1.292827	-5.431038
113.N	1.292827	-3.121160	-5.431038
114.N	1.855070	-.768395	2.322423
115.N	-.768395	-1.855070	2.322423
116.N	-1.855070	.768395	2.322423
117.N	.768395	1.855070	2.322423
118.C	2.147284	-2.099205	2.159462
119.C	3.002722	-.033997	2.159462
120.C	3.605905	-2.259221	1.995994
121.C	4.147270	-.952249	1.995994
122.C	4.443819	-3.376786	1.914459
123.C	5.530003	-.754506	1.914459
124.C	5.837103	-3.179779	1.857030
125.C	6.375899	-1.879012	1.857030
126.CL	3.828922	-4.993756	1.925976
127.CL	6.238575	.823662	1.925976
128.CL	6.906138	-4.550625	1.805534
129.CL	8.101155	-1.665599	1.805534
130.C	-2.099205	-2.147284	2.159462
131.C	-.033997	-3.002722	2.159462
132.C	-2.259221	-3.605905	1.995994
133.C	-.952249	-4.147270	1.995994
134.C	-3.376786	-4.443819	1.914459

135.C	-.754506	-5.530003	1.914459
136.C	-3.179779	-5.837103	1.857030
137.C	-1.879012	-6.375899	1.857030
138.CL	-4.993756	-3.828922	1.925976
139.CL	.823662	-6.238575	1.925976
140.CL	-4.550625	-6.906138	1.805534
141.CL	-1.665599	-8.101155	1.805534
142.C	-2.147284	2.099205	2.159462
143.C	-3.002722	.033997	2.159462
144.C	-3.605905	2.259221	1.995994
145.C	-4.147270	.952249	1.995994
146.C	-4.443819	3.376786	1.914459
147.C	-5.530003	.754506	1.914459
148.C	-5.837103	3.179779	1.857030
149.C	-6.375899	1.879012	1.857030
150.CL	-3.828922	4.993756	1.925976
151.CL	-6.238575	-.823662	1.925976
152.CL	-6.906138	4.550625	1.805534
153.CL	-8.101155	1.665599	1.805534
154.C	2.099205	2.147284	2.159462
155.C	.033997	3.002722	2.159462
156.C	2.259221	3.605905	1.995994
157.C	.952249	4.147270	1.995994
158.C	3.376786	4.443819	1.914459
159.C	.754506	5.530003	1.914459
160.C	3.179779	5.837103	1.857030
161.C	1.879012	6.375899	1.857030
162.CL	4.993756	3.828922	1.925976
163.CL	-.823662	6.238575	1.925976
164.CL	4.550625	6.906138	1.805534
165.CL	1.665599	8.101155	1.805534
166.N	3.120618	1.292602	2.112973
167.N	1.292602	-3.120618	2.112973
168.N	-3.120618	-1.292602	2.112973
169.N	-1.292602	3.120618	2.112973
170.Lu	.000000	.000000	3.745693
171.N	1.843087	.763431	5.155602
172.N	.763431	-1.843087	5.155602
173.N	-1.843087	-.763431	5.155602
174.N	-.763431	1.843087	5.155602
175.C	2.988595	.033924	5.379458
176.C	2.137244	2.089268	5.379458
177.C	4.110661	.941095	5.652334
178.C	3.572131	2.241221	5.652334
179.C	5.466907	.720465	5.884799
180.C	4.375132	3.356242	5.884799
181.C	6.280277	1.841178	6.092144
182.C	5.742736	3.138917	6.092144
183.H	5.876246	-.289435	5.890128
184.H	3.950472	4.359795	5.890128
185.H	7.350632	1.706678	6.251936
186.H	6.404486	3.990878	6.251936
187.C	.033924	-2.988595	5.379458
188.C	2.089268	-2.137244	5.379458
189.C	.941095	-4.110661	5.652334
190.C	2.241221	-3.572131	5.652334
191.C	.720465	-5.466907	5.884799
192.C	3.356242	-4.375132	5.884799
193.C	1.841178	-6.280277	6.092144

194.C	3.138917	-5.742736	6.092144
195.H	-.289435	-5.876246	5.890128
196.H	4.359795	-3.950472	5.890128
197.H	1.706678	-7.350632	6.251936
198.H	3.990878	-6.404486	6.251936
199.C	-2.988595	-.033924	5.379458
200.C	-2.137244	-2.089268	5.379458
201.C	-4.110661	-.941095	5.652334
202.C	-3.572131	-2.241221	5.652334
203.C	-5.466907	-.720465	5.884799
204.C	-4.375132	-3.356242	5.884799
205.C	-6.280277	-1.841178	6.092144
206.C	-5.742736	-3.138917	6.092144
207.H	-5.876246	.289435	5.890128
208.H	-3.950472	-4.359795	5.890128
209.H	-7.350632	-1.706678	6.251936
210.H	-6.404486	-3.990878	6.251936
211.C	-.033924	2.988595	5.379458
212.C	-2.089268	2.137244	5.379458
213.C	-.941095	4.110661	5.652334
214.C	-2.241221	3.572131	5.652334
215.C	-.720465	5.466907	5.884799
216.C	-3.356242	4.375132	5.884799
217.C	-1.841178	6.280277	6.092144
218.C	-3.138917	5.742736	6.092144
219.H	.289435	5.876246	5.890128
220.H	-4.359795	3.950472	5.890128
221.H	-1.706678	7.350632	6.251936
222.H	-3.990878	6.404486	6.251936
223.N	3.121160	-1.292827	5.431038
224.N	-1.292827	-3.121160	5.431038
225.N	-3.121160	1.292827	5.431038
226.N	1.292827	3.121160	5.431038

$\{PcLu[PcCl_{16}]\}_2$ singlet D_{4d}

Bonding energy -58.05973946 a.u.
-1579.88589594 eV

Atom	X	Y	Z (Angstrom)
1.N	1.854749	.768262	-2.319587
2.N	-.768262	1.854749	-2.319587
3.N	-1.854749	-.768262	-2.319587
4.N	.768262	-1.854749	-2.319587
5.C	2.147062	2.098962	-2.156653
6.C	3.002392	.034012	-2.156653
7.C	3.605918	2.259213	-1.994169
8.C	4.147274	.952264	-1.994169
9.C	4.443747	3.376757	-1.913980
10.C	5.529932	.754476	-1.913980
11.C	5.836813	3.179547	-1.857282
12.C	6.375529	1.878971	-1.857282
13.CL	3.828860	4.993642	-1.926127
14.CL	6.238451	-.823625	-1.926127
15.CL	6.905925	4.550401	-1.806001
16.CL	8.100846	1.665607	-1.806001
17.C	-2.098962	2.147062	-2.156653

18.C	-.034012	3.002392	-2.156653
19.C	-2.259213	3.605918	-1.994169
20.C	-.952264	4.147274	-1.994169
21.C	-3.376757	4.443747	-1.913980
22.C	-.754476	5.529932	-1.913980
23.C	-3.179547	5.836813	-1.857282
24.C	-1.878971	6.375529	-1.857282
25.CL	-4.993642	3.828860	-1.926127
26.CL	.823625	6.238451	-1.926127
27.CL	-4.550401	6.905925	-1.806001
28.CL	-1.665607	8.100846	-1.806001
29.C	-2.147062	-2.098962	-2.156653
30.C	-3.002392	-.034012	-2.156653
31.C	-3.605918	-2.259213	-1.994169
32.C	-4.147274	-.952264	-1.994169
33.C	-4.443747	-3.376757	-1.913980
34.C	-5.529932	-.754476	-1.913980
35.C	-5.836813	-3.179547	-1.857282
36.C	-6.375529	-1.878971	-1.857282
37.CL	-3.828860	-4.993642	-1.926127
38.CL	-6.238451	.823625	-1.926127
39.CL	-6.905925	-4.550401	-1.806001
40.CL	-8.100846	-1.665607	-1.806001
41.C	2.098962	-2.147062	-2.156653
42.C	.034012	-3.002392	-2.156653
43.C	2.259213	-3.605918	-1.994169
44.C	.952264	-4.147274	-1.994169
45.C	3.376757	-4.443747	-1.913980
46.C	.754476	-5.529932	-1.913980
47.C	3.179547	-5.836813	-1.857282
48.C	1.878971	-6.375529	-1.857282
49.CL	4.993642	-3.828860	-1.926127
50.CL	-.823625	-6.238451	-1.926127
51.CL	4.550401	-6.905925	-1.806001
52.CL	1.665607	-8.100846	-1.806001
53.N	1.292466	3.120289	-2.110120
54.N	-3.120289	1.292466	-2.110120
55.N	-1.292466	-3.120289	-2.110120
56.N	3.120289	-1.292466	-2.110120
57.Lu	.000000	.000000	-3.744097
58.N	.763493	1.843235	-5.153623
59.N	-1.843235	.763493	-5.153623
60.N	-.763493	-1.843235	-5.153623
61.N	1.843235	-.763493	-5.153623
62.C	.033885	2.988801	-5.377275
63.C	2.089441	2.137362	-5.377275
64.C	.941007	4.110638	-5.650273
65.C	2.241268	3.572053	-5.650273
66.C	.720560	5.467101	-5.882482
67.C	3.356311	4.375337	-5.882482
68.C	1.841241	6.280551	-6.089232
69.C	3.139066	5.742974	-6.089232
70.H	-.289371	5.876515	-5.887926
71.H	4.359940	3.950708	-5.887926
72.H	1.706769	7.351034	-6.248503
73.H	3.991098	6.404834	-6.248503
74.C	-2.988801	.033885	-5.377275
75.C	-2.137362	2.089441	-5.377275
76.C	-4.110638	.941007	-5.650273

77.C	-3.572053	2.241268	-5.650273
78.C	-5.467101	.720560	-5.882482
79.C	-4.375337	3.356311	-5.882482
80.C	-6.280551	1.841241	-6.089232
81.C	-5.742974	3.139066	-6.089232
82.H	-5.876515	-.289371	-5.887926
83.H	-3.950708	4.359940	-5.887926
84.H	-7.351034	1.706769	-6.248503
85.H	-6.404834	3.991098	-6.248503
86.C	-.033885	-2.988801	-5.377275
87.C	-2.089441	-2.137362	-5.377275
88.C	-.941007	-4.110638	-5.650273
89.C	-2.241268	-3.572053	-5.650273
90.C	-.720560	-5.467101	-5.882482
91.C	-3.356311	-4.375337	-5.882482
92.C	-1.841241	-6.280551	-6.089232
93.C	-3.139066	-5.742974	-6.089232
94.H	.289371	-5.876515	-5.887926
95.H	-4.359940	-3.950708	-5.887926
96.H	-1.706769	-7.351034	-6.248503
97.H	-3.991098	-6.404834	-6.248503
98.C	2.988801	-.033885	-5.377275
99.C	2.137362	-2.089441	-5.377275
100.C	4.110638	-.941007	-5.650273
101.C	3.572053	-2.241268	-5.650273
102.C	5.467101	-.720560	-5.882482
103.C	4.375337	-3.356311	-5.882482
104.C	6.280551	-1.841241	-6.089232
105.C	5.742974	-3.139066	-6.089232
106.H	5.876515	.289371	-5.887926
107.H	3.950708	-4.359940	-5.887926
108.H	7.351034	-1.706769	-6.248503
109.H	6.404834	-3.991098	-6.248503
110.N	3.121347	1.292904	-5.428753
111.N	-1.292904	3.121347	-5.428753
112.N	-3.121347	-1.292904	-5.428753
113.N	1.292904	-3.121347	-5.428753
114.N	1.854749	-.768262	2.319587
115.N	-.768262	-1.854749	2.319587
116.N	-1.854749	.768262	2.319587
117.N	.768262	1.854749	2.319587
118.C	2.147062	-2.098962	2.156653
119.C	3.002392	-.034012	2.156653
120.C	3.605918	-2.259213	1.994169
121.C	4.147274	-.952264	1.994169
122.C	4.443747	-3.376757	1.913980
123.C	5.529932	-.754476	1.913980
124.C	5.836813	-3.179547	1.857282
125.C	6.375529	-1.878971	1.857282
126.CL	3.828860	-4.993642	1.926127
127.CL	6.238451	.823625	1.926127
128.CL	6.905925	-4.550401	1.806001
129.CL	8.100846	-1.665607	1.806001
130.C	-2.098962	-2.147062	2.156653
131.C	-.034012	-3.002392	2.156653
132.C	-2.259213	-3.605918	1.994169
133.C	-.952264	-4.147274	1.994169
134.C	-3.376757	-4.443747	1.913980
135.C	-.754476	-5.529932	1.913980

136.C	-3.179547	-5.836813	1.857282
137.C	-1.878971	-6.375529	1.857282
138.CL	-4.993642	-3.828860	1.926127
139.CL	.823625	-6.238451	1.926127
140.CL	-4.550401	-6.905925	1.806001
141.CL	-1.665607	-8.100846	1.806001
142.C	-2.147062	2.098962	2.156653
143.C	-3.002392	.034012	2.156653
144.C	-3.605918	2.259213	1.994169
145.C	-4.147274	.952264	1.994169
146.C	-4.443747	3.376757	1.913980
147.C	-5.529932	.754476	1.913980
148.C	-5.836813	3.179547	1.857282
149.C	-6.375529	1.878971	1.857282
150.CL	-3.828860	4.993642	1.926127
151.CL	-6.238451	-.823625	1.926127
152.CL	-6.905925	4.550401	1.806001
153.CL	-8.100846	1.665607	1.806001
154.C	2.098962	2.147062	2.156653
155.C	.034012	3.002392	2.156653
156.C	2.259213	3.605918	1.994169
157.C	.952264	4.147274	1.994169
158.C	3.376757	4.443747	1.913980
159.C	.754476	5.529932	1.913980
160.C	3.179547	5.836813	1.857282
161.C	1.878971	6.375529	1.857282
162.CL	4.993642	3.828860	1.926127
163.CL	-.823625	6.238451	1.926127
164.CL	4.550401	6.905925	1.806001
165.CL	1.665607	8.100846	1.806001
166.N	3.120289	1.292466	2.110120
167.N	1.292466	-3.120289	2.110120
168.N	-3.120289	-1.292466	2.110120
169.N	-1.292466	3.120289	2.110120
170.Lu	.000000	.000000	3.744097
171.N	1.843235	.763493	5.153623
172.N	.763493	-1.843235	5.153623
173.N	-1.843235	-.763493	5.153623
174.N	-.763493	1.843235	5.153623
175.C	2.988801	.033885	5.377275
176.C	2.137362	2.089441	5.377275
177.C	4.110638	.941007	5.650273
178.C	3.572053	2.241268	5.650273
179.C	5.467101	.720560	5.882482
180.C	4.375337	3.356311	5.882482
181.C	6.280551	1.841241	6.089232
182.C	5.742974	3.139066	6.089232
183.H	5.876515	-.289371	5.887926
184.H	3.950708	4.359940	5.887926
185.H	7.351034	1.706769	6.248503
186.H	6.404834	3.991098	6.248503
187.C	.033885	-2.988801	5.377275
188.C	2.089441	-2.137362	5.377275
189.C	.941007	-4.110638	5.650273
190.C	2.241268	-3.572053	5.650273
191.C	.720560	-5.467101	5.882482
192.C	3.356311	-4.375337	5.882482
193.C	1.841241	-6.280551	6.089232
194.C	3.139066	-5.742974	6.089232

195.H	-.289371	-5.876515	5.887926
196.H	4.359940	-3.950708	5.887926
197.H	1.706769	-7.351034	6.248503
198.H	3.991098	-6.404834	6.248503
199.C	-2.988801	-.033885	5.377275
200.C	-2.137362	-2.089441	5.377275
201.C	-4.110638	-.941007	5.650273
202.C	-3.572053	-2.241268	5.650273
203.C	-5.467101	-.720560	5.882482
204.C	-4.375337	-3.356311	5.882482
205.C	-6.280551	-1.841241	6.089232
206.C	-5.742974	-3.139066	6.089232
207.H	-5.876515	.289371	5.887926
208.H	-3.950708	-4.359940	5.887926
209.H	-7.351034	-1.706769	6.248503
210.H	-6.404834	-3.991098	6.248503
211.C	-.033885	2.988801	5.377275
212.C	-2.089441	2.137362	5.377275
213.C	-.941007	4.110638	5.650273
214.C	-2.241268	3.572053	5.650273
215.C	-.720560	5.467101	5.882482
216.C	-3.356311	4.375337	5.882482
217.C	-1.841241	6.280551	6.089232
218.C	-3.139066	5.742974	6.089232
219.H	.289371	5.876515	5.887926
220.H	-4.359940	3.950708	5.887926
221.H	-1.706769	7.351034	6.248503
222.H	-3.991098	6.404834	6.248503
223.N	3.121347	-1.292904	5.428753
224.N	-1.292904	-3.121347	5.428753
225.N	-3.121347	1.292904	5.428753
226.N	1.292904	3.121347	5.428753

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Table S2. Distances between the $(N_p)_4$ plane and the planes formed by the various ligand type atoms. Bold values correspond to the substituted Pc^{Cl} ligands.

Type of atoms defining each plane	$[LuPc_2]^q$ C_{4v}			$PcLu[Pc(p\text{-}Cl_8)]^q$ C_{4v}			$PcLu[Pc(np\text{-}Cl_8)]^q$ C_{4v}			$PcLu[PcCl_{16}]^q$ C_{4v}		
	q = +1	q = 0	q = -1	q = +1	q = 0	q = -1	q = +1	q = 0	q = -1	q = +1	q = 0	q = -1
C_α	**0.18** 0.18	**0.18** 0.18	**0.20** 0.20	**0.18** 0.19	**0.18** 0.19	**0.18** 0.19	**0.19** 0.23	**0.20** 0.23	**0.21** 0.25	**0.18** 0.21	**0.19** 0.24	**0.20** 0.24
C_β	**0.38** 0.39	**0.36** 0.37	**0.40** 0.40	**0.37** 0.40	**0.35** 0.39	**0.35** 0.37	**0.41** 0.52	**0.42** 0.52	**0.46** 0.56	**0.36** 0.48	**0.40** 0.55	**0.41** 0.54
C_γ	**0.52** 0.54	**0.46** 0.48	**0.51** 0.54	**0.47** 0.54	**0.43** 0.51	**0.42** 0.47	**0.58** 0.77	**0.59** 0.77	**0.64** 0.84	**0.47** 0.69	**0.54** 0.82	**0.55** 0.81
C_μ	**0.63** 0.66	**0.54** 0.56	**0.61** 0.65	**0.55** 0.65	**0.48** 0.59	**0.45** 0.53	**0.74** 1.01	**0.73** 0.99	**0.80** 1.09	**0.53** 0.88	**0.66** 1.07	**0.67** 1.05
X_γ	**0.52** 0.55	**0.46** 0.48	**0.50** 0.53	**0.48** 0.55	**0.42** 0.51	**0.40** 0.46	**0.60** 0.79	**0.59** 0.78	**0.63** 0.84	**0.51** 0.70	**0.54** 0.83	**0.54** 0.81
X_μ	**0.71** 0.75	**0.59** 0.62	**0.68** 0.73	**0.62** 0.74	**0.51** 0.65	**0.46** 0.57	**0.86** 1.19	**0.85** 1.17	**0.93** 1.28	**0.60** 1.02	**0.79** 1.26	**0.79** 1.23
N_m	**0.23** 0.23	**0.23** 0.23	**0.25** 0.25	**0.23** 0.24	**0.23** 0.24	**0.24** 0.24	**0.25** 0.28	**0.26** 0.29	**0.28** 0.31	**0.23** 0.27	**0.25** 0.30	**0.26** 0.30