

## Supplementary Material

### Synthesis of an extremely sterically shielding *N*-heterocyclic carbene ligand

**Simone G. Weber, Christian Loos, Frank Rominger, and Bernd F. Straub\***

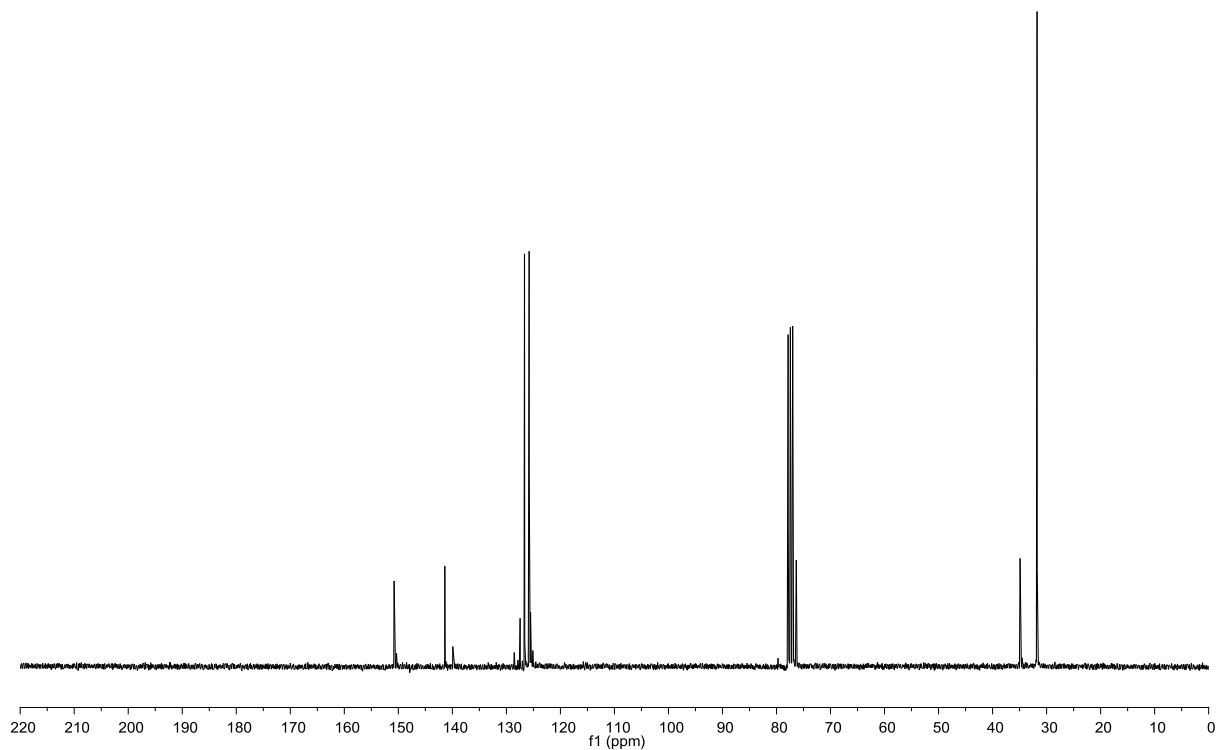
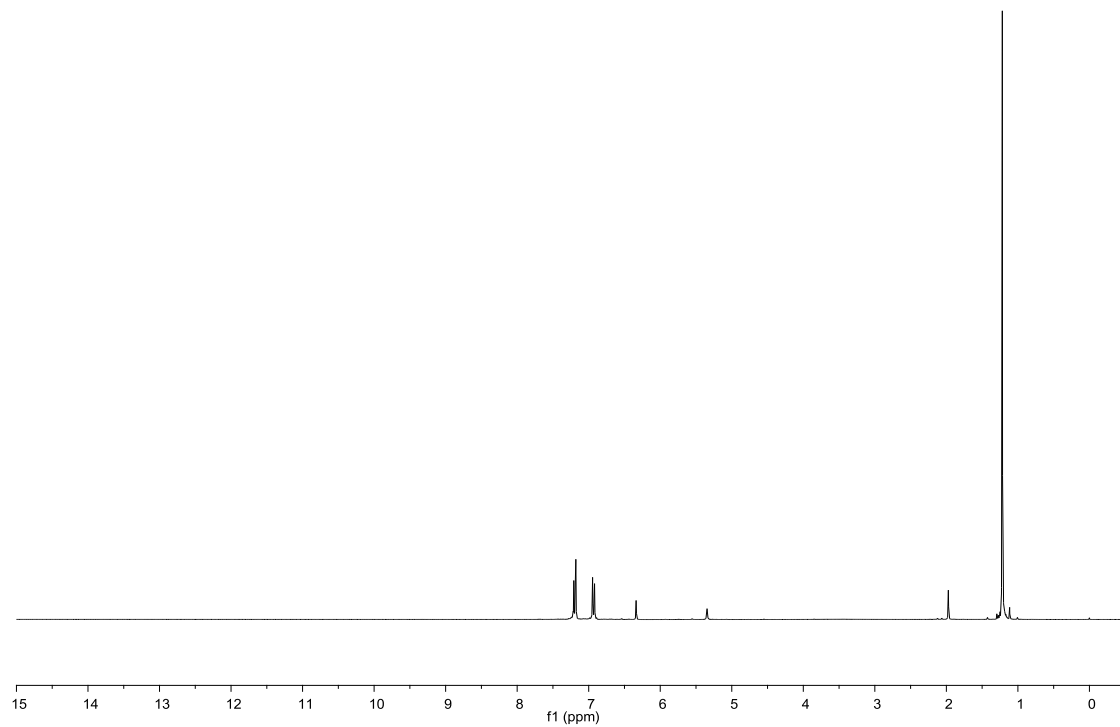
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Heidelberg, Germany*

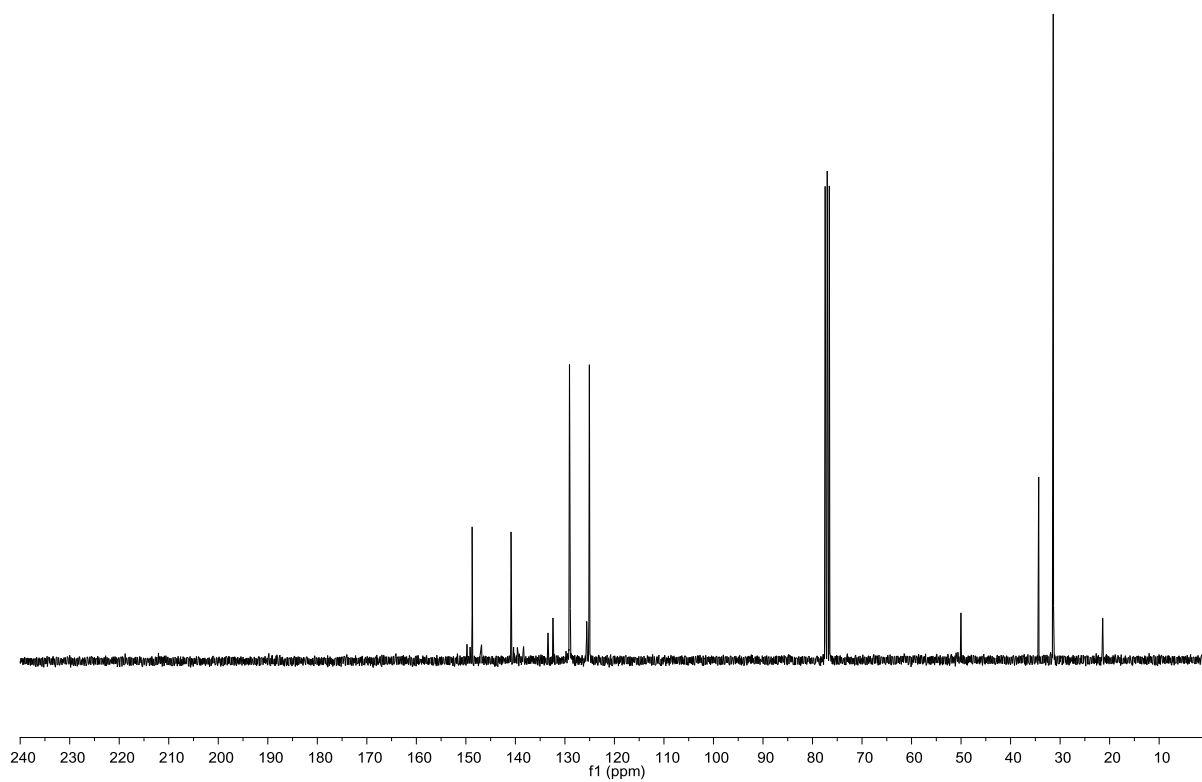
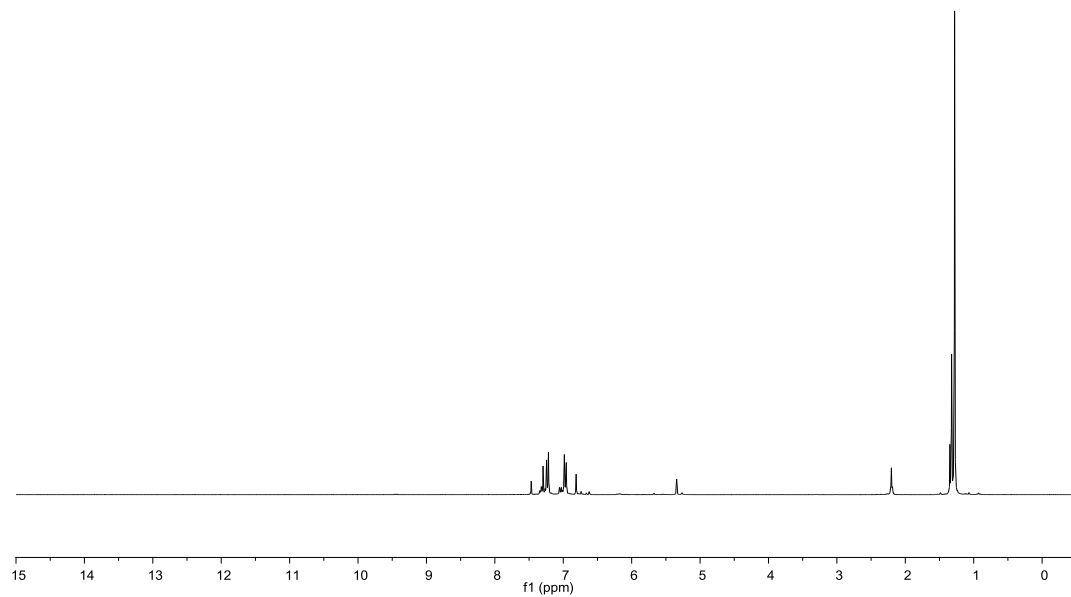
*E-mail: [straub@oci.uni-heidelberg.de](mailto:straub@oci.uni-heidelberg.de)*

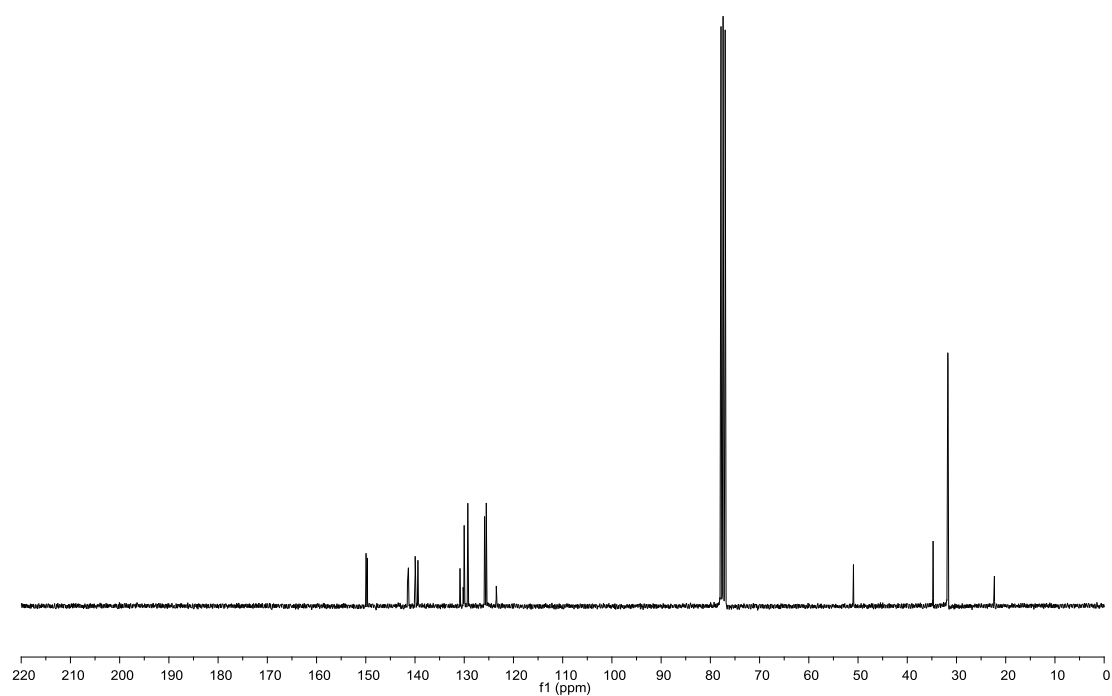
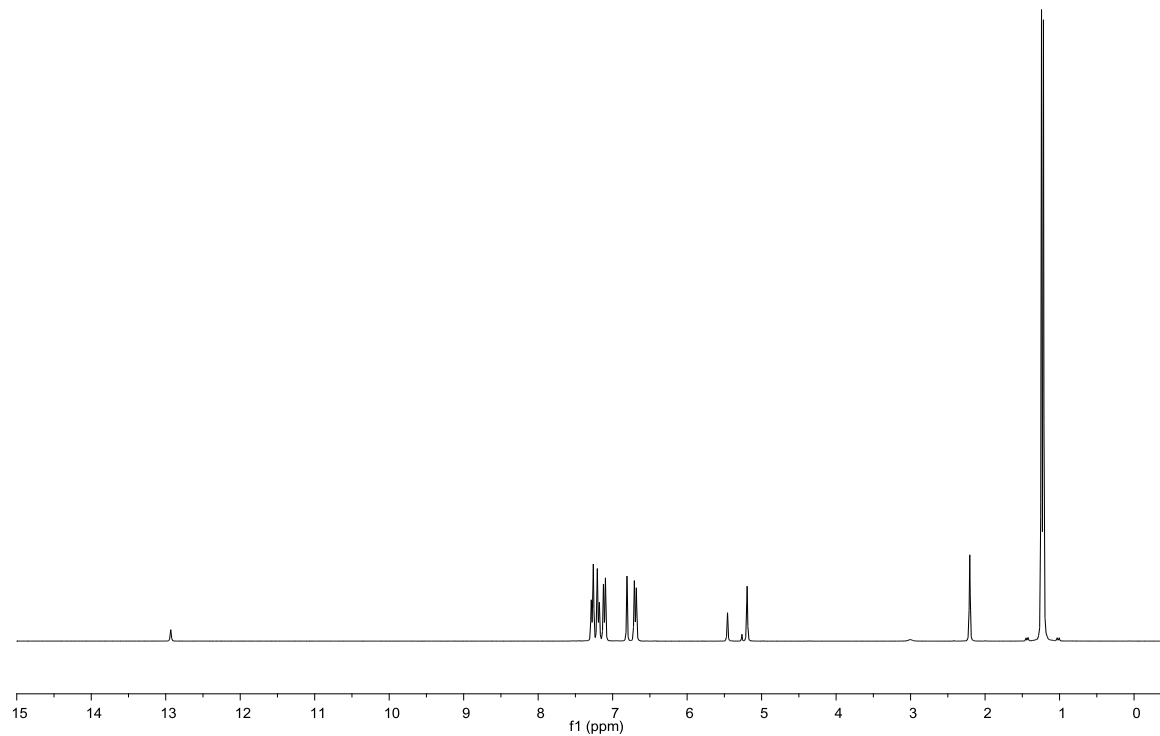
**Dedicated to Prof. Dr. Rainer Beckert on the occasion of his 60<sup>th</sup> birthday**

Figures of proton and carbon 13 spectra of compounds **1**, **2**, **3** and **4** are included.

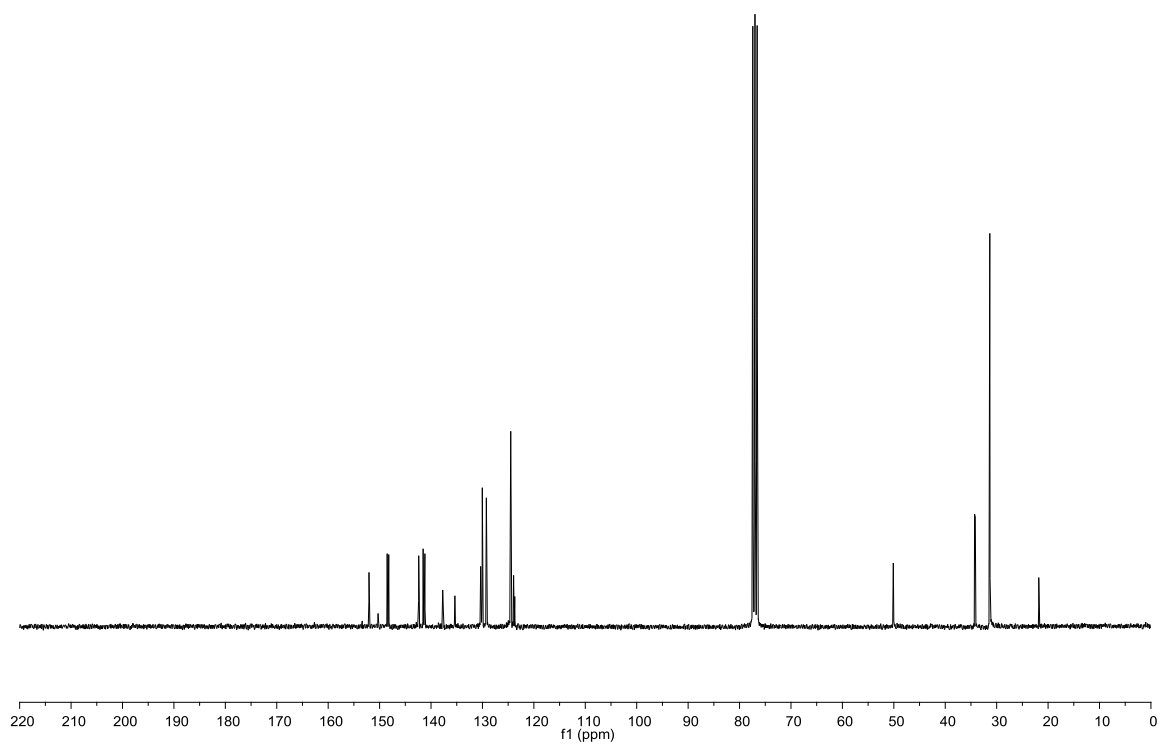
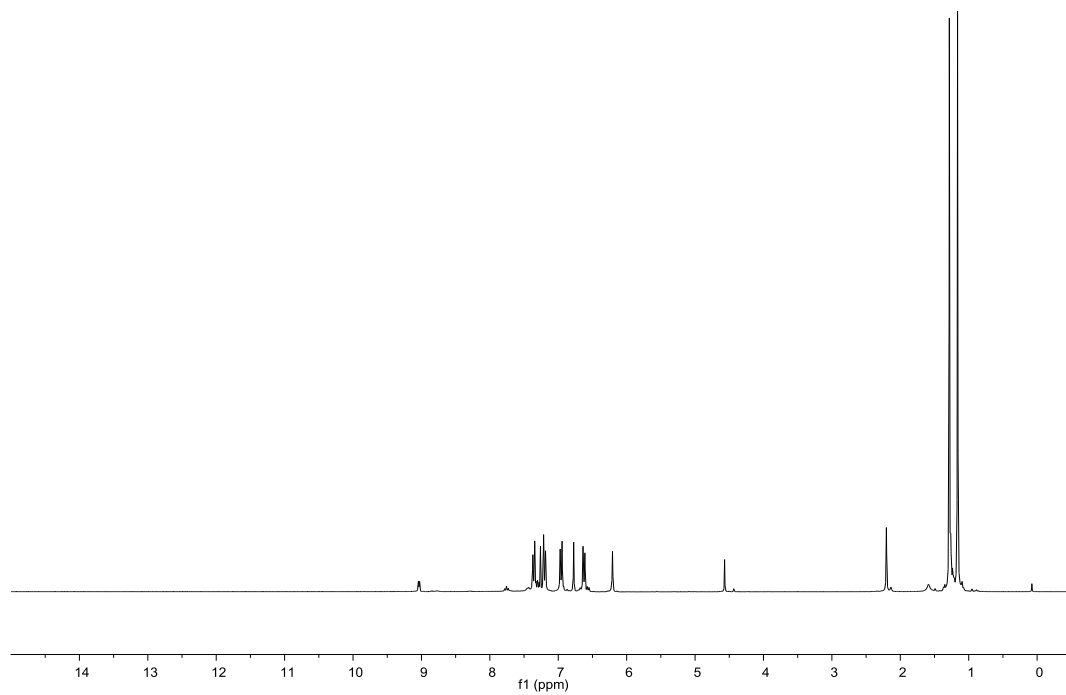
Cartesian coordinates and SCF energies from DFT structure optimizations of (IPr<sup>\*\*</sup>)AgCl, (IPr<sup>\*\*</sup>)AuCl, (IPr)Pd(py)Cl<sub>2</sub>, (IPr<sup>\*</sup>)Pd(py)Cl<sub>2</sub>, and (IPr<sup>\*\*</sup>)Pd(py)Cl<sub>2</sub> are included (BP86/LACVP<sup>\*\*</sup>, Jaguar version 7.8).

**2,6-Bis[bis(4-*tert*-butylphenyl)methyl]-4-methylaniline (1)**

***N,N'*-Bis{2,6-bis[bis(4-*tert*-butylphenyl)methyl]-4-methylphenyl}-1,4-diazabutadiene (2)**

**1,3-Bis{2,6-bis[bis(4-*tert*-butylphenyl)methyl]-4-methylphenyl}-1*H*-imidazol-3-ium chloride**  
**(3)**

***trans*-Palladium{1,3-bis{2,6-bis[bis(4-*tert*-butylphenyl)methyl]-4-methylphenyl}-1H-imidazol-2-yliden}(κ<sup>1</sup>N-pyridine) dichloride (4)**



**(IPr\*\*)AgCl**

225

Total energy:	-4636.66998447289		
Ag	0.0000000000	0.0000000000	-2.3634310026
Cl	0.0000000000	0.0000000000	-4.7016032339
C	0.0000000000	0.0000000000	-0.2740396914
N	0.7823760571	-0.7482877154	0.5719583520
C	0.4952414194	-0.4708393913	1.9108900335
H	1.0056314307	-0.9734456952	2.7262574766
C	1.8285009682	-1.6615864440	0.1549065546
C	1.4714427499	-2.9683180450	-0.2794789483
C	2.5075649887	-3.8335868733	-0.6615736389
H	2.2465572392	-4.8381474067	-1.0059851589
C	3.8622046271	-3.4535676757	-0.5945834008
C	4.1656718440	-2.1470117572	-0.1942965019
H	5.2107103939	-1.8296865881	-0.1805422654
C	3.1721474243	-1.2254870770	0.1870142134
C	0.0043709646	-3.4424734394	-0.2983141842
H	-0.5974948813	-2.5916842996	-0.6635558002
C	4.9561599557	-4.4251444659	-0.9861985034
H	4.7661180703	-5.4270215136	-0.5693675056
H	5.9388427317	-4.0860300106	-0.6245851316
H	5.0177651892	-4.5300082885	-2.0820590289
C	3.5807203425	0.2065199489	0.5695424696
H	2.6803454278	0.7067127635	0.9679405174
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C	-0.2535981597	-4.5824262134	3.3941889159
H	0.4172654957	-4.9640164467	4.1712152454
C	-1.6275419819	-4.4142518903	3.6756458448
C	-2.4406475987	-3.9588655523	2.6178416893
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C	-1.9064282713	-3.6556576311	1.3559256375
H	-2.5801619844	-3.3336609943	0.5541895132
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C	-0.2755848144	-5.9351577249	-0.8936421251
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C	-0.3156804770	-4.3091935618	-2.6721712228
H	-0.3035751665	-3.2695862092	-3.0194909184
C	-0.5330155774	-7.8235447149	-4.2851732022
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C	4.1758748376	0.4255417627	3.0412486698
H	3.1131233122	0.6046611104	3.2369109517
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H	5.2490117610	2.4137127551	0.5083334879
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H	-1.6815656315	-2.8321497470	5.9965018610
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C	-5.1104766157	-3.0403578075	-1.5504601359
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C	-4.9475855575	-3.7627588936	-4.0033095360
C	2.1869202696	4.7654683862	5.0719714804
C	1.4779522675	3.9047410493	6.1512931655
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H	1.8333293964	4.1785394647	7.1592879244
H	1.6815656315	2.8321497470	5.9965018610
C	3.7105905728	4.5336506764	5.1722648678
H	4.2614702344	5.1355375226	4.4311766772
H	3.9722121496	3.4757040569	5.0038896104
H	4.0701083174	4.8167521711	6.1747565836
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H	0.8283356424	6.4929939999	5.3252132946
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H	-0.3830090946	8.3768938627	-6.1978082771
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H	2.0842103575	8.5254821192	-5.6794311619
H	2.1442578020	6.7692883431	-5.3661284560
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H	1.0715110377	9.4479518365	-2.8936271823
H	-0.6699017808	9.3449414979	-3.2457488104
H	0.4499179346	9.9972861160	-4.4710694726
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H	-7.2194194322	1.9730707956	5.4203235802
H	-6.0770264995	1.0065633732	6.3825011866
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C	-8.9073470130	-0.1081185448	4.6700984660
H	-9.1833886902	-0.9551126746	4.0207689848
H	-9.1125458312	0.8255988690	4.1216469107
H	-9.5673202251	-0.1263592332	5.5523241076
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H	-7.9665117394	-1.5035203215	6.7933721259
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C	-4.1095571494	-3.4718728609	-5.2667482701
H	-3.0307737013	-3.5443761765	-5.0556694421
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H	-4.3547458603	-4.1997543604	-6.0571058731
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H	-5.2542044611	-5.5296451083	-2.6990604255
H	-3.5928295257	-5.3556501519	-3.3145700767
H	-4.8962416756	-5.9223524551	-4.3974312095
C	-6.4542607002	-3.6202457340	-4.3390180870
H	-7.0816304071	-3.8229217839	-3.4558168656
H	-6.7424955619	-4.3296495105	-5.1336867507
H	-6.6861597541	-2.6005128866	-4.6883797209

**(IPr\*\*)AuCl**

225

Total energy: -4626.40172833302

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Cl	0.0000000000	0.0000000000	4.5979635975
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N	-0.7936923790	-0.7458834956	-0.5883175727

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C	-1.8590162936	-1.6530884513	-0.1931913669
C	-3.2021269725	-1.2092456135	-0.2141231741
C	-4.2022191693	-2.1346393571	0.1422008171
H	-5.2470969505	-1.8069690202	0.1385391090
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C	-2.5641306903	-3.8648872526	0.4920114179
H	-2.3155464527	-4.8955149178	0.7719371911
C	-1.5213981456	-2.9886910584	0.1556165185
C	-3.6192488473	0.2206531023	-0.5889428438
H	-2.7274113345	0.7196117610	-1.0155295588
C	-5.0103068058	-4.4301408386	0.8666838913
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H	-6.1572936105	-1.4056413405	-6.2309801520
H	-7.8769346483	-1.5232443825	-6.7019203039
C	-7.3211586202	1.1300031682	-6.0573333724
H	-7.5082279183	2.0885318791	-5.5408287218
H	-8.0268534937	1.0508701788	-6.9051965757
H	-6.3016097650	1.1725599233	-6.4803511023
C	-8.9816631344	-0.1014882634	-4.6404704229
H	-9.2592484626	0.8091021390	-4.0789729874
H	-9.2023971767	-0.9792392720	-4.0064728245

H	-9.6396528666	-0.1627718432	-5.5261665320
C	-4.0016113047	1.0499197137	0.6485107824
C	-3.4421585377	0.7514651291	1.9031169312
H	-2.8158957414	-0.1395673159	2.0283631030
C	-3.6466076853	1.5814766986	3.0141752610
H	-3.1600663171	1.3026207558	3.9549880587
C	-4.4283559453	2.7484199471	2.9253299761
C	-5.0080993659	3.0306952079	1.6675715663
H	-5.6363288855	3.9226674008	1.5446462209
C	-4.7989324485	2.2088238164	0.5513670031
H	-5.2642865006	2.4727202187	-0.4068492496
C	-4.6642313855	3.6873531130	4.1268586897
C	0.4972405771	-3.6793939657	-1.2806100592
C	-0.2954428448	-4.0702943349	-2.3778918969
H	-1.3783648750	-4.1975602507	-2.2461234722
C	0.2813169947	-4.3130768786	-3.6346787545
H	-0.3752823757	-4.6187784388	-4.4605826915
C	1.6686077638	-4.1726499224	-3.8613182690
C	2.4517400678	-3.7765447637	-2.7566071489
H	3.5346662028	-3.6507797612	-2.8653115279
C	1.8796827950	-3.5353189685	-1.4973831991
H	2.5302719908	-3.2581941451	-0.6559567867
C	2.2640653579	-4.4718165051	-5.2552211034
C	0.1244880826	-4.7266644913	1.0015595810
C	0.2272251292	-6.0172342150	0.4551173248
H	0.2473370501	-6.1458960087	-0.6336281475
C	0.3089834377	-7.1511884213	1.2802509176
H	0.3805702650	-8.1354146464	0.8039261539
C	0.2831558927	-7.0431808736	2.6827701161
C	0.2096655947	-5.7377484055	3.2229176638
H	0.2080963705	-5.5988350988	4.3118811562
C	0.1351878373	-4.6034529091	2.4058978563
H	0.0662660233	-3.6051891555	2.8597218360
C	0.3597269822	-8.2646285989	3.6226832896
C	-4.3055820914	5.1440761935	3.7316693889
H	-4.9205005988	5.5124019019	2.8912742179
H	-3.2453689463	5.2226201047	3.4307968285
H	-4.4717526909	5.8237211646	4.5886348248
C	-3.8031639998	3.2936823037	5.3490700196
H	-3.9757296238	4.0106080263	6.1729111358

H	-2.7244118841	3.3038360242	5.1107178896
H	-4.0570588000	2.2885197322	5.7316388366
C	-6.1627543357	3.6227126606	4.5299593603
H	-6.8209695304	3.9077872648	3.6890496402
H	-6.3696892942	4.3095753515	5.3728021618
H	-6.4450200970	2.6009496941	4.8441691654
C	3.7984269146	-4.2994259625	-5.2848181884
H	4.3021936336	-4.9888604971	-4.5827030474
H	4.1047924613	-3.2694898745	-5.0245703503
H	4.1807951575	-4.5170057286	-6.2989666524
C	1.9312666363	-5.9363266263	-5.6511921304
H	0.8421458808	-6.1186078654	-5.6801525846
H	2.3709815776	-6.6492236908	-4.9302654308
H	2.3387481864	-6.1677549112	-6.6534539909
C	1.6440808449	-3.5072839484	-6.3003985294
H	0.5444351541	-3.6017201176	-6.3472643086
H	2.0438893221	-3.7205921735	-7.3096695908
H	1.8801387830	-2.4552402155	-6.0561934483
C	0.3913342286	-9.5990514279	2.8450988661
H	1.2767111534	-9.6761047866	2.1879070293
H	-0.5094060607	-9.7266926048	2.2163505531
H	0.4275057629	-10.4450998344	3.5544710673
C	-0.8835013526	-8.2820255078	4.5524360483
H	-0.8392458281	-9.1500498908	5.2369133677
H	-1.8165922930	-8.3590985578	3.9648248804
H	-0.9521185545	-7.3712054407	5.1729884365
C	1.6483890158	-8.1651384136	4.4828777241
H	2.5496401051	-8.1610627343	3.8434335752
H	1.7206350927	-9.0250556472	5.1754088678
H	1.6635038342	-7.2411395972	5.0877297377
N	0.7936923790	0.7458834956	-0.5883175727
C	0.4941991579	0.4706731451	-1.9251147416
H	1.0052173177	0.9837998572	-2.7359532829
C	1.8590162936	1.6530884513	-0.1931913669
C	3.2021269725	1.2092456135	-0.2141231741
C	4.2022191693	2.1346393571	0.1422008171
H	5.2470969505	1.8069690202	0.1385391090
C	3.9118795775	3.4574442356	0.4902030559
C	2.5641306903	3.8648872526	0.4920114179
H	2.3155464527	4.8955149178	0.7719371911

C	1.5213981456	2.9886910584	0.1556165185
C	3.6192488473	-0.2206531023	-0.5889428438
H	2.7274113345	-0.7196117610	-1.0155295588
C	5.0103068058	4.4301408386	0.8666838913
H	6.0109112043	3.9884551289	0.7202096695
H	4.9273166815	4.7347816600	1.9269417434
H	4.9541753567	5.3540082642	0.2613435130
C	0.0619841622	3.4721350176	0.1339134242
H	-0.5477818950	2.6726507542	0.5985152347
C	4.6612182851	-0.1944786439	-1.7160079292
C	6.0430976957	-0.0480711290	-1.4872310436
H	6.4243337347	-0.0123353297	-0.4596892340
C	6.9569520985	0.0263866045	-2.5503239898
H	8.0207513476	0.1362921289	-2.3121590202
C	6.5377612062	-0.0580500475	-3.8929230117
C	5.1519086353	-0.2136349361	-4.1158428793
H	4.7699840875	-0.2744583341	-5.1434509490
C	4.2384846629	-0.2919895567	-3.0563618412
H	3.1697922345	-0.4223728642	-3.2739296606
C	7.5034155340	0.0685635391	-5.0906038354
C	7.1922538867	1.3924648204	-5.8426670892
H	7.3063841014	2.2636386582	-5.1725989103
H	6.1572936105	1.4056413405	-6.2309801520
H	7.8769346483	1.5232443825	-6.7019203039
C	7.3211586202	-1.1300031682	-6.0573333724
H	7.5082279183	-2.0885318791	-5.5408287218
H	8.0268534937	-1.0508701788	-6.9051965757
H	6.3016097650	-1.1725599233	-6.4803511023
C	8.9816631344	0.1014882634	-4.6404704229
H	9.2592484626	-0.8091021390	-4.0789729874
H	9.2023971767	0.9792392720	-4.0064728245
H	9.6396528666	0.1627718432	-5.5261665320
C	4.0016113047	-1.0499197137	0.6485107824
C	3.4421585377	-0.7514651291	1.9031169312
H	2.8158957414	0.1395673159	2.0283631030
C	3.6466076853	-1.5814766986	3.0141752610
H	3.1600663171	-1.3026207558	3.9549880587
C	4.4283559453	-2.7484199471	2.9253299761
C	5.0080993659	-3.0306952079	1.6675715663
H	5.6363288855	-3.9226674008	1.5446462209

C	4.7989324485	-2.2088238164	0.5513670031
H	5.2642865006	-2.4727202187	-0.4068492496
C	4.6642313855	-3.6873531130	4.1268586897
C	-0.4972405771	3.6793939657	-1.2806100592
C	0.2954428448	4.0702943349	-2.3778918969
H	1.3783648750	4.1975602507	-2.2461234722
C	-0.2813169947	4.3130768786	-3.6346787545
H	0.3752823757	4.6187784388	-4.4605826915
C	-1.6686077638	4.1726499224	-3.8613182690
C	-2.4517400678	3.7765447637	-2.7566071489
H	-3.5346662028	3.6507797612	-2.8653115279
C	-1.8796827950	3.5353189685	-1.4973831991
H	-2.5302719908	3.2581941451	-0.6559567867
C	-2.2640653579	4.4718165051	-5.2552211034
C	-0.1244880826	4.7266644913	1.0015595810
C	-0.2272251292	6.0172342150	0.4551173248
H	-0.2473370501	6.1458960087	-0.6336281475
C	-0.3089834377	7.1511884213	1.2802509176
H	-0.3805702650	8.1354146464	0.8039261539
C	-0.2831558927	7.0431808736	2.6827701161
C	-0.2096655947	5.7377484055	3.2229176638
H	-0.2080963705	5.5988350988	4.3118811562
C	-0.1351878373	4.6034529091	2.4058978563
H	-0.0662660233	3.6051891555	2.8597218360
C	-0.3597269822	8.2646285989	3.6226832896
C	4.3055820914	-5.1440761935	3.7316693889
H	4.9205005988	-5.5124019019	2.8912742179
H	3.2453689463	-5.2226201047	3.4307968285
H	4.4717526909	-5.8237211646	4.5886348248
C	3.8031639998	-3.2936823037	5.3490700196
H	3.9757296238	-4.0106080263	6.1729111358
H	2.7244118841	-3.3038360242	5.1107178896
H	4.0570588000	-2.2885197322	5.7316388366
C	6.1627543357	-3.6227126606	4.5299593603
H	6.8209695304	-3.9077872648	3.6890496402
H	6.3696892942	-4.3095753515	5.3728021618
H	6.4450200970	-2.6009496941	4.8441691654
C	-3.7984269146	4.2994259625	-5.2848181884
H	-4.3021936336	4.9888604971	-4.5827030474
H	-4.1047924613	3.2694898745	-5.0245703503



H	-4.1807951575	4.5170057286	-6.2989666524
C	-1.9312666363	5.9363266263	-5.6511921304
H	-0.8421458808	6.1186078654	-5.6801525846
H	-2.3709815776	6.6492236908	-4.9302654308
H	-2.3387481864	6.1677549112	-6.6534539909
C	-1.6440808449	3.5072839484	-6.3003985294
H	-0.5444351541	3.6017201176	-6.3472643086
H	-2.0438893221	3.7205921735	-7.3096695908
H	-1.8801387830	2.4552402155	-6.0561934483
C	-0.3913342286	9.5990514279	2.8450988661
H	-1.2767111534	9.6761047866	2.1879070293
H	0.5094060607	9.7266926048	2.2163505531
H	-0.4275057629	10.4450998344	3.5544710673
C	0.8835013526	8.2820255078	4.5524360483
H	0.8392458281	9.1500498908	5.2369133677
H	1.8165922930	8.3590985578	3.9648248804
H	0.9521185545	7.3712054407	5.1729884365
C	-1.6483890158	8.1651384136	4.4828777241
H	-2.5496401051	8.1610627343	3.8434335752
H	-1.7206350927	9.0250556472	5.1754088678
H	-1.6635038342	7.2411395972	5.0877297377

**(IPr)Pd(py)Cl<sub>2</sub>**

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Total energy: -2455.73564626750

Pd	11.4532813805	-1.8279707073	-6.1423980677
Cl	11.9792981827	0.2820960024	-7.0962669096
Cl	10.9427016633	-3.9726916106	-5.2594525646
C	9.6265184616	-1.1928240228	-5.7151525062
N	9.2137352765	-0.6547689931	-4.5180034065
C	7.8565064917	-0.3254741940	-4.5669081476
H	7.3484429906	0.1152699306	-3.7143271490
C	7.4103655641	-0.6643832903	-5.8108569059
H	6.4298107896	-0.5861535449	-6.2708457725
N	8.5023816449	-1.1916055084	-6.5074521459
N	13.4449708705	-2.4904056441	-6.5284984457
C	14.1003087660	-2.1053724073	-7.6498300063
H	13.5441552239	-1.4386678093	-8.3145109896

C	15.4132088610	-2.5069573998	-7.9196101938
H	15.8966673809	-2.1773241401	-8.8438314679
C	16.0819075731	-3.3176481412	-6.9923165708
H	17.1127196190	-3.6400408909	-7.1731668476
C	15.4043566266	-3.7067994429	-5.8286166320
H	15.8833056152	-4.3371994100	-5.0739191740
C	14.0851359787	-3.2830211434	-5.6339656018
H	13.4931969048	-3.5877542083	-4.7670349486
C	10.0307465538	-0.4183607368	-3.3349120460
C	10.6951556401	0.8302787471	-3.2100446490
C	11.4393378971	1.0471301038	-2.0346556830
H	11.9713829720	1.9951330167	-1.9086593607
C	11.5081300627	0.0789952495	-1.0275300495
C	10.8185620370	-1.1298922643	-1.1652919176
H	10.8680284170	-1.8748677293	-0.3653268122
C	10.0577629271	-1.4086938663	-2.3178034791
C	10.5661051420	1.9451742378	-4.2498869387
H	10.3136809908	1.4791598743	-5.2170691550
H	12.0974969432	0.2724734091	-0.1241673573
C	9.2490447662	-2.7043187512	-2.4027955620
H	9.0600518749	-2.9154568484	-3.4690230605
C	8.3878270809	-1.6395124290	-7.8896767994
C	8.5143128928	-0.6755032496	-8.9245290367
C	8.3258035425	-1.1212953541	-10.2474639280
H	8.4214412570	-0.4058799124	-11.0700741561
C	8.0191410414	-2.4574310353	-10.5260860333
C	7.8812543293	-3.3806607946	-9.4842591240
H	7.6308186425	-4.4210520257	-9.7131051604
C	8.0543864109	-2.9964080757	-8.1397929971
C	7.8117587312	-4.0070472108	-7.0179838506
H	8.3426823589	-3.6519696787	-6.1190558757
H	7.8797610434	-2.7803363729	-11.5639330863
C	8.7764877265	0.8067314026	-8.6499207116
H	9.2508720192	0.8876565503	-7.6569736935
C	11.8785730671	2.7238076770	-4.4694890200
H	11.7520326135	3.4304588152	-5.3072484640
H	12.1668811454	3.3172515910	-3.5829100435
H	12.7036166171	2.0425814029	-4.7293233366
C	9.4235368789	2.9138193615	-3.8566523503
H	9.3130884289	3.7068693112	-4.6171856571

H	8.4535195041	2.3954650268	-3.7671073467
H	9.6353756897	3.4000330904	-2.8874072896
C	10.0054945060	-3.9238548547	-1.8387686729
H	9.4241478573	-4.8415454648	-2.0319979399
H	10.9850026360	-4.0391659838	-2.3274792033
H	10.1533509465	-3.8552927331	-0.7458303581
C	7.8894432907	-2.5376109820	-1.6804272296
H	7.2968807662	-3.4663166364	-1.7568816642
H	8.0383039965	-2.3169088999	-0.6081253374
H	7.2882088368	-1.7184645614	-2.1102251721
C	6.3003166576	-4.0951404560	-6.6937767788
H	6.1250435495	-4.8064879028	-5.8673810110
H	5.8854825531	-3.1180913485	-6.3913341063
H	5.7277444634	-4.4459238736	-7.5713626776
C	8.3802206979	-5.4044069613	-7.3356789995
H	8.2772684145	-6.0549807245	-6.4507829454
H	7.8445439546	-5.8957186815	-8.1681631697
H	9.4514608903	-5.3466654315	-7.5840521948
C	9.7557047194	1.4392657768	-9.6592388724
H	9.9926396688	2.4711072615	-9.3480075382
H	10.6999002193	0.8747601496	-9.6981437373
H	9.3278982716	1.4961955011	-10.6764003306
C	7.4452934739	1.5977363793	-8.6299056814
H	7.6353768584	2.6646767566	-8.4180081426
H	6.9337278731	1.5318137640	-9.6068609518
H	6.7492716331	1.2210424087	-7.8613926870

**(IPr\*)Pd(py)Cl<sub>2</sub>**

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Total energy: -4068.21294112011

Pd	11.5811505436	-1.7509661243	-6.1959898926
Cl	12.2681475522	0.5175867421	-6.1149508609
Cl	10.8465011662	-3.9999203717	-6.3216453787
C	9.7419336331	-1.1795397783	-5.7121548041
N	9.3318812109	-0.5855100633	-4.5372441920
C	7.9606915824	-0.3067432613	-4.5845579624
H	7.4454495389	0.1515309816	-3.7482582885
C	7.5149012271	-0.7010607843	-5.8067855703
H	6.5305632350	-0.6541759330	-6.2582950539
N	8.6041201898	-1.2566779193	-6.4869090637
N	13.5880984799	-2.3590851088	-6.7110779712
C	14.4160426139	-1.5172211719	-7.3801982348
H	14.0024469585	-0.5303548641	-7.6064904298
C	15.7177640841	-1.8847009017	-7.7377253531
H	16.3442513192	-1.1729991652	-8.2833938216
C	16.1901014347	-3.1563914554	-7.3863837582
H	17.2060292720	-3.4683133602	-7.6514630454
C	15.3356794099	-4.0202595502	-6.6880980359
H	15.6565948544	-5.0224754813	-6.3892094613
C	14.0413866396	-3.5927408663	-6.3721616801
H	13.3233300067	-4.2329711904	-5.8518581847
C	10.1225575494	-0.2688825916	-3.3545894885
C	10.3151231191	1.0959583622	-2.9946203425
C	10.9899386744	1.3703913753	-1.7925863609
H	11.1663346052	2.4185392891	-1.5269512208
C	11.4570691401	0.3560982532	-0.9404817308
C	11.2549861944	-0.9760085404	-1.3293460549
H	11.6328707941	-1.7865792777	-0.6976092854
C	10.5947524857	-1.3176972333	-2.5254513548
C	9.7985475715	2.2695180880	-3.8469668777
H	9.8751264101	1.9522635310	-4.9041075880
C	12.1457050908	0.6946773638	0.3656613755
H	12.8380298888	-0.1056369861	0.6754120636
H	11.4111115477	0.8279832112	1.1824214195
H	12.7178455400	1.6343928288	0.2867430771

C	10.3818473955	-2.7964832291	-2.8642521123
H	10.4092557476	-2.8972335879	-3.9646337538
C	8.4421859775	-1.8756165307	-7.7952084115
C	9.0318531626	-1.2834062184	-8.9409408985
C	8.8041064752	-1.8840736835	-10.1924109826
H	9.2727363053	-1.4332621279	-11.0733876358
C	8.0119881958	-3.0338368502	-10.3441449668
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H	6.8273929345	-4.4927149517	-9.2760682816
C	7.6188200078	-3.0299422400	-7.9106719467
C	6.8830127980	-3.6668490008	-6.7193936201
H	7.5013450675	-3.4969792232	-5.8181394519
C	7.7788335245	-3.6447286036	-11.7095883492
H	7.0552470338	-3.0492010307	-12.2968746873
H	7.3788712203	-4.6685278096	-11.6290153491
H	8.7131044532	-3.6860196211	-12.2953378745
C	9.8454151796	0.0125785603	-8.8643115353
H	10.4076515429	0.0040428276	-7.9115655756
C	8.3238813404	2.5958425945	-3.5721632061
C	7.5367421296	3.1368719574	-4.6090531585
H	7.9782528202	3.2735782904	-5.6033093090
C	6.1965201471	3.4814863888	-4.3882300380
H	5.5999980105	3.8900888164	-5.2116975031
C	5.6168117824	3.2942041210	-3.1225126587
C	6.3909676666	2.7606417059	-2.0817409622
H	5.9494356516	2.6079941776	-1.0901432066
C	7.7347325261	2.4154326559	-2.3050446000
H	8.3301729374	1.9921421856	-1.4889310039
C	10.6726511542	3.5367588638	-3.7087289902
C	11.9361536323	3.5775469436	-4.3344662078
H	12.2786140071	2.7013957062	-4.8955748702
C	12.7515376525	4.7138649954	-4.2372442201
H	13.7258727586	4.7214038374	-4.7393132055
C	12.3270949885	5.8347112014	-3.5045311269
C	11.0752394500	5.8028241273	-2.8738448851
H	10.7255159169	6.6686153333	-2.2996149869
C	10.2548942090	4.6665783415	-2.9775686757
H	9.2744852898	4.6665014986	-2.4913465828
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C	9.0189402879	-3.3314215896	-2.4177240116

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C	7.1206418731	-3.4251184563	-0.8838823026
H	6.5981663846	-3.0317664226	-0.0041702340
C	6.5828825607	-4.5097285710	-1.5927814569
C	7.2586329586	-5.0039367862	-2.7217960265
H	6.8482863899	-5.8475001527	-3.2879697028
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H	12.9657161891	-2.5825764715	-3.6040345209
C	13.9449268169	-4.1600898785	-2.4811556073
H	14.9358587487	-3.9373853676	-2.8937208250
C	13.7836137657	-5.2023939587	-1.5523519978
C	12.5103051387	-5.4715156772	-1.0337962531
H	12.3725809311	-6.2822485465	-0.3091537274
C	11.4012084843	-4.7070012523	-1.4370430741
H	10.4104517469	-4.9296905550	-1.0277538435
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H	11.9075743315	-1.6988961592	-9.1795669772
C	12.9455976471	-0.9212209784	-10.9194884534
H	13.7165365645	-1.7002249122	-10.8969093201
C	12.9710885044	0.0693513810	-11.9162282639
C	11.9756652687	1.0548535457	-11.9316916620
H	11.9837582419	1.8321309239	-12.7044558646
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H	10.1892318994	1.8316170573	-10.9824940808
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C	8.9625430619	1.2638838443	-8.8342331233
C	7.6892118816	1.3192335491	-9.4309828017
H	7.2717568779	0.4200002373	-9.8978629003
C	6.9519444459	2.5150001514	-9.4350037505
H	5.9614449466	2.5397604418	-9.9040840197
C	7.4799917689	3.6740946650	-8.8480748978
C	8.7491057221	3.6284496718	-8.2455176852
H	9.1734449325	4.5278234943	-7.7845404862

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H	10.4705726732	2.3918106041	-7.7650150903
H	6.9068114330	4.6081303778	-8.8582091433
C	6.7423454345	-5.1972920063	-6.8668302509
C	7.9066879002	-5.9941238143	-6.8414477471
H	8.8824512112	-5.5066621286	-6.7336096095
C	7.8256027732	-7.3870858717	-6.9666259641
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C	6.5784033182	-8.0135160016	-7.1250311527
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H	5.6101419351	-3.4252038326	-4.3292885816
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H	5.1112006351	-2.4656533867	-8.5156433933
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**(IPr\*\*)Pd(py)Cl<sub>2</sub>**

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H	7.4093034717	0.2352611391	-3.8632476933
C	7.5654869062	-0.6506698170	-5.9065698102

H	6.6102507494	-0.5772466991	-6.4171099487
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H	16.1129286716	-1.7986461976	-8.6052624951
C	15.9426937590	-3.6960199013	-7.5400756023
H	16.8714814894	-4.1199754539	-7.9372902651
C	15.1539915717	-4.4216820360	-6.6365554478
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H	10.0402191736	-2.9894914232	-3.7195113433
C	8.5648421489	-1.8019918467	-7.8693034454
C	9.1134280699	-1.0878685476	-8.9659854144
C	8.8470480019	-1.5552779780	-10.2676939367
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H	6.9880080688	-2.5316637320	-12.3975424344
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H	8.6741481121	-3.0587325424	-12.5825549315
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C	8.3266563621	2.6209294455	-3.4661336994
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C	6.1304674069	3.4968887150	-4.0951710005
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C	6.3284547820	-4.0127059893	-0.7958561885
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C	14.7164793543	-6.1918375735	-0.8865415245
C	11.0497286555	0.1915034961	-9.9235497020
C	11.9434437042	-0.8944371619	-10.0116532905
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C	7.1609837705	-5.3310517029	-7.3378493742
C	8.3703315412	-6.0366732719	-7.4921810543
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H	4.9985893713	6.0766026970	-8.3903480068

H	5.5957274992	4.8162940572	-7.2729960107
C	7.6921474496	6.4384581414	-8.0841333158
H	7.7745622644	6.1791450858	-7.0144328026
H	7.1073944800	7.3718065577	-8.1600266486
H	8.7070406162	6.6501818660	-8.4637953601
C	6.5029695639	-9.6496269193	-10.0135939342
H	6.4776602458	-10.6966530544	-10.3677316548
H	7.0511570741	-9.0496066830	-10.7609649926
H	5.4637976325	-9.2799048343	-9.9824827046
C	8.6130795352	-10.1467546391	-8.7485014553
H	8.5584520235	-11.1971455739	-9.0858235754
H	9.1484368739	-10.1346119687	-7.7827965891
H	9.2215453539	-9.5921027760	-9.4844026765
C	6.3969803947	-10.4247408899	-7.6036636861
H	6.3644949568	-11.4806449369	-7.9292037426
H	5.3573732208	-10.0731206574	-7.4950131742
H	6.8697808542	-10.3886243001	-6.6066500840
C	1.2770810755	-0.7962099510	-6.3381273127
H	1.0349559074	-1.3548536584	-7.2589637064
H	1.9390778283	0.0434388634	-6.6139850339
H	0.3324682276	-0.3712397931	-5.9557479308
C	2.0798804661	-0.8481963957	-3.9700289949
H	2.7904365506	-0.0171752988	-4.1240500199
H	2.4421401164	-1.4447732286	-3.1159444107
H	1.1055702946	-0.4168124097	-3.6779228514
C	0.9775590356	-2.8932333716	-4.9690952650
H	0.8395177647	-3.5157872768	-5.8703399379
H	-0.0161248662	-2.5365498735	-4.6408806957
H	1.3882190625	-3.5408560550	-4.1751034980