On the use of localized orbitals for the bonding analysis of organometallic compounds

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Supporting Information

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1. Supporting Figures

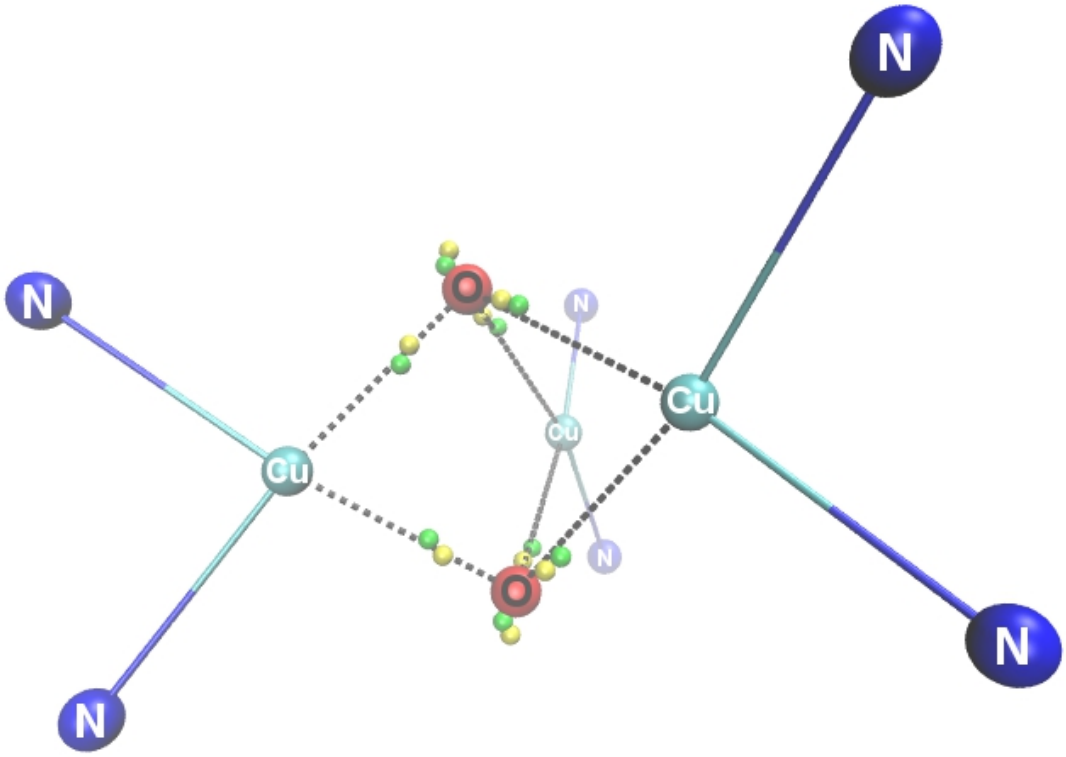

Figure S1. $(TMEDA)_3Cu_3O_2^{3+}$ complex. Only core atoms and the centroids of the localized orbitals are shown for the sake of clarity (each centroid accounts for one electron, spin-up and –down in green and yellow, respectively; some centroids are hidden below the atom's spheres, in particular those of Cu) .

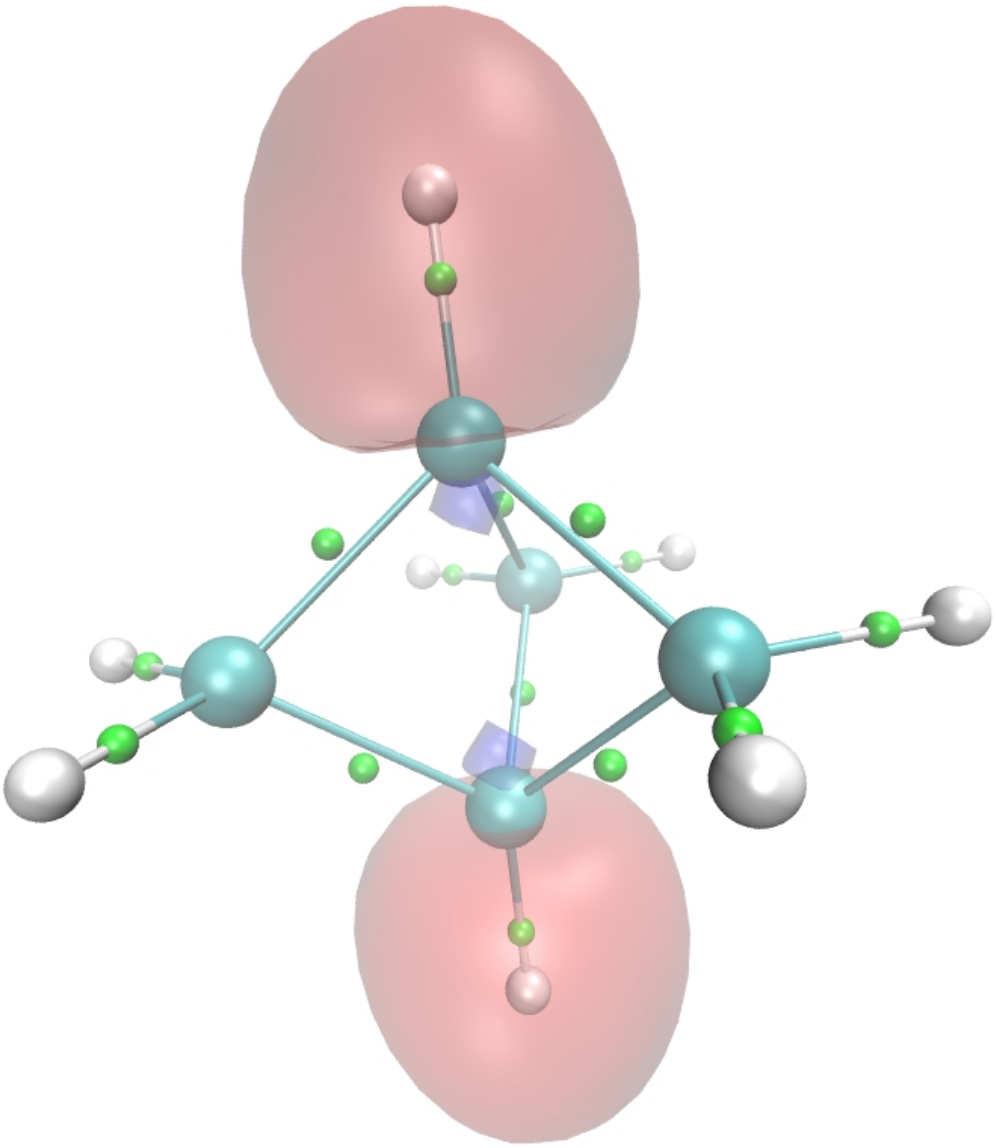

Figure S2. bicyclo[1.1.1]pentane. Centroids of the localized orbitals are shown as small green dots (each centroid accounts for two electrons). The isosurfaces of the localized orbitals corresponding to the two C – H bonds at the bridgehead C atoms are also shown.

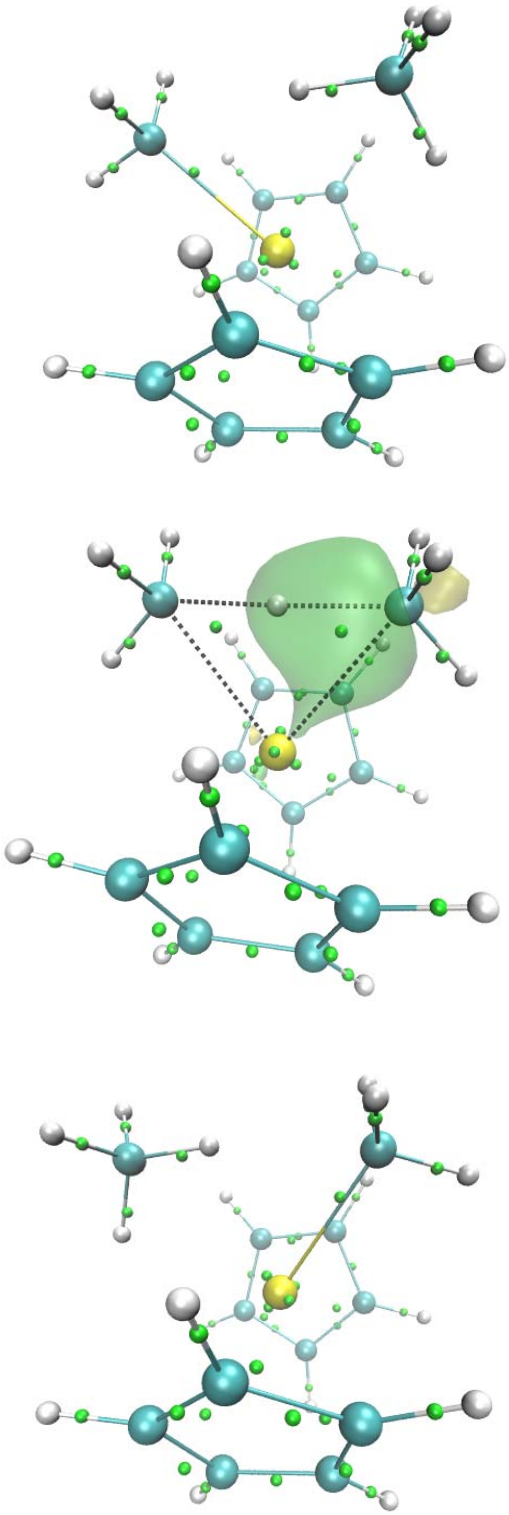

Figure S3. $Cp_2Sc(CH_4)(CH_3)$. Reactants (top panel), transition state (middle) and products (bottom) structures. The centroids of the localized orbitals are shown as small green dots. In the middle panel the dotted lines highlight braking and forming bonds. An isosurface of a relevant localized orbital is also shown.

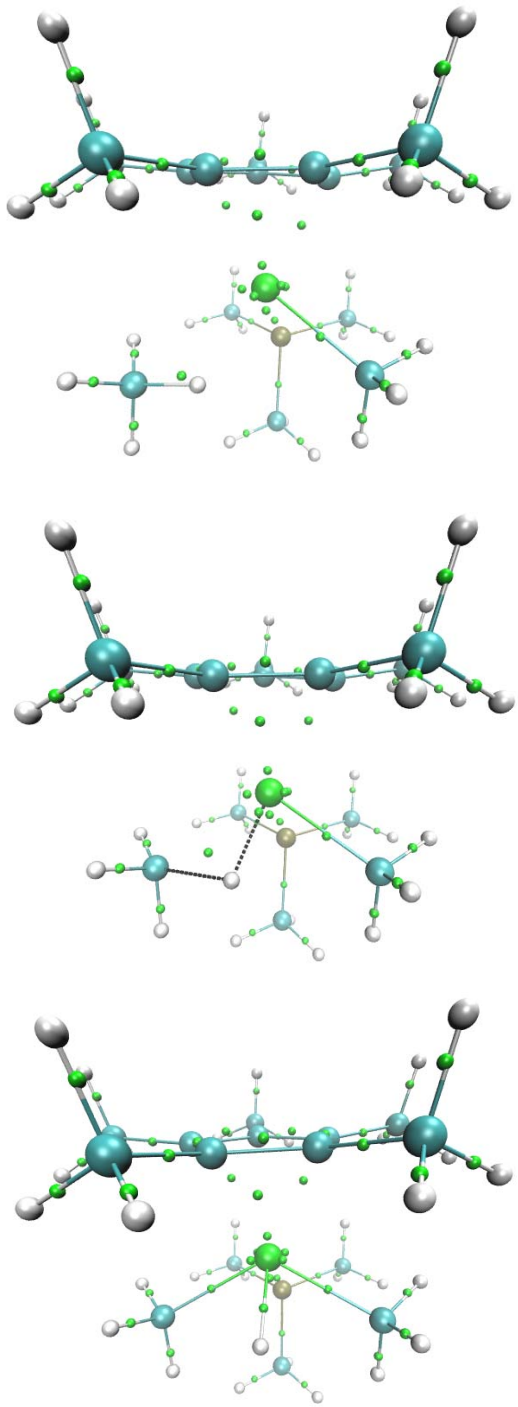

Figure S4. $Cp^*Ir(PMe_3)(CH_4)(CH_3)^+$. Reactants (top panel), transition state (middle) and products (bottom) structures. The centroids of the localized orbitals are shown as small green dots. In the middle panel the dotted lines highlight braking and forming bonds.

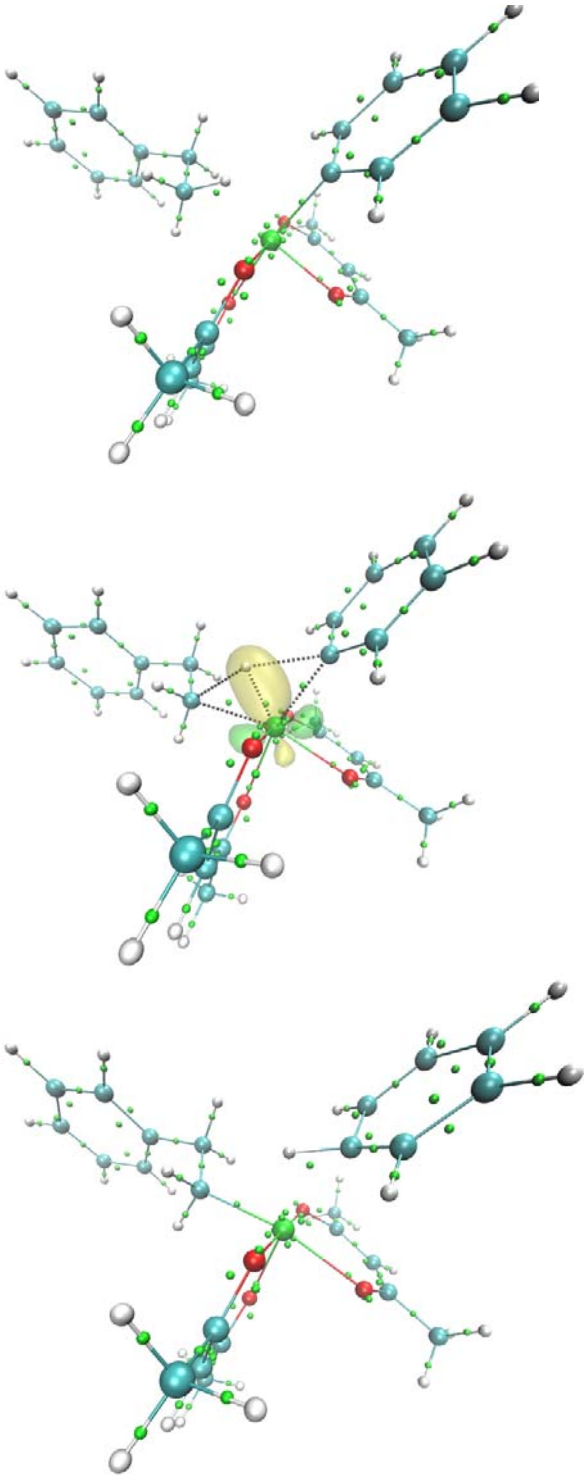

Figure S5. $(acac)_2Ir(CH_2CH_2Ph)(C_6H_6)$. Reactants (top panel), transition state (middle) and products (bottom) structures. The centroids of the localized orbitals are shown as small green dots. In the middle panel the dotted lines highlight braking and forming bonds. An isosurface of a relevant localized orbital is also shown.

2. A further example: Pd^{IV} vs Pd^{II} complexes.

The procedure proposed by Sit *et al*. to assign oxidation states was applied to complexes (bpy)$Pd(Cl)_2(CF_3)_2$ (**1**) and (bpy)$Pd(Cl)_2(CH_3)_2$ (**2**) (bpy = 2,2'-bipyridine). We used Bader's Atoms in Molecules theory to reveal which orbitals have Pd character (listed in Table S1). As may be appreciated, for each complex we have 7 orbitals localized on Pd. These are the semicore s and p and the non-bonding t2g d orbitals. Now we have to decide how to assign the electrons of each Pd – X bond. Sit *et al*. proposed to look at the position of the Wannier center and the shape of the orbital. In both complexes, the centers of Pd – Cl and Pd – N orbitals are displaced towards Cl / N and the electrons are thus assigned to Cl / N. On the contrary, in both complexes, the centers of the Pd – C orbitals are placed midway from Pd and C. However, visual inspection of the Pd – C orbitals reveals that they appear very similar in shape to the Pd – Cl orbitals (see Figure S6) and thus the electrons belong to C. This choice leads to assign oxidation state IV to Pd in both **1** and **2**.

Table S1. For complexes 1 and 2, the orbital number (wf#) and its population on Pd are given. A further label indicates which other atom shares the orbital.

-- 1 –		**-- 2 –**	
wf#	popul.	wf#	popul
1	1.93	1	1.92
2	1.94	2	1.94
3	1.94	3	1.95
4	1.93	4	1.94
51	0.35 (N)	35	0.32 (N)
53	0.26 (N)	37	0.21 (N)
56	1.94	40	0.31 (Cl)
60	0.88 (C)	43	1.03 (C)
61	1.94	44	1.93
62	1.94	46	1.09 (C)
63	0.57 (Cl)	47	1.93
64	0.94 (C)	48	0.51 (Cl)
66	0.40 (Cl)	50	1.94

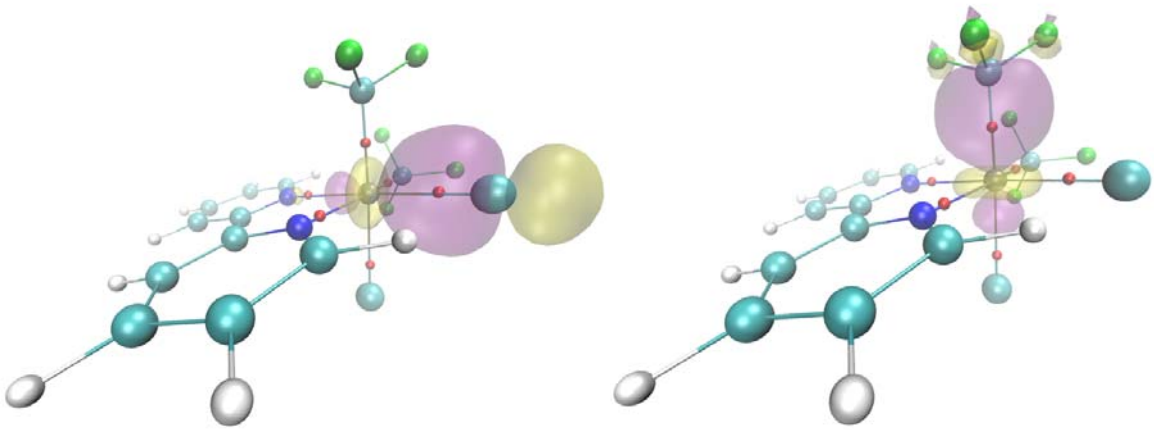

Figure S6. Complex 1 in ball and stick and isosurface of orbital #63 (Pd – Cl , left) or #60 (Pd – C, right). The red dots mark the position of the Wannier centers of all Pd – X bonds.

Results have been compared to those computed for the square planar (bpy)Pd(Cl)(CX_3) (X=F,H) i.e. we removed the axial ligands from complexes 1 and 2. From the table below it may be appreciated that now there are 8 orbitals localized on Pd (the semicore s and p, and 4 d orbitals corresponding to a d^8 configuration). The shape of the Wannier functions of the Pd – C bonds are similar to complexes 1 and 2, but now the Wannier centers are displaced towards the C. Electron counting gives Pd^{II}.

Table S2. For complexes (bpy)Pd(Cl)(CX_3) (X=F,H), the orbital number (wf#) and its population on Pd are given. A further label indicates which other atom shares the orbital.

-- (bpy)Pd(Cl)(CF_3) --		-- (bpy)Pd(Cl)(CH_3) --	
wf#	popul.	wf#	popul
1	1.96	1	1.96
2	1.94	2	1.88
3	1.94	3	1.94
4	1.96	4	1.94
38	0.30 (N)	30	0.31 (N)
39	0.26 (N)	33	0.23 (N)
46	0.45 (Cl)	37	0.40 (Cl)
47	0.78 (C)	39	0.94 (C)
49	1.94	41	1.95
50	1.90	42	1.96
51	1.94	44	1.94
53	1.90	45	1.87

Of interest, we report the Pd atomic charges computed according to Bader's,[1] Mulliken's[2] and Lowdin's[3] population analysis. As may be appreciated from Table S3, neither methods based on population analysis schemes[4, 5] nor methods based on the partitioning of the electron density[6] reproduce integer variations which are expected from a change in the metal oxidation state (actually, this observation was interpreted as a compensation mechanism in the metal-ligand orbital mixing[6]). Furthermore, variations in the metal charge are dependent on the ligands involved.[4]

Table S3. Pd atomic charge (a.u.).

Complex\Charge	**Barder**	**Mulliken**	**Lowdin**
1	0.72	-0.04	-0.88
2	0.69	0.14	-0.69
(bpy)Pd(Cl)(CF_3)	0.48	0.07	-0.46
(bpy)Pd(Cl)(CH_3)	0.43	0.12	-0.37

References

[1] R. F. W. Bader, *Acc. Chem. Res.* **1985**, *18*, 9-15.
[2] R. S. Mulliken, *J. Chem. Phys.* **1955**, *23*, 1833-1840.
[3] P. O. Lowdin, *Physical Review* **1955**, *97*, 1474-1489.
[4] G. Aullon and S. Alvarez, *Theor. Chem. Acc.* **2009**, *123*, 67-73.
[5] P. H. L. Sit, R. Car, M. H. Cohen and A. Selloni, *Inorg. Chem.* **2011**, *50*, 10259-10267.
[6] H. Raebiger, S. Lany and A. Zunger, *Nature* **2008**, *453*, 763-766.

3. Computation of localized orbitals in gaussian09[1]

The multi-step job shown below (using here Cl_2 as a test case) provides Boys localized orbitals in the .chk file. This file has to be processed in order to extract the orbital centroids. Using the bash scripting environment under linux and the g09 utilities formchk, cubegen and cubman, the analysis would proceed as follows (cl2.chk is the .chk file from the g09 calculation, and 7 is the number of valence orbitals in Cl_2).

1. Format the .chk file using formchk:

```
formchk cl2.chk cl2.fchk
```

2. Generate .cube files for each localized orbital using cubegen (these may be visualized by some visualization software):

```
for i in `seq 1 7`; do echo $i; cubegen 0 MO=$i cl2.fchk $i.cube 0 h; done
```

3. Compute the orbital density using the cubman utility:

```
for i in `seq 1 7`; do printf '%s\n' SQ $i.cube y $i\squared.cube y | cubman; done
```

4. Use the cubman utility to compute the orbital centroids (DipAE in the output):

```
for i in `seq 1 7`; do printf '%s\n' P $i\squared.cube y | cubman; done |grep "DipAE=" | awk '{print "X  ", -$2*0.529177, -$3*0.529177, -$4*0.529177}'
```

INPUT file:

```
%Chk=cl2
#p pbepbe SDDAll Symmetry=None NoSymm

scf

0 1
Cl   0. 0. 0.
Cl   0. 0. 2.2026

--Link1--
%Chk=cl2
#p pbepbe SDDAll Geom=Check Guess(NoSymm,Read,Local,Save,Only) Pop=Full
Symmetry=None NoSymm

localization

0 1
```

As a second example, we provide the localized orbitals of $PdCl_4^{2-}$ computed with Gaussian 09 according the Pipek-Mezey criterion. This option is set up adding

"IOp(4/9=20212)"

to the job specification (the first "2" is the one that indicates that the population method be used). The Boys and Pipek-Mezey[2] criteria provide similar localized orbitals (see Figure S6). The main difference is that the Pipek-Mezey scheme maintains the σ-π separation (not shown). Both localization criteria indicate a Pd^{II} oxidation state for $PdCl_4^{2-}$ (Table S1).

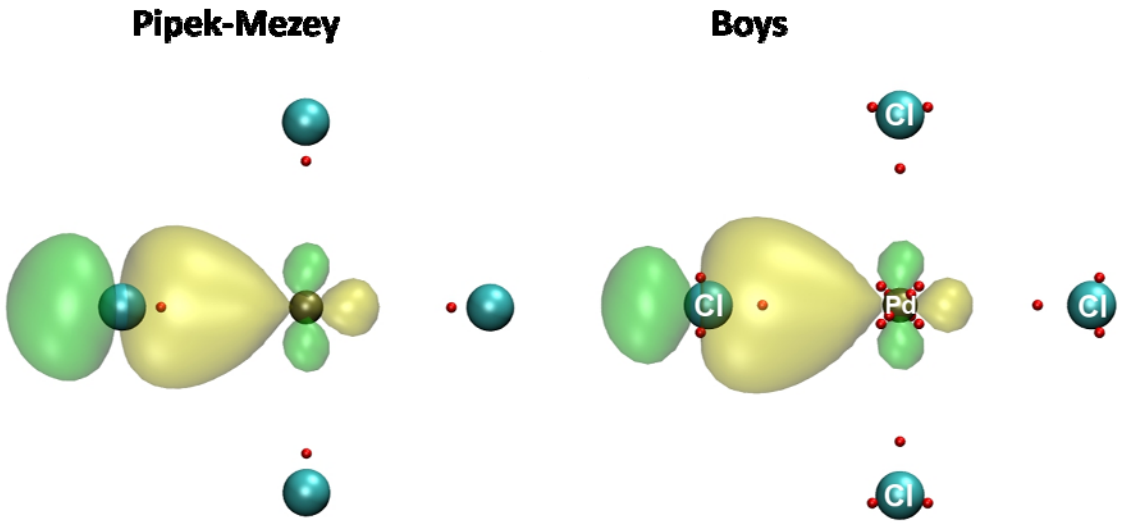

Figure S7. Localized orbital centroids (red dots) and Pd – Cl bond orbital in $PdCl_4^{2-}$ according to the Pipek-Mezey (left panel) and Boys (right) localization criteria. Some centroids are hidden below the atom's spheres, especially in the Pipek-Mezey scheme.

Table S4. Orbital electron population[a] of Pd in $PdCl_4^{2-}$ in the Pipek-Mezey and Boys localised orbital representations.

Orbital	Pipek-Mezey	Boys	Orbital	Pipek-Mezey	Boys
1	1.99	1.97	**13**	0.36	0.37
2	2.00	1.98	**14**	0.02	0.02
3	2.00	1.97	**15**	0.02	0.02
4	2.00	1.98	**16**	0.02	0.02
5	0.00	0.02	**17**	0.02	1.97
6	0.00	0.02	**18**	0.01	0.02
7	0.00	0.02	**19**	0.01	0.02
8	0.00	0.02	**20**	0.01	0.02
9	0.36	0.37	**21**	1.92	1.97
10	0.36	0.37	**22**	1.95	1.98
11	0.01	0.37	**23**	1.95	0.02
12	0.36	0.02	**24**	1.97	1.98

[a] Atomic electron populations have been computed integrating the orbital density within the atomic basins determined according to Bader's Atoms in Molecules theory.[1]

[1] Gaussian 09, Revision **A.1**, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

[2] J. Pipek, P.G. Mezey, *J. Chem. Phys.* **1989,** 90, 4916-4926.

3. Cartesian coordinates of atoms and orbital centroids in the complexes analyzed

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$PdCl_4^{2-}$

Pd	7.000000	7.000000	7.000000
Cl	9.660044	7.000000	6.999994
Cl	6.999998	9.660044	7.000001
Cl	4.339957	6.999999	7.000006
Cl	7.000002	4.339957	6.999998
X	6.737244	6.737257	6.884502
X	6.848615	7.151350	6.683567
X	7.262731	7.262742	6.884440
X	6.848724	6.848689	7.316499
X	6.615794	9.767571	7.212596
X	7.384217	4.232420	7.212569
X	9.767591	6.615737	7.212477
X	4.232336	6.616167	7.213249
X	6.999968	5.091239	7.004544
X	8.908767	7.000011	7.004510
X	7.000033	8.908773	7.004534
X	7.383893	9.767670	7.213130
X	5.091227	6.999987	7.004577
X	6.999731	4.247286	6.562600
X	7.000247	9.752731	6.562608
X	4.247313	6.999601	6.562602
X	6.737324	7.262687	7.115609
X	6.616115	4.232324	7.213142
X	9.767632	7.383838	7.213242
X	4.232375	7.384267	7.212462
X	7.262700	6.737310	7.115544
X	7.151347	7.151311	7.316460
X	9.752748	7.000385	6.562604
X	7.151311	6.848652	6.683528

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[Pt(NHC(Dip)$_2$)(SiMe$_2$Ph)$_2$]

Pt	9.999265	10.000624	9.181725
C	9.998808	10.000738	7.083385
C	10.537625	10.413421	4.889725
N	10.846419	10.659241	6.224865
C	11.966558	11.483855	6.599939
C	11.735581	12.827971	6.953031
C	12.861489	13.615239	7.234544
C	14.151114	13.090396	7.146377
C	14.344275	11.756062	6.791109
C	13.253857	10.917911	6.519022
C	10.334256	13.414554	7.047122
C	13.478431	9.446533	6.196558
Si	11.511301	10.312620	10.923900
C	12.340909	8.685810	11.413947
C	12.859334	11.383467	10.121064
C	11.160747	11.295313	12.509548
C	9.921380	13.613657	8.519800
C	10.195215	14.717258	6.235630
C	14.367707	9.264193	4.951186
C	14.049809	8.698746	7.418576
C	10.748409	12.640795	12.419868
C	10.557869	13.427366	13.559006
C	10.787609	12.883386	14.828819
C	11.206989	11.555324	14.942755
C	11.387423	10.772927	13.796055
H	11.111917	10.852116	4.085895
H	12.722296	14.655343	7.522390
H	15.008945	13.723216	7.364549
H	15.352811	11.350645	6.741040
H	9.639678	12.682466	6.616636
H	12.504130	8.996220	5.973715
H	11.706358	8.072790	12.064804
H	12.571472	8.093262	10.518895
H	13.285292	8.889434	11.938890
H	13.276792	10.937012	9.213829
H	12.488989	12.381688	9.861833
H	13.670277	11.504022	10.854398
H	10.607824	14.297787	9.036627
H	9.921650	12.643603	9.049860
H	8.910042	14.037844	8.582472
H	10.483283	14.572991	5.185616
H	10.819455	15.522655	6.645011
H	9.154565	15.068555	6.260160
H	15.374950	9.672264	5.109859
H	13.940335	9.769770	4.074550
H	14.478277	8.198154	4.710042
H	13.362304	8.762251	8.273650
H	15.016550	9.115448	7.730445
H	14.203384	7.637262	7.181062
H	10.564516	13.079486	11.438657
H	10.231753	14.460930	13.459645
H	10.641860	13.490937	15.719794
H	11.385057	11.122564	15.925450
H	11.695427	9.734929	13.909612
C	9.462502	9.582911	4.890011
N	9.152065	9.340645	6.225296
C	8.031891	8.516121	6.600649
C	8.262965	7.171983	6.953013
C	7.136992	6.384341	7.233296
C	5.847249	6.908950	7.144927
C	5.654096	8.243650	6.790834
C	6.744608	9.082042	6.519728
C	9.664525	6.585538	7.047263
C	6.520631	10.553369	6.197278
Si	8.487335	9.686934	10.923886
C	7.658435	11.313630	11.414656
C	7.139010	8.616827	10.120701
C	8.838476	8.703682	12.509024
C	10.077454	6.387016	8.520084
C	9.803267	5.282681	6.236114
C	5.632321	10.735393	4.951218

C	5.949463	11.301764	7.418995
C	9.251594	7.358435	12.419100
C	9.443880	6.572130	13.558113
C	9.215440	7.116208	14.828098
C	8.794425	8.443725	14.942359
C	8.611965	9.225678	13.795681
H	8.888833	9.142799	4.086522
H	7.276087	5.343825	7.519630
H	4.989493	6.275535	7.361789
H	4.645481	8.648934	6.740231
H	10.359110	7.317504	6.616597
H	7.495313	11.003039	5.974849
H	8.293681	11.926593	12.064906
H	7.427447	11.905890	10.519547
H	6.714369	11.110354	11.940321
H	6.720941	9.064345	9.214265
H	7.509360	7.618985	9.860059
H	6.328571	8.495412	10.854433
H	9.391285	5.702758	9.037131
H	10.076821	7.357227	9.049818
H	11.088996	5.963316	8.583009
H	9.514349	5.426747	5.186325
H	9.179407	4.477345	6.646193
H	10.843964	4.931553	6.259950
H	4.625051	10.327062	5.109015
H	6.060822	10.229497	4.075287
H	5.521870	11.801313	4.709586
H	6.637092	11.238311	8.273973
H	4.982536	10.885756	7.731196
H	5.796554	12.363227	7.180949
H	9.435349	6.919926	11.437769
H	9.770792	5.538834	13.458523
H	9.363299	6.509026	15.718971
H	8.617091	8.876503	15.925158
H	8.302967	10.263372	13.909425
X	8.674783	8.734843	15.601992
X	12.490666	8.306948	10.815895
X	6.069352	10.625437	5.580444
X	7.378439	8.599908	6.303909
X	10.722780	12.103991	14.774668
X	13.509591	13.363278	7.196219
X	6.488850	6.636238	7.194960
X	9.808968	10.246997	4.909399
X	9.843493	6.483562	7.775547
X	10.616625	15.249498	6.514465
X	12.395229	13.059139	7.345263
X	10.668495	13.171921	14.202259
X	11.304932	11.158836	14.377096
X	12.581848	11.243091	6.874281
X	6.194109	8.675685	6.653764
X	10.957580	11.966623	12.449303
X	13.126596	11.077967	9.527689
X	10.191188	9.749305	4.910175
X	8.731049	7.722147	14.755430
X	11.315136	11.008749	6.389706
X	7.508389	11.692317	10.816584
X	7.042675	11.158445	11.755306
X	4.962196	10.460279	5.064625
X	10.957731	13.037381	13.065710
X	9.710530	5.931863	6.644125
X	10.916800	10.701969	4.365832
X	14.722857	13.514784	7.290767
X	9.042015	8.032486	12.448645
X	9.247676	13.897465	8.548037
X	7.169899	10.849500	6.047416
X	9.333860	6.827619	14.201441
X	15.037794	9.539155	5.065171
X	10.625887	12.934549	11.758542
X	12.005642	9.281592	11.224231
X	14.695363	8.982502	7.617278
X	9.083776	9.293391	4.366353
X	7.231640	5.688567	7.423694
X	10.725636	10.240335	6.459968
X	12.435398	13.203762	6.794718

X	6.622653	8.556102	10.614017
X	11.921852	8.295188	11.839671
X	10.415520	10.659608	6.437301
X	8.400995	9.918429	13.874691
X	9.272427	9.760090	6.459460
X	8.750323	9.089607	11.918491
X	9.031543	8.926435	13.202555
X	12.766790	14.310751	7.425874
X	10.387363	14.614084	5.535255
X	10.403789	12.861514	13.092742
X	13.364175	10.195618	6.351768
X	9.373971	7.064783	11.757700
X	5.303781	11.018462	7.617917
X	9.502776	9.858565	9.931151
X	5.275552	6.484195	7.288458
X	11.248607	10.909443	11.918868
X	10.385645	14.072896	8.857678
X	9.636576	9.885520	9.155663
X	9.610561	5.385706	5.535881
X	13.930105	9.374412	5.579997
X	6.228442	10.903034	6.807346
X	13.770605	9.097129	6.806787
X	6.408489	11.255768	7.981262
X	5.886922	7.705564	7.219936
X	13.804303	11.324224	6.653306
X	9.043235	6.961632	13.065157
X	9.663115	5.877553	13.493441
X	8.683307	8.991260	6.390362
X	10.288190	14.068122	6.643784
X	11.820263	12.142801	6.772513
X	9.787734	10.322898	9.265474
X	10.498557	5.057261	6.256656
X	10.467404	10.138548	10.052795
X	5.925468	10.396374	4.369579
X	6.634497	9.804319	6.352604
X	7.603271	6.940255	7.344752
X	13.376049	11.443632	10.614076
X	14.075274	9.603018	4.369079
X	13.590849	8.744759	7.980896
X	9.315384	6.706511	15.425321
X	5.851995	12.006655	7.249474
X	10.689063	13.293332	15.426104
X	15.016945	11.479635	6.754527
X	11.597736	10.079975	13.874933
X	8.951445	6.884392	6.994236
X	10.357340	9.883545	9.219697
X	9.252824	9.427217	5.640115
X	10.123414	7.071877	6.756050
X	7.682936	9.019644	10.374017
X	8.077922	11.704219	11.839967
X	7.392426	7.962179	9.957197
X	5.565328	11.447161	4.798203
X	14.111099	12.293647	7.220603
X	10.062616	9.828191	8.885514
X	11.327112	11.264208	15.602324
X	10.339165	14.122127	13.494482
X	14.434756	8.552354	4.798499
X	10.967877	11.072559	13.203211
X	12.605908	12.038361	9.958470
X	7.993465	10.717934	11.224799
X	10.246342	10.295167	9.190336
X	9.613382	5.927696	8.858114
X	14.139361	12.446301	6.668612
X	10.751285	6.103522	8.548465
X	9.940824	10.176782	8.890316
X	8.178251	7.857200	6.773036
X	11.510027	11.227019	13.163378
X	10.155315	13.516789	7.775340
X	12.315424	10.980606	10.374479
X	8.489464	8.771626	13.162878
X	9.582814	9.340881	6.438426
X	7.563145	6.796364	6.793990
X	9.279186	7.895782	14.773684
X	9.875351	12.928150	6.756051

X	11.047210	13.115644	6.994180
X	12.620004	11.399984	6.303265
X	9.382109	4.750478	6.515402
X	12.956890	8.841210	11.754136
X	10.000280	9.998599	9.511580
X	7.416579	8.756818	6.874899
X	12.829380	9.150000	6.046443
X	9.926105	12.973488	8.864212
X	11.271119	12.276862	14.755552
X	6.871335	8.923004	9.527875
X	4.981388	8.519990	6.753930
X	9.597004	7.138092	13.091836
X	14.147696	7.993832	7.249385
X	5.859331	7.553538	6.667743
X	10.746427	10.571058	5.639755
X	9.999422	10.001058	7.708687
X	9.499958	14.942778	6.256639
X	9.991732	9.616605	9.257606
X	8.695225	8.839898	14.376696
X	10.072454	7.027301	8.864320

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$[Pd_3(dmpe)_2(1\text{-}(SiH_2),2\text{-}(SiH)\text{-}C_6H_4)_2(1,2\text{-}(SiH)_2C_6H_4)]$

Pd	10.999969	10.860100	9.388386
Pd	13.749277	10.404035	9.943234
Pd	8.385857	11.701098	10.180769
P	15.513058	11.267296	8.705042
P	14.836978	8.369626	9.894048
P	6.479305	10.942272	9.100099
P	7.689843	13.849368	9.662463
Si	11.151582	12.107204	7.367364
Si	10.604574	9.284663	7.665552
Si	12.634142	12.540571	10.250409
Si	9.350227	9.558773	10.668280
Si	11.884727	9.549291	11.267463
Si	10.384514	12.502797	11.286821
C	12.153487	13.694565	7.704938
C	12.310669	14.663950	6.697890
C	13.076145	15.816092	6.914430
C	13.699740	16.013748	8.152652
C	13.556673	15.056655	9.162712
C	12.792019	13.891603	8.953424
C	9.405960	7.959893	8.322369
C	9.010488	6.884754	7.504292
C	8.112122	5.916951	7.967036
C	7.597179	6.011141	9.266048
C	7.982342	7.072056	10.090954
C	8.877322	8.060156	9.631596
C	11.587362	10.435011	12.900013
C	11.985868	9.868700	14.129025
C	11.795370	10.545877	15.332718
C	11.199203	11.816379	15.330521
C	10.785496	12.387008	14.127260
C	10.960755	11.715173	12.899134
C	16.526211	9.793947	8.165235
C	16.553516	8.704845	9.248611
C	16.729551	12.295150	9.622268
C	15.325688	12.193345	7.135358
C	15.166039	7.355962	11.386662
C	14.166347	7.129658	8.717946
C	5.426126	12.452569	8.789085
C	6.301826	13.665356	8.432875
C	5.279433	9.748818	9.808091
C	6.745296	10.271847	7.414036
C	6.930254	14.844978	11.007622
C	8.820592	15.049206	8.868655
H	11.846714	11.502032	6.192170
H	9.844856	12.555379	6.800595
H	9.986356	9.713833	6.376376
H	11.845090	8.580293	7.236203
H	13.287352	13.038236	11.498948
H	9.102218	9.193472	12.093323
H	11.995719	8.091634	11.577893
H	10.254654	13.965088	11.584904
H	11.831536	14.518431	5.729137
H	13.185476	16.555548	6.123247
H	14.293218	16.909235	8.327868
H	14.041479	15.215092	10.126288
H	9.408184	6.801004	6.492398
H	7.819022	5.090765	7.321937
H	6.902818	5.257568	9.633517
H	7.586080	7.135446	11.104764
H	12.452724	8.883809	14.135345
H	12.109736	10.092410	16.270864
H	11.054857	12.352345	16.266603
H	10.316912	13.370951	14.133700
H	16.043772	9.413270	7.252765
H	17.540649	10.112204	7.884627
H	17.145199	9.038770	10.113760
H	17.014490	7.777060	8.879722
H	17.027620	11.778996	10.543184
H	17.618734	12.516309	9.017677
H	16.239405	13.235903	9.906352
H	16.287186	12.301122	6.616985

H	14.611326	11.666736	6.489456
H	14.910247	13.186343	7.350120
H	14.205568	7.010358	11.791017
H	15.800268	6.489053	11.161577
H	15.650408	7.979755	12.148379
H	13.163239	6.835210	9.055113
H	14.053593	7.589828	7.728453
H	14.807253	6.241361	8.647680
H	4.685622	12.245562	8.002843
H	4.867811	12.641232	9.718037
H	5.709993	14.589947	8.371869
H	6.780243	13.518722	7.453037
H	4.994088	10.070443	10.817102
H	4.381267	9.651966	9.184303
H	5.774538	8.770981	9.881685
H	5.798390	10.143414	6.874288
H	7.407892	10.944744	6.855031
H	7.254849	9.302682	7.500916
H	7.697099	15.038713	11.769248
H	6.533425	15.799041	10.637583
H	6.124826	14.269202	11.480289
H	9.654790	15.254405	9.552941
H	9.243207	14.599854	7.960908
H	8.314662	15.990415	8.618717
X	10.864784	12.059763	13.499898
X	12.070820	14.379957	7.375186
X	11.577028	10.175767	14.698141
X	16.108454	10.416151	8.408396
X	9.276124	6.826649	6.824696
X	13.109633	15.937958	7.675098
X	6.675956	15.464486	10.745543
X	5.915419	14.270974	8.408100
X	12.729451	13.374386	9.456615
X	11.762588	13.080823	7.606620
X	13.043938	11.403158	9.998762
X	5.070980	12.571202	9.407893
X	16.842384	8.094571	9.001956
X	7.711084	7.113772	10.768958
X	16.918062	11.943095	10.215606
X	8.563706	6.394670	7.726224
X	15.068148	12.826576	7.292365
X	5.099419	9.974372	10.462552
X	11.103229	12.174531	15.960711
X	17.305037	12.426473	9.211194
X	14.109040	7.441627	8.080111
X	5.786305	10.264812	9.506923
X	11.558573	8.746678	7.351235
X	13.809235	10.683826	9.724555
X	10.669203	10.710614	9.496818
X	13.381616	14.370238	8.844322
X	12.300576	9.206083	14.131015
X	8.909037	7.537424	7.910724
X	8.039003	11.858231	10.134571
X	10.726279	12.010380	12.262564
X	10.470577	13.048180	14.129868
X	7.167602	10.724691	7.063354
X	8.279838	11.408838	10.006210
X	9.354157	7.234040	8.103745
X	15.581724	6.795827	11.218064
X	9.870708	8.479979	8.094555
X	8.651480	7.365437	9.852585
X	13.634161	15.544429	8.665625
X	6.879432	13.750097	8.962707
X	11.989443	14.568906	6.046708
X	14.868284	11.834229	6.726683
X	13.491800	10.544638	10.149203
X	11.707607	10.087620	12.260224
X	4.699285	9.702455	9.387006
X	11.046348	11.345267	8.417270
X	9.344237	15.172256	9.325905
X	10.771742	11.882174	14.691953
X	5.610028	9.125412	9.847071
X	7.917137	5.363997	7.532601
X	15.824018	8.556644	9.507024

X	14.098468	16.613312	8.271987
X	6.403774	14.459025	11.300665
X	15.485336	7.773249	11.869653
X	17.190334	10.009502	7.994180
X	15.966715	12.248926	6.814652
X	8.319791	11.896141	10.492447
X	5.873695	11.816213	8.909159
X	9.147180	8.019236	8.978775
X	5.878720	13.052132	8.621683
X	14.601104	6.557359	8.686829
X	8.468822	15.656335	8.714843
X	10.734182	9.773879	10.573060
X	11.031175	10.503365	9.453491
X	8.675178	11.623655	9.967358
X	9.075207	14.745649	8.282696
X	13.944626	10.653728	10.143547
X	13.117168	12.892922	11.188279
X	12.788795	10.055432	10.547438
X	16.400328	12.900011	9.795830
X	14.459963	7.659911	9.218813
X	13.575728	15.661745	7.483552
X	14.834881	11.048692	9.136087
X	7.783479	6.535191	9.688026
X	7.703220	6.233883	8.537519
X	8.641179	11.558716	10.392037
X	16.523209	9.254769	8.715191
X	11.388185	12.321142	10.524821
X	11.293920	12.129724	14.631758
X	7.247096	14.422580	10.431905
X	10.915058	10.930037	9.773053
X	10.141252	12.456380	6.945997
X	7.164008	11.119087	9.540199
X	6.112410	10.198574	7.078820
X	13.147598	16.310646	6.382409
X	16.197144	9.548769	7.572050
X	11.979760	8.430007	11.487503
X	9.062346	8.633399	10.033746
X	8.318069	11.811987	9.819586
X	13.866863	10.256111	10.262904
X	10.131334	9.634426	6.686018
X	15.030652	7.788037	10.748261
X	10.882585	10.845916	9.066248
X	7.130770	5.507543	9.514040
X	6.625442	13.563187	7.797734
X	15.406752	11.792604	7.811277
X	16.929035	8.929323	9.823460
X	11.790841	10.141674	13.501322
X	13.818078	10.263232	9.593110
X	8.216040	7.666909	9.648446
X	7.065140	9.651798	7.488778
X	11.044312	10.950975	13.010635
X	8.000535	13.110963	9.889034
X	13.445288	10.393506	9.752204
X	13.886480	15.164571	9.806895
X	11.170294	11.195395	9.406071
X	8.158555	11.517739	10.405658
X	12.006031	10.243284	15.964253
X	11.686821	11.631006	6.479336
X	13.524385	6.947966	8.952988
X	11.284524	10.779628	9.138086
X	8.533815	12.028062	10.138006
X	13.662086	10.058894	9.952575
X	7.437026	14.964840	11.490013
X	12.099734	10.423209	14.639777
X	14.393314	9.070026	9.981549
X	14.538392	7.137860	11.632449
X	6.627009	10.565918	8.136435
X	8.858704	10.668818	10.371284
X	8.140593	5.921227	8.735635
X	9.487948	11.977755	10.698337
X	12.921173	14.636824	9.044692
X	4.951017	12.311483	8.268229
X	8.327396	14.537689	9.207405
X	10.273821	13.621275	11.489092

X	12.689901	15.243853	6.796237
X	14.119337	10.315521	9.890795
X	9.179440	9.298544	11.737201
X	12.467783	13.784440	8.333827
X	10.750168	11.112992	9.424005
X	16.217642	11.851720	9.231103
X	11.530518	11.197642	12.960179
X	10.810334	10.241607	8.646890
X	11.499410	11.181978	15.349771
X	11.299203	10.819679	9.568271
X	12.539010	14.112996	7.184870

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$[(L_2Cu)_3S_2]^{3+}$(L = $Me_2NCH_2CH_2NMe_2$)

Cu	7.188734	10.610069	8.989510
S	8.128607	9.079359	10.395407
N	6.466903	11.944257	10.412794
C	5.309032	11.327995	11.123333
H	4.901473	12.033302	11.863408
H	5.646672	10.425003	11.643698
H	4.517076	11.060643	10.415411
S	8.127724	9.083324	7.584501
N	6.262868	11.831500	7.575069
C	7.497386	12.325310	11.420504
H	7.086310	13.065187	12.124177
H	8.367823	12.761502	10.917304
H	7.805330	11.438168	11.984854
C	6.044690	13.162693	9.646522
H	6.943736	13.761991	9.455926
H	5.369021	13.781569	10.258259
C	5.372313	12.757995	8.349051
H	4.428600	12.232364	8.541151
H	5.130631	13.646881	7.744324
C	7.322622	12.597902	6.854277
H	6.865439	13.272009	6.113939
H	7.984553	11.897025	6.334347
H	7.912551	13.196195	7.557291
C	5.456632	11.077249	6.575029
H	4.969805	11.773874	5.875344
H	4.686011	10.487727	7.083934
H	6.113966	10.411643	6.004885
Cu	9.916228	9.113951	8.989554
Cu	7.282642	7.508955	8.989830
N	11.431265	9.061185	10.410599
N	6.444479	6.215488	10.409723
C	11.475185	10.378201	11.114179
C	7.551215	5.518419	11.129577

H	12.287840	10.382458	11.856494
H	7.138889	4.817049	11.871058
H	10.523254	10.543719	11.630364
H	8.164037	6.262345	11.650222
H	11.644034	11.192396	10.401050
H	8.180868	4.960240	10.428191
N	11.425441	9.292934	7.573251
N	6.646955	6.109464	7.574604
C	11.255295	7.982972	11.424356
C	5.598369	6.927801	11.408921
H	12.104587	7.979519	12.125098
H	5.155134	6.208413	12.114527
H	11.202525	7.007956	10.927026
H	4.791959	7.465413	10.897678
H	10.334506	8.159103	11.991360
H	6.214842	7.636530	11.972409
C	12.700907	8.827326	9.643987
C	5.599314	5.246352	9.639276
H	12.784103	7.749032	9.460039
H	4.632804	5.728789	9.446720
H	13.571400	9.119827	10.252957
H	5.397070	4.348842	10.245812
C	12.676346	9.605366	8.342422
C	6.287905	4.871894	8.342222
H	7.216126	4.318783	8.534804
H	12.691724	10.686563	8.528384
H	5.643988	4.218431	7.731456
H	13.564384	9.369671	7.734223
C	5.458957	6.656194	6.855206
C	11.562959	7.991560	6.853038
H	5.099071	5.927202	6.112938
H	12.374638	8.053888	6.112225
H	5.746175	7.577342	6.336866
H	10.625283	7.765533	6.333848
H	4.647494	6.874650	7.557968
H	11.789582	7.183728	7.557478

C	7.704099	5.784011	6.575482
C	11.171993	10.370790	6.575715
H	7.343170	5.015304	5.874902
H	12.019466	10.449819	5.877605
H	8.596283	5.405680	7.087448
H	11.045200	11.330681	7.088983
H	7.959765	6.685039	6.007233
H	10.267549	10.135720	6.004158
X	7.921377	8.603840	10.368305
X	5.231307	13.336375	7.955817
X	7.011685	13.028916	6.378492
X	5.861768	4.460213	7.944959
X	5.057044	11.795791	11.598857
X	7.217203	12.801500	11.870204
X	5.238573	6.173986	6.378268
X	13.259576	9.030257	10.039781
X	11.726335	10.407537	6.130040
X	11.367270	8.607354	10.841888
X	6.480613	11.511498	7.880660
X	6.018495	7.396767	11.766163
X	11.087321	10.998006	6.930914
X	5.150962	11.539638	6.128130
X	11.809858	7.995294	11.871674
X	5.951481	5.073433	8.990713
X	5.321876	6.451376	11.859774
X	11.707813	7.469770	7.335117
X	5.917400	11.522665	7.149544
X	7.287745	7.512909	8.990251
X	6.645570	13.539024	9.512577
X	11.218765	7.345643	11.079575
X	7.822569	9.495870	10.365714
X	7.190881	10.608602	8.989704
X	7.694426	11.727372	11.778039
X	12.091424	8.048069	6.377147
X	6.277863	12.461609	10.097412
X	5.484196	4.663107	10.033764

X	5.661807	7.265941	6.524659
X	12.666647	10.315543	8.473127
X	4.973576	5.579907	9.504532
X	6.090549	5.795218	10.092429
X	5.888105	12.232789	7.893968
X	11.044850	9.056570	10.102028
X	9.911092	9.113895	8.989489
X	12.735676	8.117847	9.514553
X	13.247167	9.438739	7.947086
X	7.194521	10.605605	8.989054
X	4.954681	10.691001	6.927358
X	5.598532	13.551675	10.044436
X	6.703527	12.165539	7.268464
X	7.957801	5.159429	10.649273
X	7.753821	12.122680	6.522545
X	8.641658	9.133961	10.372620
X	7.456158	5.288238	6.127836
X	11.328915	9.747343	7.148558
X	6.485386	5.583521	7.891102
X	7.286247	7.513324	8.989193
X	8.642757	9.047458	7.606906
X	6.822907	6.455469	7.882333
X	7.282730	7.515532	8.989962
X	4.762534	12.396584	8.483545
X	7.269055	5.068761	11.605886
X	11.495223	8.744329	7.266986
X	6.895288	12.113559	10.842058
X	5.072767	7.280285	11.054999
X	10.935690	7.853832	6.521871
X	11.039852	9.265217	7.881422
X	5.971340	11.694630	10.714099
X	7.836978	8.654720	7.609237
X	5.903554	10.637684	6.213417
X	5.545391	10.731301	11.455298
X	7.949083	6.021532	11.461525
X	10.839309	10.475297	11.443507

X	8.288196	5.539705	6.929918
X	12.005387	10.364940	11.591067
X	7.284410	7.510874	8.989757
X	7.188272	10.604275	8.989246
X	10.568108	10.204261	6.213375
X	9.914024	9.112943	8.989511
X	8.133308	9.076219	8.989442
X	7.356989	7.645660	8.990222
X	8.067325	12.607510	11.071642
X	12.671011	9.215476	8.993071
X	7.703720	12.982764	7.335694
X	9.907960	9.113605	8.989542
X	11.461492	9.617725	10.709355
X	6.906937	4.526438	8.477026
X	7.866084	6.390466	6.214914
X	9.913976	9.113192	8.989615
X	4.798063	11.155429	10.639090
X	5.717661	12.945724	8.997791
X	7.903024	9.550964	7.617743
X	7.192290	10.607156	8.989956
X	4.935168	6.797543	7.336122
X	6.139383	6.329255	7.269145
X	7.087073	5.963167	7.148698
X	6.642252	6.549847	10.102778
X	11.961447	9.418442	7.890637
X	6.083124	6.506073	10.835684
X	6.663784	11.612911	10.104747
X	7.267766	10.482438	8.989324
X	9.757420	9.110617	8.989660
X	6.905217	5.909181	10.715410
X	10.639737	8.110102	11.783392
X	11.583075	10.903816	10.626368
X	11.974900	8.969710	10.094709
Y	10.936603	7.853871	6.521589
Y	5.236831	13.327438	7.956976
Y	7.009169	13.022906	6.387147

Y	6.906657	4.526359	8.477485
Y	6.279752	12.458779	10.083288
Y	7.213804	12.797801	11.858378
Y	5.245381	6.174774	6.387055
Y	12.672422	9.215564	8.993035
Y	11.725204	10.402395	6.141706
Y	11.355353	8.602255	10.838899
Y	7.773364	8.442946	9.881844
Y	6.084891	6.519156	10.832707
Y	5.326939	6.450280	11.847821
Y	5.901687	10.639691	6.212351
Y	12.001972	10.359103	11.582611
Y	7.957606	5.160533	10.649545
Y	11.808260	8.000241	11.859841
Y	12.087532	8.053544	6.385677
Y	7.741485	9.700394	8.094644
Y	7.865141	6.387901	6.213800
Y	5.064084	11.795323	11.589973
Y	6.705585	6.636786	9.983541
Y	6.905798	12.105831	10.839189
Y	11.958105	9.418412	7.904425
Y	7.693291	11.730023	11.779211
Y	11.316579	9.751513	7.151656
Y	5.604316	13.542981	10.043197
Y	5.489406	4.672501	10.032593
Y	4.936199	6.798043	7.335857
Y	11.086147	10.996599	6.930988
Y	7.187259	10.602725	8.989326
Y	11.217511	7.346946	11.079499
Y	5.920030	11.509439	7.152705
Y	13.249664	9.029766	10.038568
Y	8.123568	9.078548	10.799334
Y	6.915834	5.915146	10.710163
Y	8.857100	9.105290	8.095380
Y	11.485660	8.737846	7.271972
Y	7.452446	5.291877	6.139624

Y	7.198365	10.595050	8.989501
Y	6.550255	11.430864	7.999363
Y	7.758812	9.708676	9.883608
Y	5.889881	12.229696	7.908124
Y	8.287565	5.541402	6.930026
Y	7.096957	5.971356	7.151553
Y	9.898807	9.112795	8.989572
Y	4.973644	5.579620	9.504087
Y	7.289490	7.511273	8.990383
Y	11.582221	10.903126	10.626689
Y	6.487123	5.586675	7.905345
Y	5.971556	11.682413	10.708762
Y	4.762564	12.396863	8.483961
Y	7.265944	5.074697	11.597015
Y	7.281612	7.517145	8.989929
Y	4.956454	10.690656	6.927463
Y	7.753279	12.123552	6.522256
Y	9.910990	9.113902	8.989509
Y	5.544854	10.732077	11.455551
Y	5.074531	7.280774	11.054898
Y	12.735871	8.118073	9.514091
Y	7.191725	10.606752	8.990006
Y	5.156315	11.540870	6.140375
Y	10.642398	8.109798	11.784579
Y	9.915017	9.112735	8.989485
Y	7.789579	8.435958	8.098012
Y	11.706930	7.470426	7.334821
Y	5.950733	5.072146	8.990737
Y	6.714278	12.160402	7.273385
Y	10.939115	9.246624	7.999212
Y	12.666887	10.315379	8.473534
Y	8.857882	9.083129	9.884459
Y	6.092152	5.798503	10.078131
Y	8.066837	12.605801	11.071551
Y	11.971571	8.969363	10.080894
Y	5.716844	12.946950	8.997760

Y	7.291354	7.524724	8.989878
Y	7.703612	12.981675	7.335427
Y	5.867052	4.469237	7.946123
Y	13.237286	9.438488	7.948294
Y	6.645275	13.539053	9.512087
Y	6.708796	11.518423	9.985474
Y	7.196295	10.607596	8.988957
Y	5.661264	7.265111	6.524330
Y	10.943221	9.065848	9.983466
Y	6.861594	6.554182	7.999558
Y	7.285734	7.513494	8.989084
Y	7.948598	6.020654	11.461832
Y	8.123147	9.081930	7.180603
Y	10.570672	10.204762	6.212132
Y	6.016679	7.394588	11.767360
Y	10.840191	10.475337	11.443816
Y	6.138865	6.341384	7.274376
Y	9.906610	9.113473	8.989565
Y	4.799109	11.155011	10.639364
Y	11.451361	9.623446	10.704201

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$[(L_2Cu)_3O_2]^{3+}$(L = $Me_2NCH_2CH_2NMe_2$)

Cu	7.312969	10.417186	8.990559
O	8.334002	9.101409	10.138309
N	6.619370	11.735395	10.410075
C	5.448995	11.143086	11.125940
H	5.037084	11.865565	11.847487
H	5.774505	10.247887	11.666339
H	4.660821	10.870979	10.414801
O	8.334588	9.102568	7.841556
N	6.445357	11.633421	7.576048
C	7.662921	12.093322	11.413484
H	7.273195	12.833826	12.129045
H	8.534697	12.521151	10.905181
H	7.959760	11.189724	11.956697
C	6.201313	12.959621	9.647633
H	7.100286	13.562304	9.466179
H	5.518753	13.573997	10.256172
C	5.543376	12.560057	8.337921
H	4.597403	12.033676	8.516254
H	5.309066	13.450275	7.732436
C	7.512434	12.401270	6.869755
H	7.062644	13.090885	6.138284
H	8.167836	11.699670	6.343370
H	8.104913	12.985324	7.583302
C	5.656621	10.874200	6.563202
H	5.175983	11.563188	5.851660
H	4.878113	10.286934	7.063301
H	6.329988	10.207760	6.012742
Cu	9.822311	9.116381	8.990138
Cu	7.411991	7.700460	8.989452
N	11.258260	9.102765	10.390400
N	6.637350	6.423167	10.405878
C	11.282149	10.435627	11.064288
C	7.755196	5.724755	11.106563

H	12.085611	10.449816	11.817225
H	7.354180	5.010105	11.842393
H	10.320069	10.596962	11.560740
H	8.367063	6.467517	11.628992
H	11.462805	11.236368	10.338898
H	8.378536	5.178470	10.389504
N	11.254786	9.265317	7.588485
N	6.812429	6.316983	7.572472
C	11.023882	8.046700	11.415118
C	5.810334	7.139620	11.419283
H	11.842945	8.055428	12.150331
H	5.373269	6.427780	12.136359
H	10.989655	7.063045	10.934122
H	4.997425	7.679507	10.920025
H	10.075217	8.250803	11.922768
H	6.445881	7.847659	11.962483
C	12.542200	8.839530	9.647281
C	5.788204	5.446370	9.648462
H	12.615312	7.757059	9.486025
H	4.815766	5.922194	9.468423
H	13.402597	9.137600	10.267616
H	5.599700	4.548040	10.257912
C	12.522861	9.593596	8.332862
C	6.462387	5.075897	8.338196
H	7.391149	4.519473	8.516116
H	12.540607	10.678426	8.494559
H	5.808874	4.426003	7.734485
H	13.397351	9.341984	7.711830
C	5.613334	6.848288	6.855757
C	11.363942	7.950627	6.887229
H	5.242209	6.104877	6.133285
H	12.156703	8.006751	6.125380
H	5.892828	7.759404	6.316286
H	10.409405	7.730905	6.399188
H	4.810944	7.078953	7.565740
H	11.610500	7.152386	7.595840

C	7.870692	6.016866	6.567477
C	10.944757	10.323408	6.585916
H	7.519498	5.255599	5.853528
H	11.760692	10.385310	5.849669
H	8.766754	5.638025	7.072625
H	10.842376	11.293143	7.085206
H	8.113418	6.934728	6.021198
H	10.011473	10.062410	6.075786
X	8.834524	9.106302	8.208031
X	5.382020	6.353174	6.389987
X	7.205544	12.846127	6.398566
X	6.134082	5.276379	8.993565
X	5.191257	11.625274	11.590878
X	5.881161	12.744896	8.993163
X	7.853396	11.492008	11.763563
X	11.555945	8.073022	11.868934
X	10.876759	10.953936	6.933714
X	12.519180	9.215978	8.989932
X	7.052635	11.897564	10.838164
X	11.800194	10.420780	11.535765
X	9.839931	9.113805	8.990061
X	5.531529	6.662909	11.880938
X	11.801806	8.998609	10.072594
X	5.158170	5.776000	9.521651
X	6.029276	4.665567	7.945240
X	9.817235	9.115499	8.990099
X	5.406861	13.140239	7.943886
X	8.460108	5.772737	6.917838
X	6.432284	12.258654	10.100107
X	7.479809	5.262356	11.580743
X	6.889572	11.968348	7.275403
X	6.108929	10.435570	6.209791
X	4.940684	10.965384	10.639424
X	10.732705	7.816900	6.578309
X	8.236560	12.369706	11.060810
X	7.312461	10.419110	8.993222

X	5.809373	7.451528	6.509595
X	13.072811	9.415940	7.933439
X	5.681383	4.861273	10.045239
X	13.082401	9.045767	10.046431
X	7.252945	6.178671	7.143981
X	7.940760	11.928803	6.531341
X	11.303036	8.708212	7.300364
X	10.334640	10.144651	6.262097
X	12.513913	10.303792	8.448292
X	8.159571	5.374004	10.616140
X	11.124761	9.713208	7.170746
X	7.628973	5.518706	6.108191
X	8.833961	9.096635	9.772234
X	7.420504	7.719304	8.991483
X	7.310590	10.414743	8.990622
X	6.237642	7.605975	11.768050
X	6.300786	6.529392	7.266858
X	6.803020	13.338519	9.519732
X	8.173359	9.397298	8.000405
X	5.095384	6.999445	7.341746
X	5.149632	10.487473	6.910159
X	6.279337	5.996808	10.099836
X	6.639235	11.337050	7.877459
X	6.120001	11.495903	10.715307
X	6.282784	6.712667	10.838566
X	11.520792	7.438338	7.372992
X	5.348950	11.336302	6.105482
X	11.873604	8.010309	6.409918
X	9.825260	9.115112	8.990251
X	8.169898	9.390892	9.965422
X	7.896978	12.776583	7.358231
X	8.025749	6.627935	6.215754
X	6.966698	6.631706	7.871067
X	6.106496	11.324681	7.144103
X	8.170800	8.803808	9.983015
X	10.647068	10.530478	11.378914

X	7.412110	7.698939	8.986557
X	10.999701	7.406556	11.079355
X	7.103239	6.116952	10.704440
X	6.794709	11.427491	10.108882
X	10.402707	8.188294	11.736950
X	11.160396	8.656213	10.818170
X	7.328238	10.393753	8.988721
X	7.408099	7.690793	8.989393
X	5.280253	7.495169	11.072723
X	12.569215	8.129666	9.532261
X	5.675487	10.551065	11.472785
X	8.167096	8.808820	8.010936
X	11.476171	10.342493	6.131483
X	7.408198	7.700905	8.989536
X	8.427437	9.098418	7.536800
X	7.082768	4.728225	8.463792
X	6.064013	12.037737	7.885031
X	11.791669	9.397680	7.907122
X	6.653976	5.785333	7.882867
X	10.777946	9.223879	8.036964
X	11.269980	9.667856	10.665974
X	4.931802	12.197713	8.463600
X	8.426539	9.107056	10.443224
X	7.396050	12.577064	11.873536
X	10.779922	9.099321	9.942989
X	7.405509	7.704615	8.989781
X	6.807276	6.727319	10.104313
X	8.154375	6.224360	11.442090
X	9.833922	9.116903	8.990143
X	7.308480	10.426952	8.990349
X	5.750287	13.346047	10.043807
X	7.303340	10.414259	8.990244
X	11.396772	10.948812	10.567677
Y	8.918784	9.114831	8.342062
Y	6.299145	6.541161	7.271606
Y	7.204167	12.836010	6.408445

Y	6.133398	5.275018	8.993527
Y	5.675935	10.551288	11.471604
Y	5.880441	12.746122	8.993189
Y	7.393471	12.566102	11.859058
Y	11.000081	7.405926	11.079525
Y	11.475402	10.344308	6.126420
Y	12.518741	9.215949	8.989957
Y	6.434420	12.255797	10.085789
Y	11.801390	10.423615	11.539780
Y	8.042353	9.473813	8.088125
Y	7.264746	6.188193	7.147989
Y	11.802561	8.998804	10.077176
Y	5.542835	6.667547	11.865773
Y	6.034130	4.673329	7.946481
Y	9.817027	9.116268	8.990094
Y	5.201203	11.621283	11.581132
Y	8.459161	5.773648	6.917921
Y	5.755115	13.339198	10.042575
Y	7.477696	5.272862	11.570354
Y	10.809168	9.097410	9.985911
Y	6.109637	10.435580	6.212274
Y	7.853159	11.491232	11.761182
Y	10.731524	7.817184	6.578702
Y	12.569120	8.129614	9.532406
Y	4.931873	12.197968	8.464012
Y	5.809814	7.451307	6.510784
Y	13.076149	9.416048	7.933089
Y	5.685629	4.869594	10.043815
Y	8.159018	5.374794	10.616415
Y	5.158283	5.775734	9.521198
Y	7.308233	10.426577	8.990243
Y	11.129128	9.711589	7.169402
Y	5.281749	7.495039	11.072466
Y	11.792421	9.397593	7.902485
Y	6.870973	6.826964	9.985048
Y	9.834585	9.116972	8.990160

Y	6.802741	13.338640	9.519385
Y	6.108387	11.311219	7.147251
Y	6.838194	11.325563	9.991657
Y	7.940243	11.928545	6.532399
Y	8.918796	9.102998	9.638350
Y	5.392048	6.357945	6.400011
Y	11.306749	8.710902	7.297905
Y	7.625659	5.530056	6.123552
Y	8.469081	9.109879	7.644728
Y	7.299575	10.412616	8.990582
Y	6.283868	6.726520	10.835423
Y	11.397019	10.949183	10.567657
Y	6.119004	11.484489	10.710651
Y	7.114780	6.122855	10.698768
Y	11.521072	7.437985	7.373013
Y	6.901114	11.963336	7.280766
Y	10.332056	10.143625	6.263808
Y	11.874974	8.007569	6.405827
Y	8.025381	6.628495	6.218076
Y	5.360235	11.332526	6.120187
Y	7.006576	6.744545	7.991017
Y	7.409510	7.700484	8.989428
Y	5.150982	10.487740	6.910378
Y	7.412700	7.712127	8.988928
Y	6.238335	7.605962	11.765561
Y	11.555276	8.071249	11.873879
Y	8.051456	9.483480	9.888689
Y	9.815617	9.114655	8.990285
Y	8.068060	8.707033	9.895399
Y	7.896474	12.775843	7.357956
Y	11.164762	8.658175	10.819510
Y	6.705042	11.247910	7.993612
Y	7.082499	4.728076	8.464154
Y	6.280715	6.000648	10.084354
Y	8.153809	6.224543	11.441008
Y	10.877109	10.954624	6.933519

Y	6.656404	5.788993	7.898489
Y	5.411113	13.132804	7.945210
Y	7.403998	7.708358	8.989459
Y	12.513805	10.303826	8.448165
Y	5.096353	6.999362	7.341528
Y	8.235680	12.368894	11.060777
Y	7.313375	10.412831	8.990729
Y	4.941610	10.965547	10.639613
Y	9.840023	9.113427	8.990137
Y	13.085666	9.045875	10.046763
Y	6.065351	12.034516	7.899251
Y	10.645943	10.530134	11.378572
Y	7.407442	7.690993	8.989591
Y	8.467633	9.105720	10.335389
Y	7.314598	10.404706	8.991121
Y	8.079814	8.699199	8.085606
Y	10.400092	8.189123	11.735203
Y	10.807691	9.228464	7.993488
Y	7.064658	11.888956	10.834270
Y	11.273604	9.665579	10.668334

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$[^{Mes}DPB^{Ph}]NiH_2$

Ni	11.264890	10.398812	10.060829
P	13.161936	9.593590	10.635654
P	9.438238	11.508894	10.392058
C	9.726151	11.239319	12.182577
C	10.205432	9.954620	12.546921
C	7.760722	10.877175	10.057632
C	6.697591	11.201468	10.908182
H	6.867279	11.863211	11.758237
C	8.196001	15.351522	9.537582
H	7.292702	15.847810	9.190159
C	7.548234	10.005730	8.989679
H	8.383985	9.729480	8.347249
C	13.988604	10.726022	11.811699
C	14.412477	9.220873	9.361541
C	14.438357	11.968983	11.349135
H	14.334739	12.219730	10.293337
C	10.497810	15.447161	10.238977
H	11.398863	16.021177	10.442769
C	10.609944	9.810671	13.882808
H	11.014857	8.849072	14.202742
C	13.730520	6.061947	12.649908
H	14.561364	5.416508	12.925872
C	7.747827	6.344450	9.662691
H	7.761183	5.750292	8.746040
C	14.102188	10.419850	13.168365
H	13.744808	9.460644	13.538859
C	9.971098	12.067705	14.440104
H	9.868492	12.870658	15.166714
B	10.289773	8.678468	11.531754
C	13.950118	8.777684	8.119091
H	12.876130	8.715316	7.940134
C	6.583797	6.391538	10.420099
C	8.928035	7.832510	11.212696

C	8.196164	13.970571	9.719790
H	7.292657	13.399187	9.516522
C	7.649140	8.556350	13.322148
H	7.713366	9.647195	13.213744
H	8.444206	8.266299	14.019076
H	6.690358	8.330394	13.802656
C	12.427392	5.736328	13.019751
H	12.237602	4.830343	13.592699
C	10.491594	10.833087	14.816427
H	10.808657	10.667264	15.844627
C	8.898720	7.040103	10.035565
C	9.350152	13.319107	10.157889
C	5.435204	10.669216	10.680568
H	4.612352	10.920041	11.346058
C	11.366035	6.553827	12.646087
H	10.347556	6.272140	12.918409
C	7.756176	7.832333	12.006074
C	16.219770	8.529334	7.352859
H	16.925278	8.262771	6.569209
C	5.329379	5.705632	9.970282
H	4.690860	6.388542	9.391283
H	4.732496	5.354022	10.819838
H	5.546093	4.844555	9.327714
C	15.787135	9.321919	9.588650
H	16.153706	9.680208	10.549994
C	10.082493	6.921234	9.111040
H	11.007302	6.668545	9.644084
H	10.280126	7.861812	8.572800
H	9.907852	6.145374	8.357440
C	6.284331	9.467978	8.766860
H	6.130297	8.769727	7.947121
C	14.661100	11.342295	14.049427
H	14.737921	11.097289	15.106320
C	11.556289	7.728873	11.905191
C	9.606165	12.273660	13.115680
H	9.238890	13.249968	12.800099

C	6.620142	7.128627	11.596842
H	5.726932	7.163231	12.224914
C	9.342314	16.091106	9.800378
H	9.339690	17.169657	9.659913
C	16.686562	8.977240	8.584874
H	17.755869	9.060184	8.765706
C	12.883450	8.039018	11.553359
C	13.956336	7.215959	11.911477
H	14.970482	7.476517	11.605743
C	15.117397	12.568502	13.581861
H	15.554779	13.286688	14.271762
C	10.506215	14.069497	10.406447
H	11.414685	13.562246	10.734016
C	14.850954	8.428934	7.120019
H	14.484419	8.085958	6.155374
C	5.230381	9.800796	9.610396
H	4.244131	9.373372	9.441344
C	15.008689	12.879974	12.227610
H	15.362587	13.839579	11.857396
H	11.988914	11.575313	9.569478
H	10.489479	9.048206	10.296623
X	7.754995	5.943167	9.042293
X	5.936740	9.492216	9.407484
X	7.003101	8.400778	13.638838
X	16.027454	9.556335	10.228666
X	17.400454	9.032234	8.704536
X	15.245028	13.521326	11.981612
X	6.027976	11.092189	10.520512
X	12.303567	5.129466	13.403370
X	7.591606	15.680223	9.306005
X	9.927058	15.784085	10.024021
X	13.746612	6.784803	12.546899
X	10.096753	12.126104	13.706803
X	4.938095	5.477003	10.539670
X	13.087579	5.887163	12.847462
X	15.100794	11.780851	13.661841

X	4.884798	10.836510	11.123583
X	13.237063	8.734862	8.000216
X	7.253962	11.060236	10.488472
X	11.224442	10.617267	10.236265
X	10.703547	10.724500	15.507221
X	15.084570	9.277624	9.501552
X	8.121836	6.941955	9.790448
X	15.410190	13.050326	14.041264
X	10.452406	14.740873	10.007483
X	4.922931	6.170190	9.592454
X	6.017327	7.153538	12.022852
X	13.432500	7.655058	11.722763
X	14.584002	12.007834	13.749835
X	5.798437	9.925927	9.066293
X	7.511882	10.699793	9.427845
X	13.834370	10.786922	12.503182
X	14.604465	8.200804	6.477462
X	15.468155	8.792646	7.266148
X	9.370852	12.533219	10.260141
X	6.808248	6.584134	11.166221
X	10.772349	10.469977	14.163532
X	8.206182	7.975405	11.356373
X	12.417087	9.932637	10.331193
X	14.369619	12.131105	10.646856
X	13.868757	9.787313	13.414855
X	12.324289	7.671367	11.513561
X	6.161871	10.637000	10.847378
X	9.342815	16.812584	9.707114
X	5.479960	5.135055	9.542561
X	11.104995	10.252438	9.887457
X	8.422264	7.529723	11.640597
X	7.152335	6.354459	10.026705
X	14.453201	12.466917	11.952037
X	14.303275	9.271757	8.658251
X	16.150837	8.843199	9.086251
X	11.012700	10.372925	10.191891

X	14.391098	8.596286	7.616457
X	9.558290	11.962491	13.824128
X	13.675977	6.491154	12.054118
X	13.029164	8.720589	11.133269
X	8.947981	13.672161	9.689690
X	9.902338	12.604798	14.927363
X	13.646623	10.218696	11.302412
X	11.767663	11.198333	9.744535
X	10.245136	10.284657	14.303750
X	11.027302	8.129875	11.730545
X	11.523679	10.479230	10.107853
X	7.597417	13.594353	9.585125
X	10.225591	11.455728	14.648208
X	9.515171	8.226194	11.371032
X	5.316590	10.239143	10.146098
X	8.190446	14.658221	9.626513
X	7.691004	9.268842	13.231989
X	15.481488	8.254912	7.446497
X	8.178396	8.353148	13.770504
X	11.103997	13.731693	10.624080
X	16.140583	9.382872	8.893654
X	8.493081	11.161377	10.197202
X	10.689854	6.367222	12.833138
X	9.931309	13.666738	10.288959
X	10.292889	14.805588	10.555195
X	14.712071	11.176459	14.754622
X	10.682920	6.757411	9.470982
X	8.929814	7.441822	10.616847
X	6.634661	7.052428	10.879605
X	11.461665	7.148393	12.278548
X	10.397264	9.879891	13.214624
X	11.176093	10.607378	9.913122
X	12.389977	7.973551	11.985593
X	6.920185	9.739033	8.866297
X	14.631741	7.396141	11.707450
X	5.950908	6.037016	10.193345

X	10.880742	9.168202	14.096548
X	15.074202	12.736715	12.906171
X	11.098372	15.831942	10.374498
X	4.569154	9.516364	9.498850
X	8.778516	13.741841	10.231766
X	10.197664	7.553808	8.766379
X	11.973705	6.400451	13.007879
X	7.623982	10.258684	9.768053
X	14.973096	12.239199	11.845597
X	10.556884	9.170222	10.514327
X	14.297482	8.742622	8.850134
X	8.719100	15.630256	9.967819
X	9.699503	10.627348	12.467743
X	9.660038	11.766389	12.624912
X	6.182171	9.006438	8.217467
X	11.323210	10.329591	10.335152
X	8.312972	6.479066	10.083135
X	16.467766	8.749565	7.965003
X	14.345725	10.560113	12.405436
X	9.553748	11.391429	11.396370
X	9.506155	6.987280	9.572910
X	7.708712	8.205238	12.668456
X	8.889195	15.560034	9.427213
X	8.102537	9.825217	8.559689
X	11.337508	10.131900	10.089754
X	14.381251	10.874187	13.612342
X	14.203919	11.331073	11.557972
X	10.231034	10.794536	12.379234
X	16.692898	8.352101	6.830531
X	14.286122	5.630291	12.834522
X	11.918725	6.111490	12.512191
X	10.096600	11.125182	10.046271
X	13.886544	9.400378	9.928130
X	6.813792	11.644403	11.470475
X	9.959392	6.403267	8.607548
X	7.187100	7.472917	11.810276

X	11.399121	10.354856	9.815689
X	9.357930	12.920833	12.901737
X	10.249049	9.419557	12.106971

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[1.1.1.]propellane

C	6.514210	7.558939	7.303135
C	7.383098	6.431326	6.609468
C	6.075485	6.910148	5.999273
H	5.223850	6.228518	6.040640
H	6.137782	7.516375	5.093708
C	7.943027	7.823853	6.855618
H	8.701406	7.928145	7.633154
H	8.086111	8.468671	5.986806
C	6.827696	6.251303	8.013714
H	7.538825	6.287255	8.840454
H	6.010363	5.539484	8.142392
X	6.281370	5.778716	8.095284
X	7.840568	6.995128	6.626218
X	8.034317	8.251443	6.274669
X	5.508713	6.455303	6.030587
X	6.120366	7.314901	5.396147
X	7.303036	6.278453	8.563713
X	6.537987	7.040229	7.813157
X	8.446756	7.890252	7.375968
X	6.819359	6.501310	6.155056
X	6.949770	6.995846	6.956536
X	7.142553	7.898550	7.176544
X	6.123788	7.396435	6.711479
X	7.227180	6.138937	7.255437

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bicyclo[1.1.1]pentane

C	6.469038	7.670979	7.397861
C	7.503537	6.326742	6.579126
C	6.151812	6.915469	6.071154
H	5.286688	6.241527	6.086858
H	6.189214	7.508329	5.149212
C	7.939904	7.790986	6.893263
H	8.713312	7.918069	7.660360
H	8.110534	8.448080	6.031845
C	6.868966	6.288843	8.003892
H	7.565540	6.306815	8.850788
H	6.057736	5.567711	8.160649
H	5.869157	8.453401	7.869308
H	8.103289	5.546600	6.103878
X	6.319048	5.802554	8.106269
X	8.051956	8.233487	6.308987
X	7.905986	5.802463	6.260633
X	5.567306	6.459228	6.085063
X	7.341201	6.303814	8.575883
X	6.211896	7.351827	6.718713
X	6.066604	8.196474	7.714295
X	6.613289	7.002799	7.801623
X	6.180405	7.316855	5.447750
X	6.827488	6.552810	6.231006
X	7.211884	7.841492	7.178226
X	7.227884	6.202344	7.313002
X	7.828069	7.041201	6.692289
X	8.461675	7.874098	7.413784

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$Cp_2Sc(CH_4)(CH_3)$ Transition state

Sc	6.923748	7.078749	7.012967
C	6.962066	8.788878	5.331382
C	6.912377	9.177315	8.174711
H	6.929712	8.955390	6.756700
C	5.017362	6.056009	8.278979
C	4.496478	7.229286	7.664779
C	4.521100	7.037337	6.261501
C	9.441399	7.364592	7.017834
C	9.136986	6.446883	5.978861
C	8.594168	5.276175	6.569827
C	5.347899	5.134566	7.251265
C	5.057300	5.744710	6.003150
C	9.097282	6.757845	8.253859
C	8.569550	5.468985	7.980403
H	5.121982	5.884565	9.350035
H	4.139676	8.117085	8.182474
H	4.186520	7.751864	5.512496
H	9.860324	8.360746	6.888982
H	9.289797	6.614680	4.913654
H	8.270791	4.382360	6.039044
H	7.892578	9.328016	5.092950
H	6.914242	7.914223	4.649965
H	6.105609	9.431950	5.073578
H	5.760715	4.138008	7.394827
H	5.197929	5.292510	5.021705
H	9.214301	7.205981	9.239583
H	8.224004	4.748833	8.720124
H	6.837033	8.517188	9.063643
H	7.836709	9.764941	8.291655
H	6.050643	9.861993	8.221081
X	6.897756	6.867009	6.796681
X	6.710809	7.283292	6.978968
X	6.895299	6.945984	7.284977
X	7.192314	7.206570	6.993696
X	9.170918	7.057630	8.911389
X	4.261240	7.819905	8.011708
X	5.031722	5.369304	6.592726
X	9.721225	8.028487	6.932288
X	4.300670	7.511204	5.760243
X	8.375293	4.679794	6.218823
X	6.930405	8.174598	4.915535
X	6.339214	9.624221	8.200598
X	5.016734	5.534829	7.812399
X	8.336330	4.988296	8.471091
X	5.089371	5.945377	8.994446
X	9.234368	6.560192	5.267434
X	5.625726	4.470139	7.346735
X	9.047074	5.755295	6.295552
X	7.582007	9.140368	5.180113
X	8.852268	7.126428	7.049041
X	7.528035	9.560026	8.247361
X	9.422914	6.892325	6.493154
X	9.013638	6.005001	8.130811
X	5.153291	5.447345	5.346907
X	4.676216	6.623693	8.022428
X	6.863752	8.698087	8.739420
X	6.391784	9.209161	5.167652
X	4.310656	7.047860	6.970298
X	9.405675	7.048624	7.647836
X	8.621915	5.300940	7.286092
X	4.978911	7.196161	6.958285
X	4.713134	6.360923	6.086059
X	6.941452	8.582886	6.043577
X	5.506390	5.905936	6.480808
X	8.379189	6.203570	7.922624
X	5.473318	6.111091	7.798734
X	8.407252	6.003164	6.419929
X	6.915028	8.789271	7.545248

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$Cp^*Ir(PMe_3)(CH_4)(CH_3)^+$ Transition state

Ir	8.193364	7.958334	6.807142
P	5.898842	7.963057	7.319712
C	7.685266	9.653528	5.577365
C	7.753150	6.037506	5.675270
H	8.061686	7.453094	5.289398
C	9.707132	6.845901	8.192364
C	9.073213	7.853520	8.975761
C	9.308119	9.139775	8.341041
C	10.193617	8.913486	7.207908
C	10.396262	7.502257	7.085480
C	9.782264	5.381898	8.506883
C	8.402125	7.653341	10.301684
C	8.990865	10.483773	8.930371
C	10.868828	9.981417	6.403057
C	11.309886	6.815946	6.113532
C	5.313422	9.494440	8.157602
C	4.722179	7.781179	5.910089
C	5.359341	6.611344	8.453139
H	8.517794	9.864114	4.890406
H	6.784516	9.523363	4.961100
H	7.535359	10.536204	6.219351
H	8.116314	10.447619	9.594252
H	9.842446	10.848273	9.530375
H	8.795066	11.236613	8.153580
H	7.571890	8.354771	10.464397
H	8.025485	6.629552	10.428234
H	9.132881	7.832416	11.109594
H	8.953106	5.053904	9.148910
H	9.773070	4.763387	7.597899
H	10.721440	5.154802	9.040257
H	11.433583	7.393219	5.187404
H	12.309447	6.690038	6.563901
H	10.950426	5.811936	5.846189
H	10.239515	10.873983	6.287867
H	11.794927	10.295392	6.914734
H	11.148649	9.628653	5.401085
H	8.654441	5.637261	5.192706
H	7.489264	5.393829	6.524710
H	6.929969	6.015543	4.948927
H	4.273292	6.671394	8.624012
H	5.595819	5.634667	8.005559
H	5.877679	6.694677	9.417709
H	4.857191	6.804907	5.423499
H	3.690553	7.846500	6.288555
H	4.881618	8.575117	5.168137
H	5.877673	9.646979	9.088357
H	5.477390	10.360214	7.500367
H	4.241024	9.415117	8.392860
X	8.261507	7.815944	6.357500
X	8.469687	7.948859	7.066028
X	7.972231	8.237099	6.988766
X	8.337049	7.604667	6.677176
X	11.944063	6.748283	6.426697
X	10.391514	5.263747	8.846572
X	8.864080	10.963931	8.408001
X	5.427474	10.040233	7.719590
X	8.889892	7.773336	10.799362
X	10.444737	10.557037	6.338780
X	9.228792	5.182970	8.927811
X	8.353474	5.788949	5.366367
X	4.657295	6.672588	8.546057
X	4.842578	8.302248	5.442867
X	8.246040	9.783272	5.131557
X	11.379470	7.205288	5.512497
X	8.719140	7.751954	9.619220
X	5.245090	7.859800	6.508441
X	10.833120	7.161556	6.597307
X	9.138133	9.800785	8.626966
X	9.531833	7.350719	8.677375
X	9.772433	4.994018	7.899792
X	7.937868	6.968270	5.833511

X	4.065085	7.826244	6.179892
X	4.828952	7.143167	5.610885
X	5.691849	9.572598	8.760802
X	10.510088	9.438391	6.799883
X	7.855081	8.119656	10.388949
X	11.458887	10.162340	6.753201
X	10.126410	7.146055	7.673536
X	4.620263	9.417799	8.298298
X	5.522542	5.987262	8.145523
X	5.705937	6.683015	9.072498
X	11.056692	6.159045	5.949321
X	9.552534	10.696276	9.310234
X	8.409941	10.442273	9.363728
X	8.155825	6.976440	10.367498
X	7.210509	6.040156	5.203913
X	7.583229	5.641312	6.246678
X	10.439777	8.208599	7.235306
X	9.733023	6.121802	8.340784
X	11.043873	9.734499	5.749516
X	7.588170	10.234529	6.021900
X	7.075561	9.555097	5.176853
X	8.896723	8.682520	7.780664
X	5.606001	7.190909	7.968824
X	5.575478	8.835402	7.798102
X	9.262934	8.526218	8.736847
X	9.840270	9.062572	7.849637
X	6.850634	7.951435	7.112675
X	7.884675	8.879049	6.105529
X	8.374384	8.239965	6.653154
X	9.007530	7.347528	8.069962
X	7.857506	7.919902	6.586164
X	9.691371	8.034050	6.914546
X	7.987611	7.758161	7.090050

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$(acac)_2Ir(CH_2CH_2Ph)(C_6H_6)$ Transition state

Ir	11.877612	9.985737	9.631074
O	12.133327	10.960869	7.854299
O	11.343480	11.805577	10.620512
O	13.789306	10.657166	10.157728
O	11.610850	9.071104	11.432585
C	9.731487	9.858607	9.280204
C	12.853024	8.301059	8.902449
H	11.041889	8.946570	8.832909
C	12.015104	12.230543	7.703337
C	11.654986	13.177672	8.677721
C	11.353516	12.939948	10.035227
C	14.344672	10.374955	11.274240
C	13.771557	9.639467	12.330494
C	12.491167	9.063238	12.368040
C	12.318331	12.696113	6.298043
C	10.995534	14.110950	10.922917
C	15.749673	10.909348	11.424072
C	12.040972	8.334289	13.611830
C	7.458660	8.882400	9.777723
C	6.712262	8.543575	8.637859
C	5.337824	8.789891	8.577237
C	4.682504	9.383635	9.660077
C	5.412904	9.726491	10.801991
C	6.786943	9.477532	10.857708
C	8.954375	8.648052	9.827695
C	12.641617	7.013819	9.430780
C	13.823606	8.447523	7.894690
C	14.571329	7.350874	7.451778
C	14.360209	6.080408	7.995098
C	13.388986	5.917258	8.986164
H	11.723446	12.110001	5.580456
H	12.115255	13.765687	6.156986
H	13.379448	12.499090	6.072867
H	9.992751	13.949517	11.350116
H	11.700233	14.149920	11.769271
H	11.013628	15.070981	10.390281
H	16.392342	10.442190	10.660013
H	15.751770	11.993150	11.227888
H	16.172049	10.715275	12.418746
H	11.849393	7.276998	13.366007
H	12.782507	8.386585	14.419545
H	11.088343	8.762198	13.961940
H	11.607585	14.213656	8.344320
H	14.385561	9.508220	13.220538
H	7.215624	8.073309	7.788207
H	4.775479	8.512815	7.682045
H	3.607658	9.574163	9.616075
H	4.909165	10.186067	11.656112
H	7.350502	9.744428	11.756226
H	9.433562	10.764094	9.828234
H	9.497841	10.021351	8.215065
H	9.203059	7.742364	9.248334
H	9.272516	8.460571	10.863618
H	11.884675	6.864636	10.204002
H	13.205539	4.929018	9.417183
H	14.943715	5.224998	7.645951
H	15.325149	7.493651	6.672215
H	13.996657	9.430053	7.454347
X	12.014546	10.339918	9.562848
X	11.610501	10.126771	9.374089
X	11.992710	10.053668	9.980771
X	11.560415	9.932038	9.849445
X	11.809287	9.296374	11.789331
X	12.319973	11.389869	7.893555
X	14.036860	10.359583	10.422888
X	11.116808	12.119546	10.358383
X	5.098958	9.247767	10.279745
X	13.943394	9.098105	7.600493
X	12.538514	8.374683	14.141569
X	12.181104	13.406723	6.214990

X	9.582886	9.957227	8.569934
X	15.733159	11.613458	11.299118
X	11.463793	14.123464	11.461872
X	4.995693	9.087234	9.109047
X	12.133936	6.914691	9.945740
X	14.750066	5.505285	7.762951
X	7.052574	8.229977	8.070206
X	11.873434	12.686300	8.219858
X	13.144753	9.318460	12.303640
X	9.116567	8.049129	9.434027
X	7.163121	9.656929	11.459880
X	11.542166	13.038512	9.361043
X	14.183357	9.548820	12.926018
X	14.175172	6.693642	7.603986
X	13.187213	8.189126	8.185663
X	4.960253	8.605643	7.979435
X	11.338041	8.934357	11.475553
X	12.051132	10.772127	8.305712
X	13.935950	10.822701	9.948381
X	11.274714	11.790245	10.916130
X	3.963001	9.510228	9.628686
X	12.873235	6.498816	8.924208
X	14.054015	9.959668	11.769595
X	11.626649	13.872760	8.454373
X	7.054638	9.439840	10.152857
X	11.605013	9.564451	9.303415
X	11.853502	11.326964	7.779454
X	11.993206	8.879331	11.624836
X	7.101078	8.708364	9.198188
X	15.048041	10.640663	11.362691
X	10.342453	13.991735	11.185822
X	12.162231	12.472658	7.003879
X	16.149380	10.594023	10.926706
X	13.266768	5.254483	9.274611
X	15.075393	7.450228	6.929907
X	5.197763	9.767747	10.057652
X	11.175261	13.539136	10.469480
X	6.100757	9.608762	10.840292
X	11.424621	8.625474	13.827558
X	11.010165	14.745120	10.561452
X	16.021481	10.776281	12.087708
X	9.340177	9.244699	9.553331
X	12.273891	8.702538	12.994642
X	14.199100	7.907143	7.673903
X	13.008575	12.564183	6.173799
X	13.881011	5.981552	8.493647
X	6.086422	8.976492	8.612629
X	11.922178	12.310889	5.844578
X	11.925892	7.651939	13.433783
X	13.837084	10.757406	10.608561
X	11.584224	12.182478	10.469995
X	5.078281	10.034018	11.374485
X	14.573424	6.800750	8.005266
X	9.152410	8.529957	10.511293
X	8.212953	8.772442	9.797632
X	11.733503	9.297634	11.006516
X	12.370585	9.016764	9.198588
X	9.550296	10.450891	9.645130
X	12.729033	7.669149	9.186788
X	12.216596	10.788520	7.615928
X	13.354902	10.469060	10.091300
X	10.684546	9.707023	9.321590
X	11.454370	11.446571	10.353153
X	5.985080	8.456523	8.835781
X	11.589088	12.923636	8.717846
X	13.578909	9.752491	12.167158
X	6.951713	8.921029	10.372448
X	13.268157	6.599994	9.336556
X	13.578219	8.306545	8.592251
X	11.986098	9.645791	9.762031
X	12.138691	9.923913	9.356343