

Supporting information

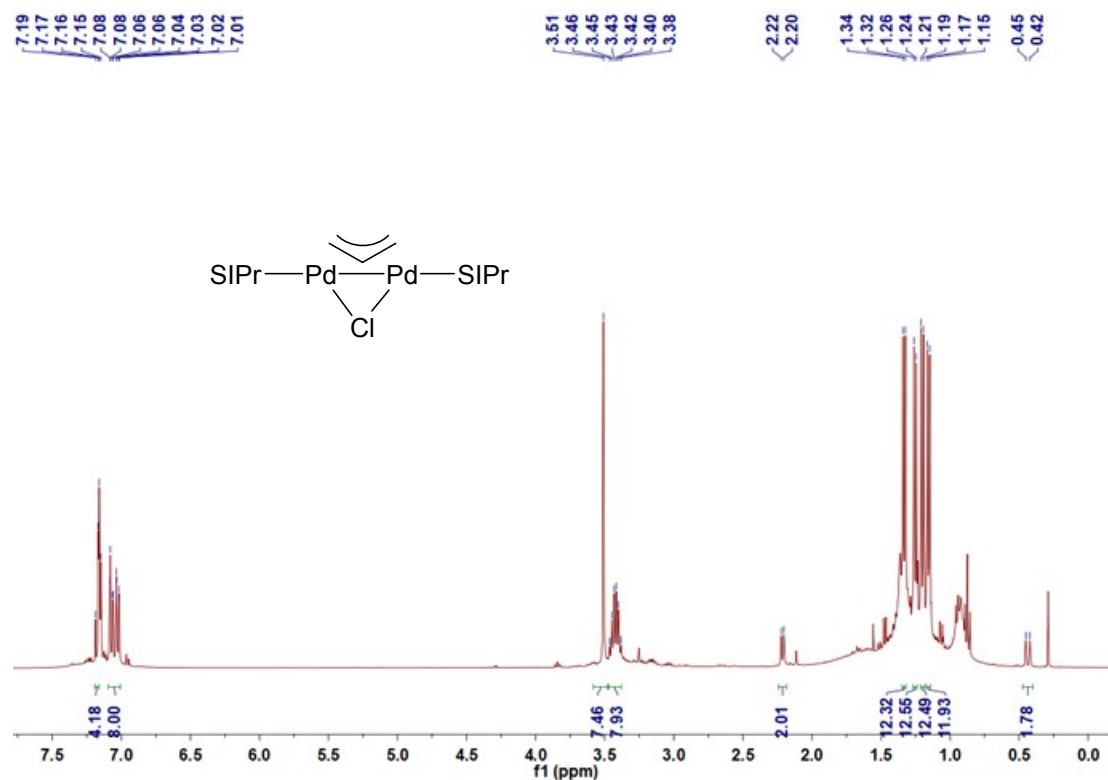
For

**Conversion of off-cycle Pd(I)-NHC dimers into highly-efficient
cross-coupling catalysts**

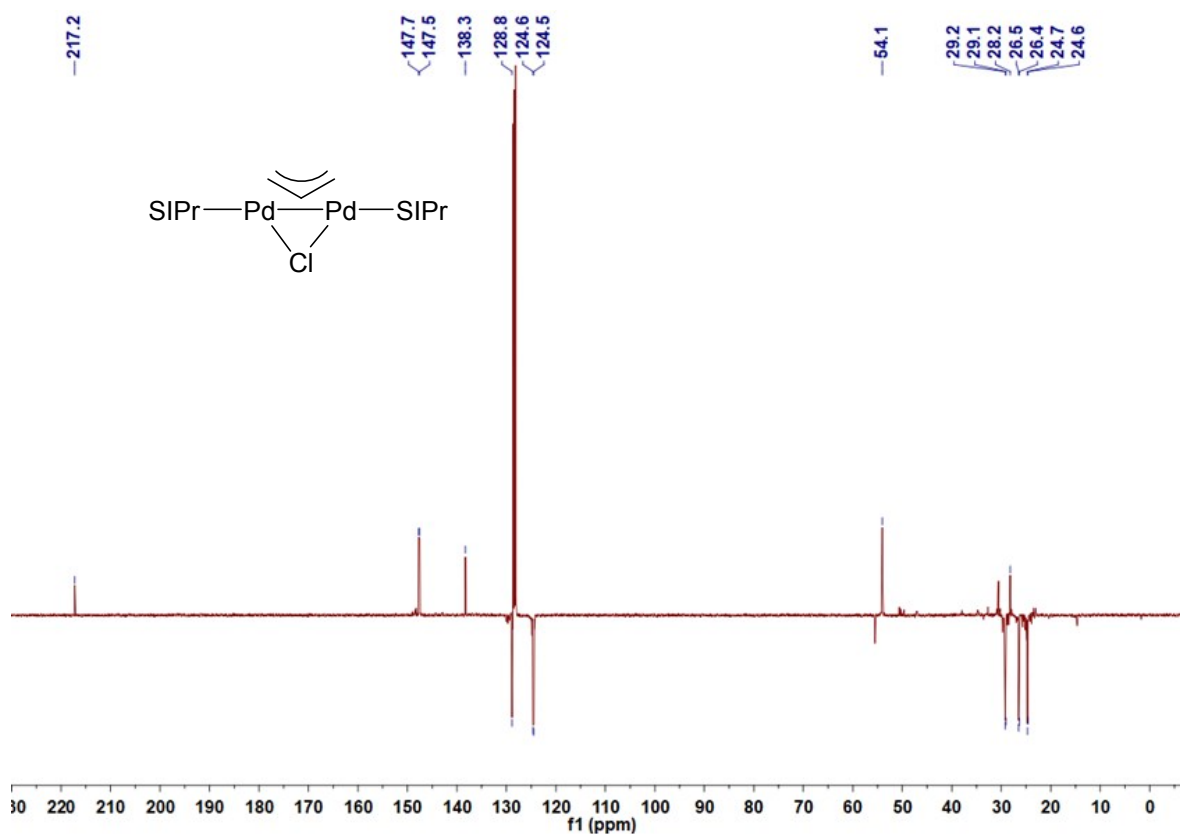
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Catherine S. J. Cazin* and Steven P. Nolan*

¹ H NMR and ¹³ C NMR spectra.....	S1
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DFT Optimized Cartesian Coordinates	S9

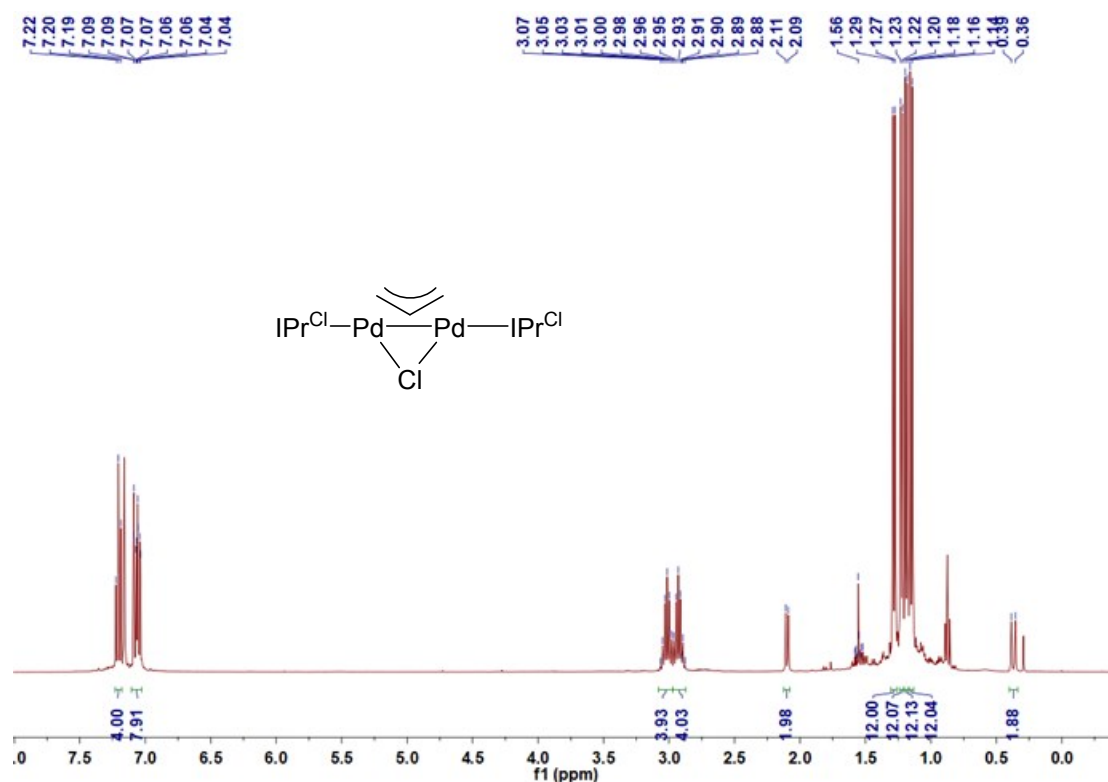
^1H NMR and ^{13}C NMR spectra



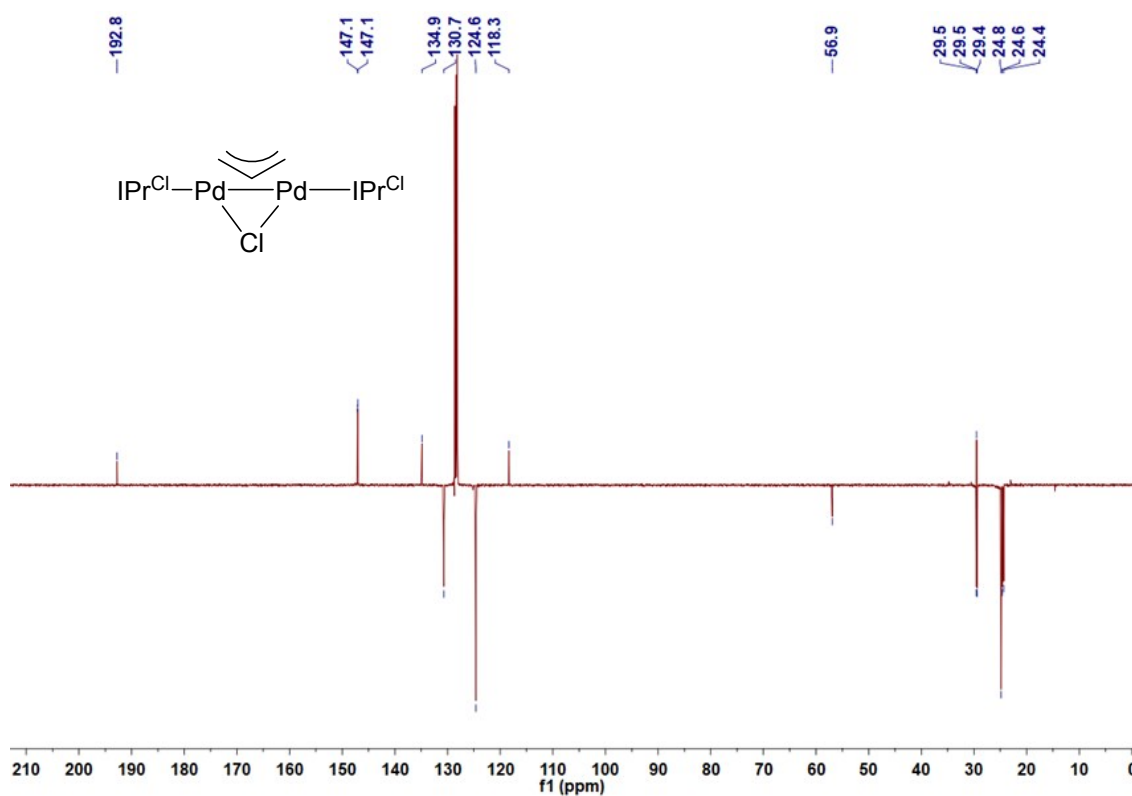
^1H NMR spectrum of $[\text{Pd}_2(\mu\text{-Cl})(\mu\text{-}\eta^3\text{-allyl})(\text{SIPr})_2]$ in C_6D_6 at 298 K (400 MHz)



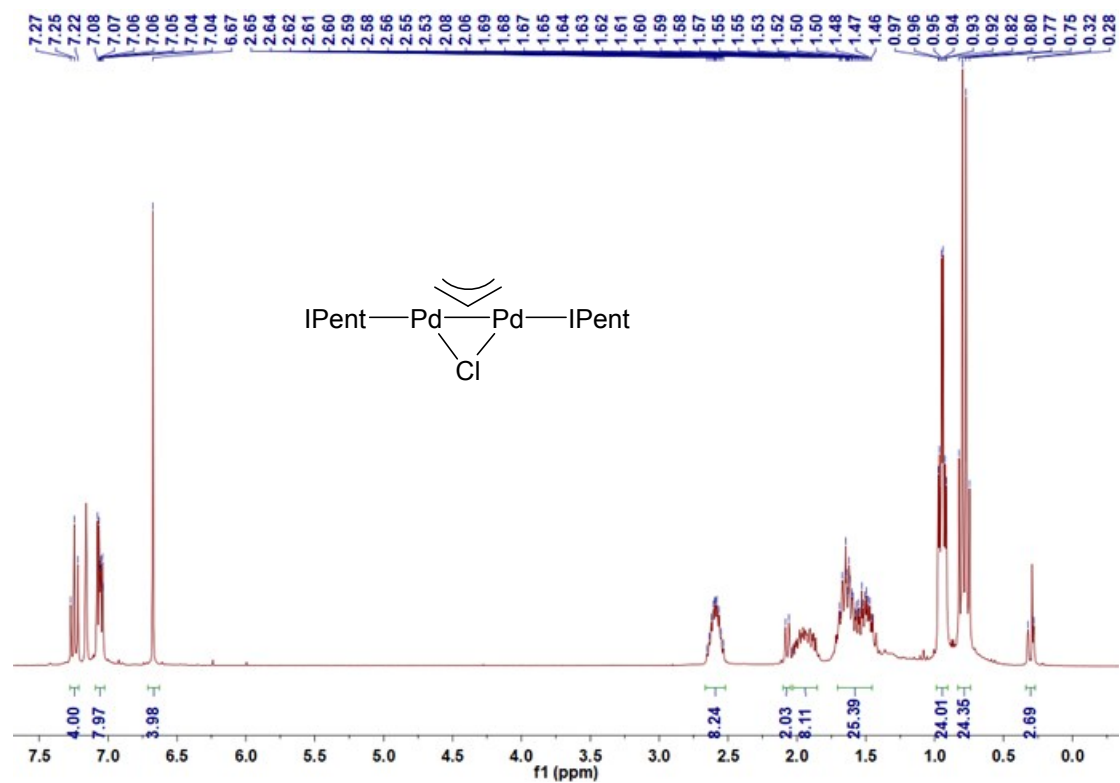
^{13}C NMR spectrum of $[\text{Pd}_2(\mu\text{-Cl})(\mu\text{-}\eta^3\text{-allyl})(\text{SIPr})_2]$ in C_6D_6 at 298 K (100 MHz)



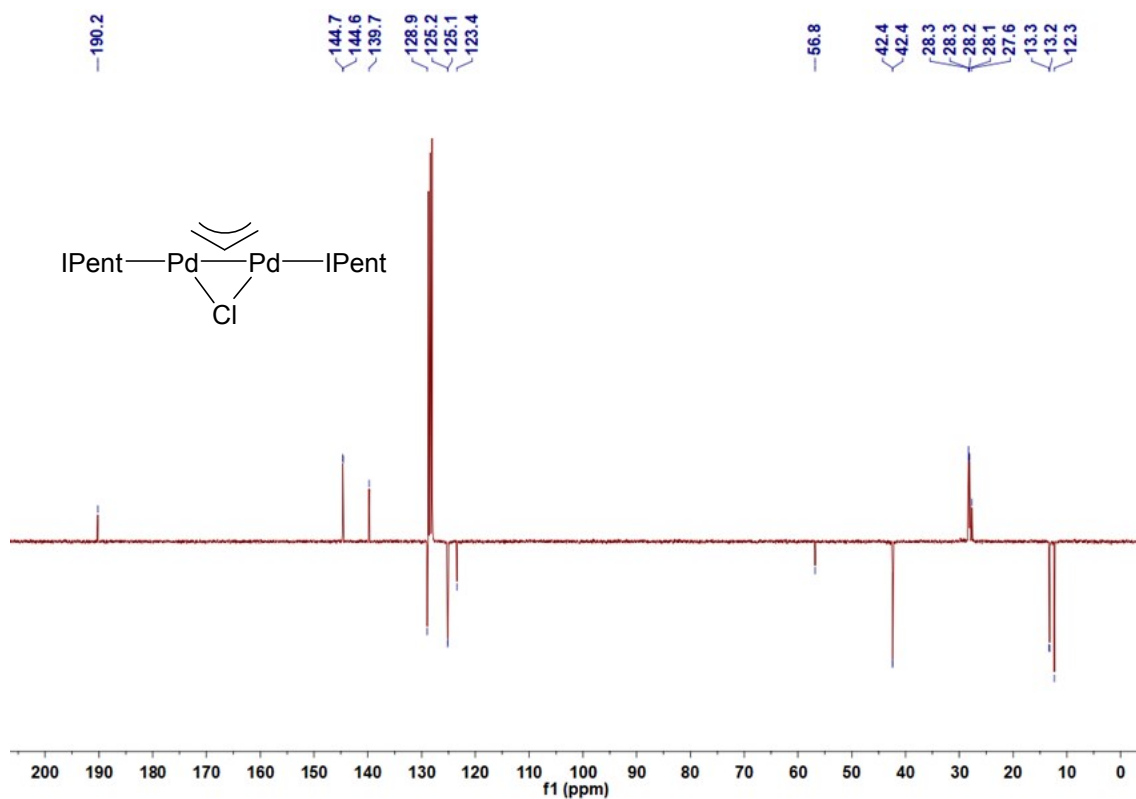
^1H NMR spectrum of $[\text{Pd}_2(\mu\text{-Cl})(\mu\text{-}\eta^3\text{-allyl})(\text{IPr}^{\text{Cl}})_2]$ in C_6D_6 at 298 K (400 MHz)



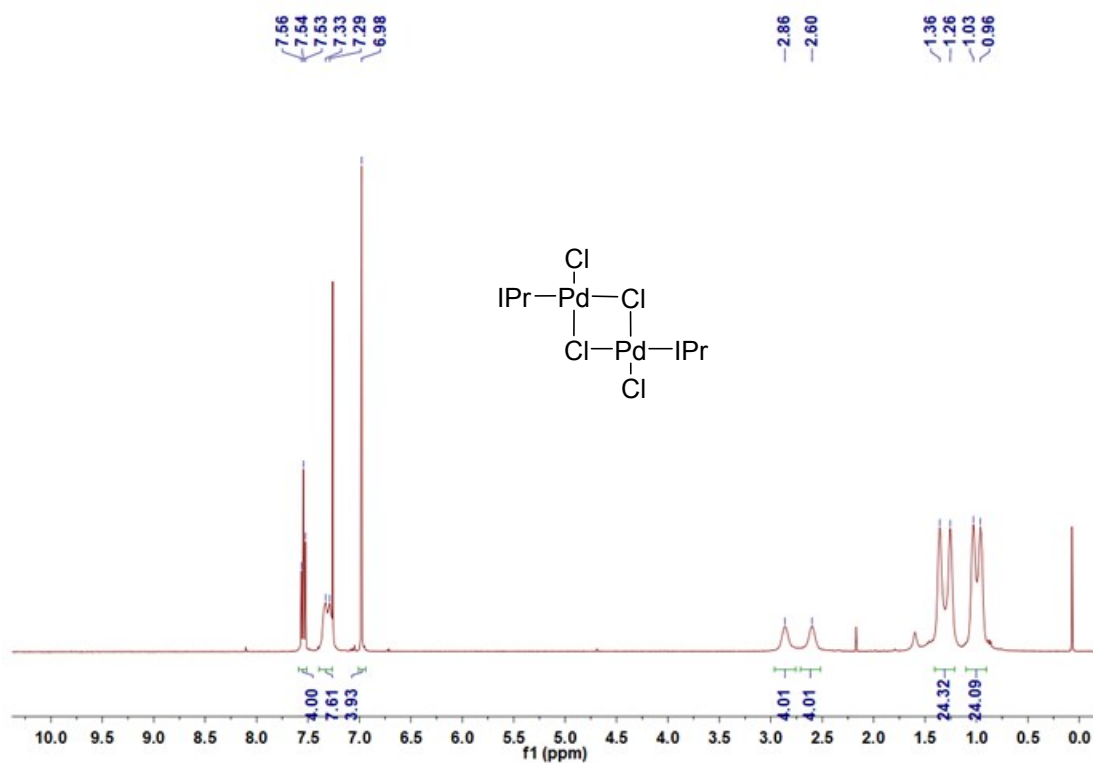
^{13}C NMR spectrum of $[\text{Pd}_2(\mu\text{-Cl})(\mu\text{-}\eta^3\text{-allyl})(\text{IPr}^{\text{Cl}})_2]$ in C_6D_6 at 298 K (100 MHz)



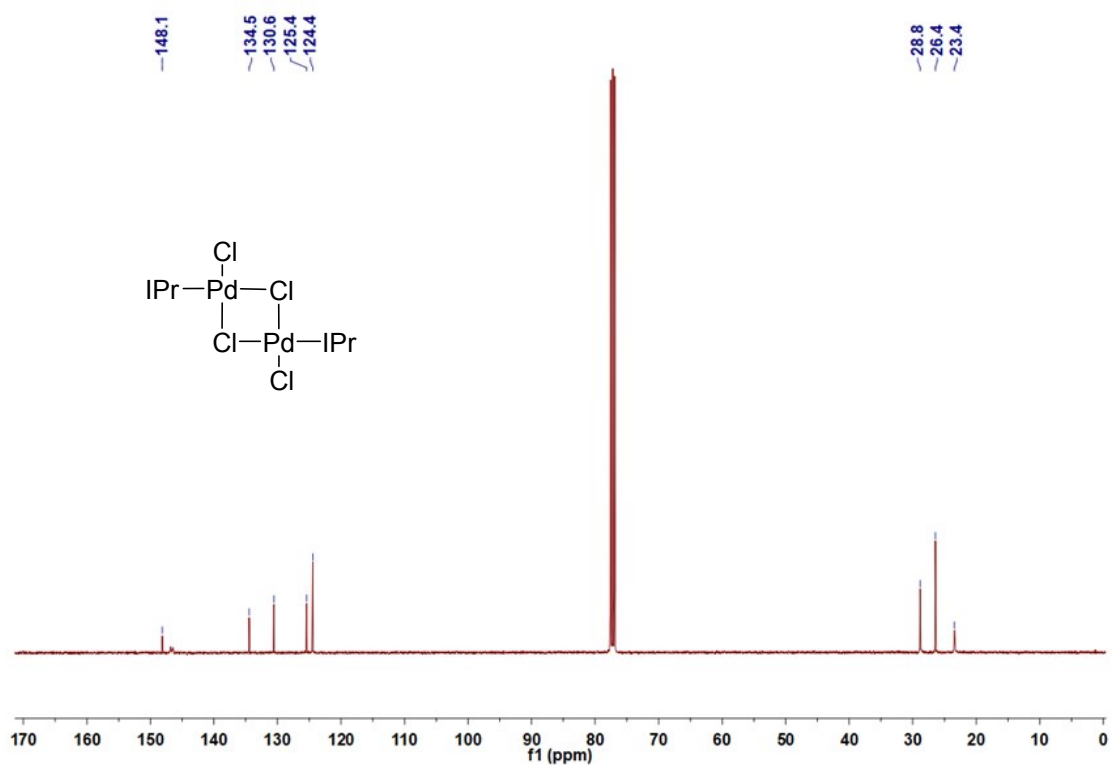
¹H NMR spectrum of $[\text{Pd}_2(\mu\text{-Cl})(\mu\text{-}\eta^3\text{-allyl})(\text{IPent})_2]$ in C_6D_6 at 298 K (300 MHz)



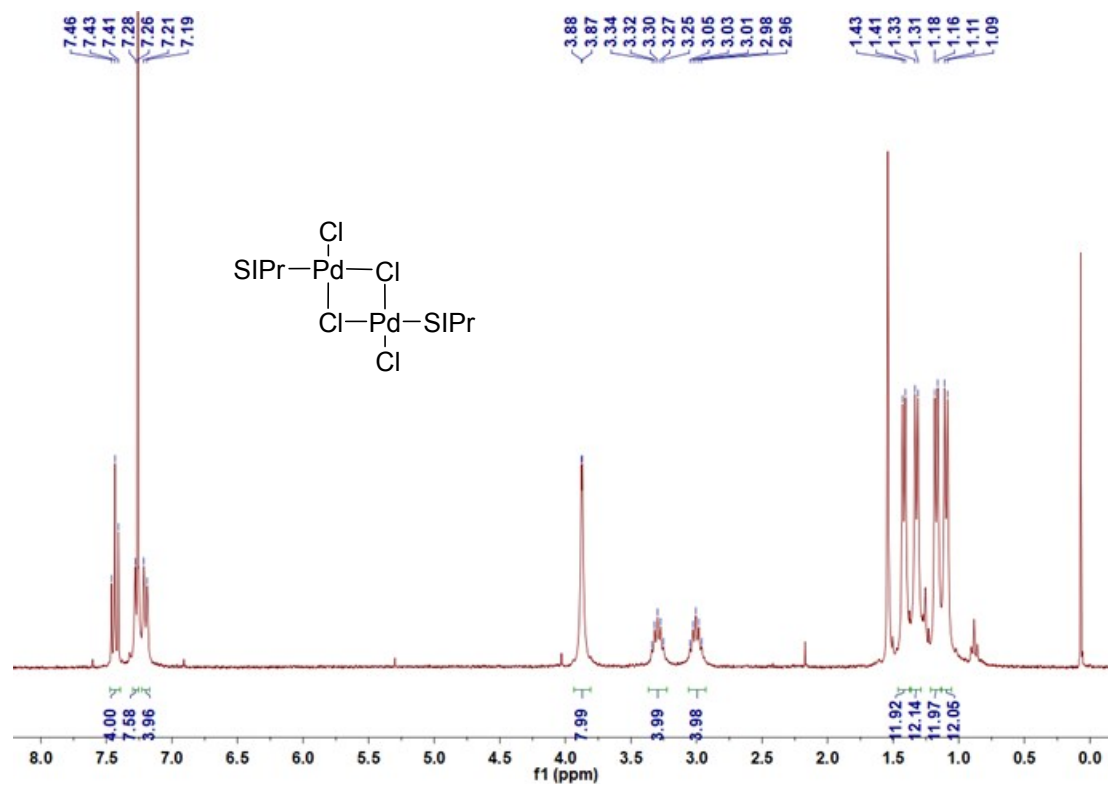
¹³C NMR spectrum of $[\text{Pd}_2(\mu\text{-Cl})(\mu\text{-}\eta^3\text{-allyl})(\text{IPent})_2]$ in C_6D_6 at 298 K (75 MHz)



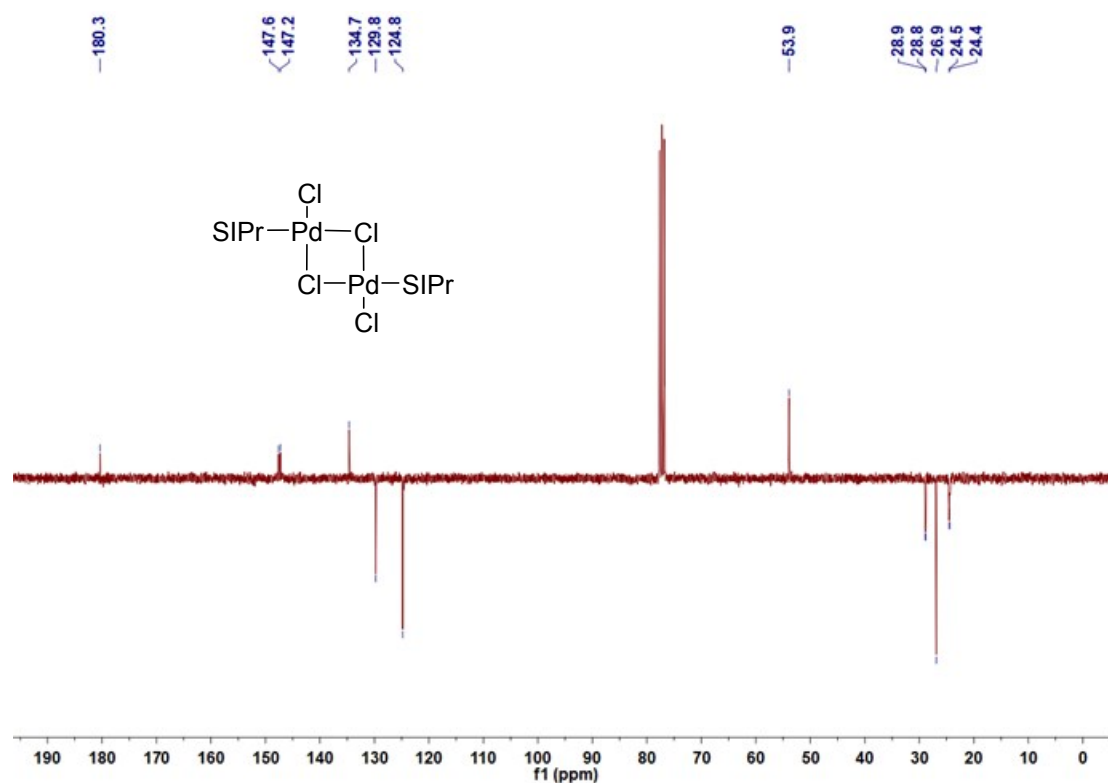
¹H NMR spectrum of [PdCl(μ-Cl)(IPr)]₂ in CDCl₃ at 298 K (400 MHz)



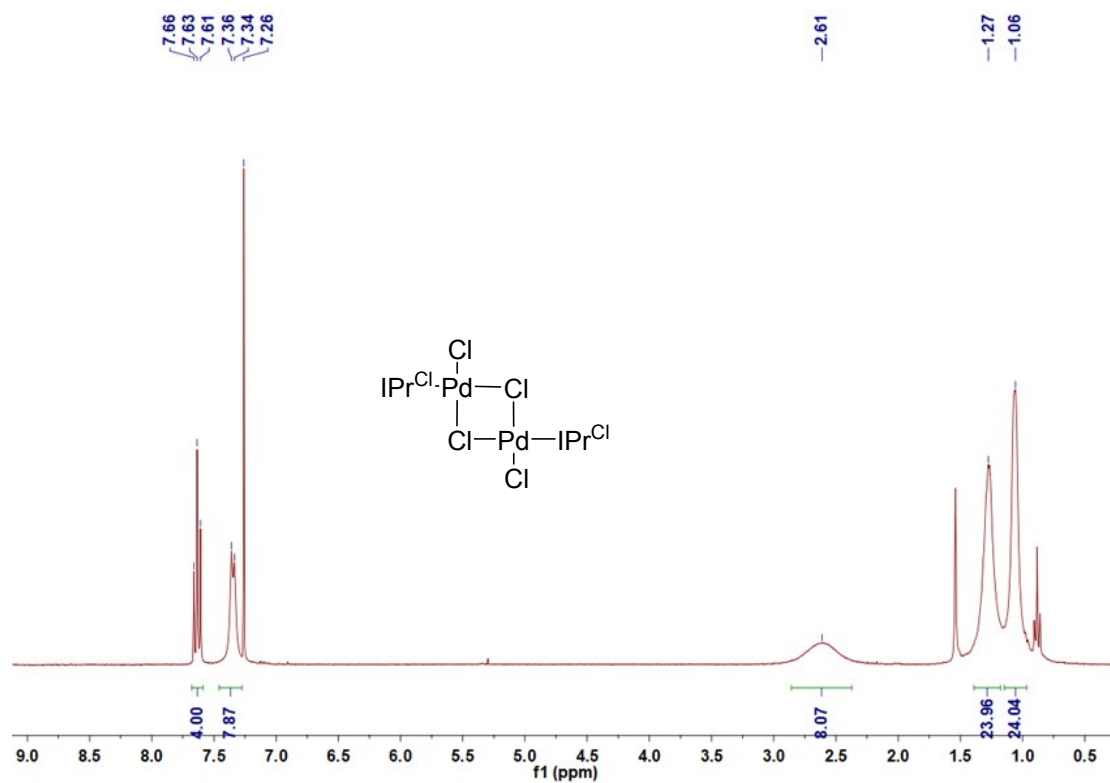
¹³C NMR spectrum of [PdCl(μ-Cl)(IPr)]₂ in CDCl₃ at 298 K (100 MHz)



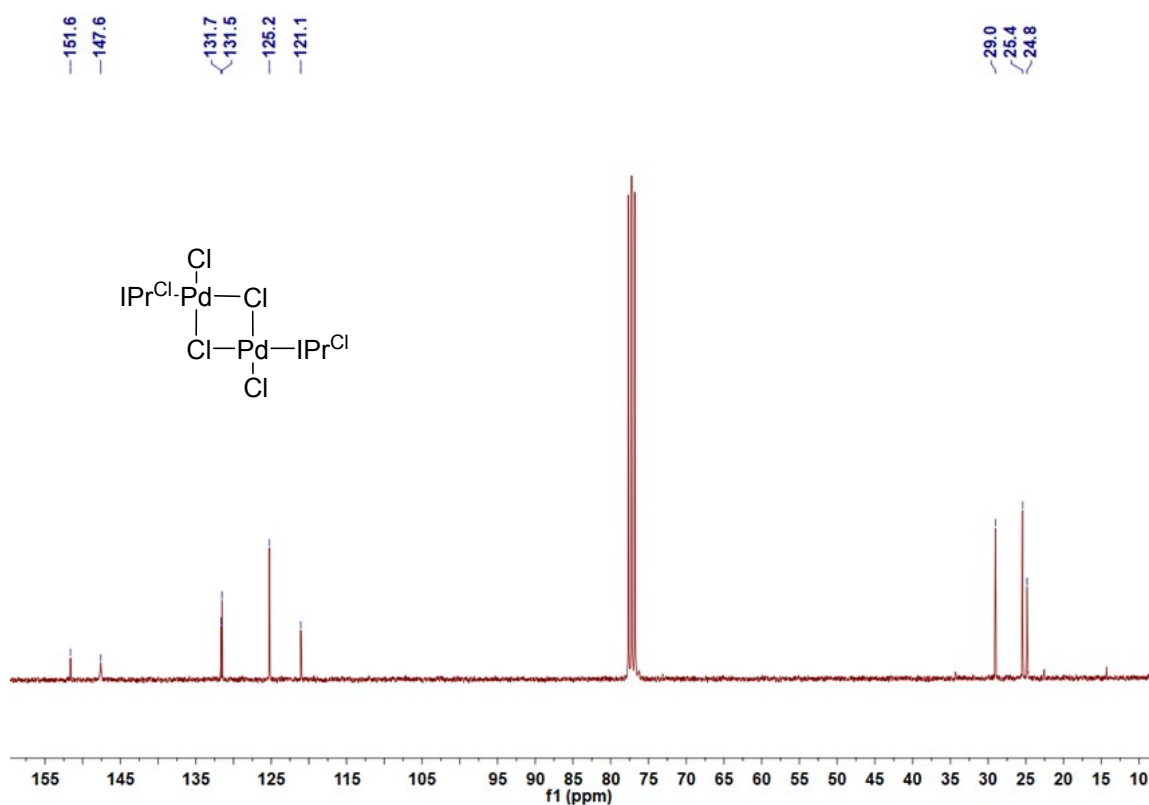
^1H NMR spectrum of $[\text{PdCl}(\mu\text{-Cl})(\text{SiPr})_2]_2$ in CDCl_3 at 298 K (300 MHz)



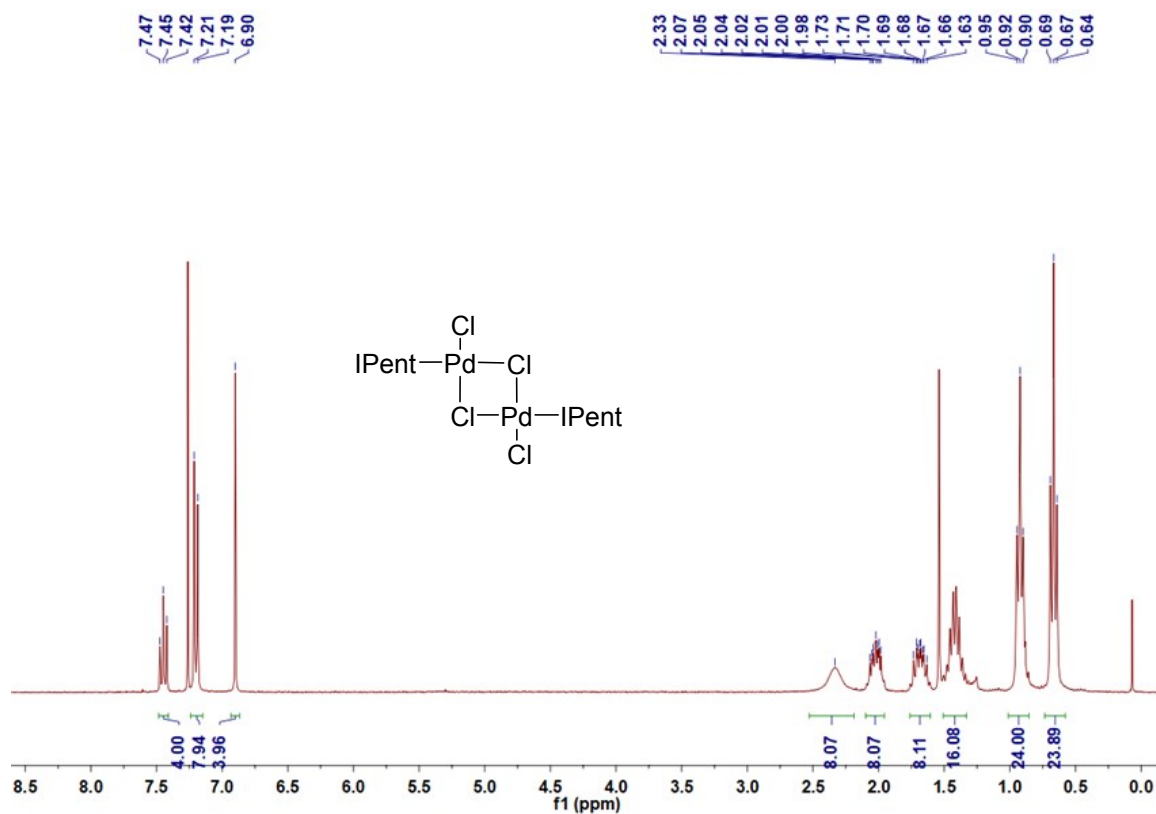
^{13}C NMR spectrum of $[\text{PdCl}(\mu\text{-Cl})(\text{SiPr})_2]_2$ in CDCl_3 at 298 K (75 MHz)



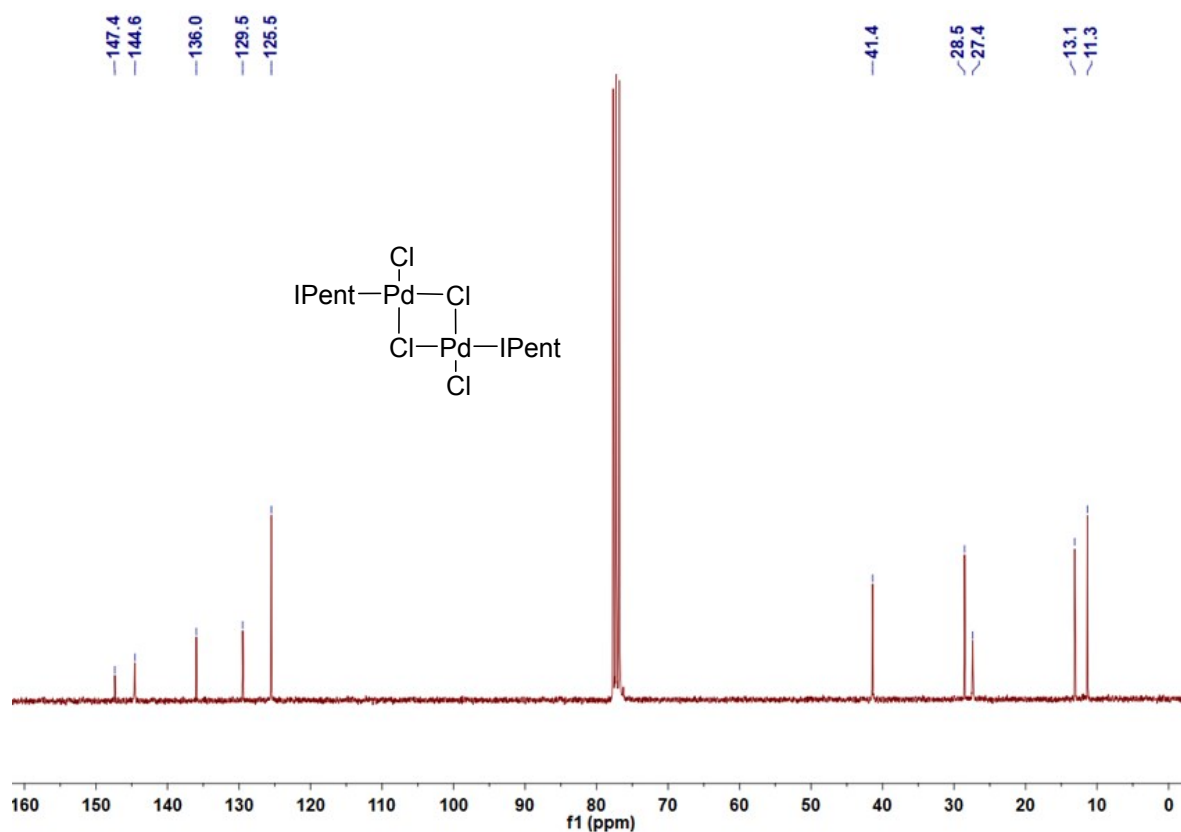
¹H NMR spectrum of [PdCl(μ-Cl)(IPrCl)]₂ in CDCl₃ at 298 K (300 MHz)



¹³C NMR spectrum of [PdCl(μ-Cl)(IPrCl)]₂ in CDCl₃ at 298 K (75 MHz)



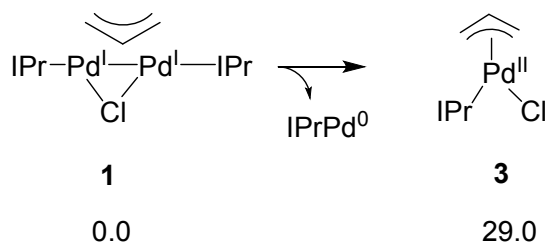
¹H NMR spectrum of [PdCl(μ-Cl)(IPent)]₂ in CDCl₃ at 298 K (300 MHz)



¹³C NMR spectrum of [PdCl(μ-Cl)(IPent)]₂ in CDCl₃ at 298 K (75 MHz)

DFT Calculations

Disproportionation



Dimerization

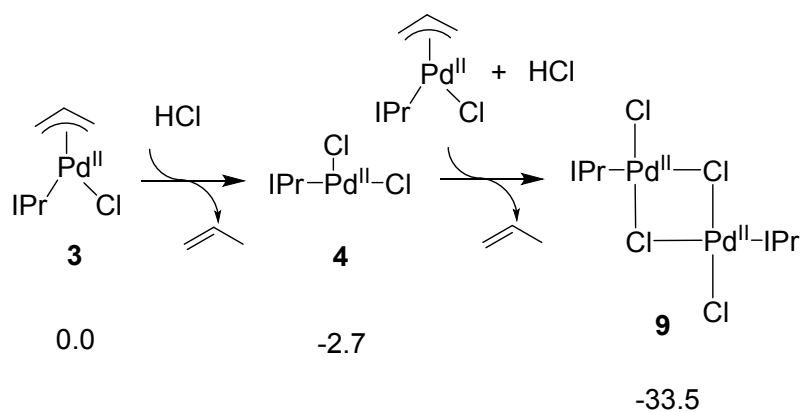


Figure S1. Disproportionation mechanism followed by dimerization in acetone. Free energies are in kcal.mol⁻¹.

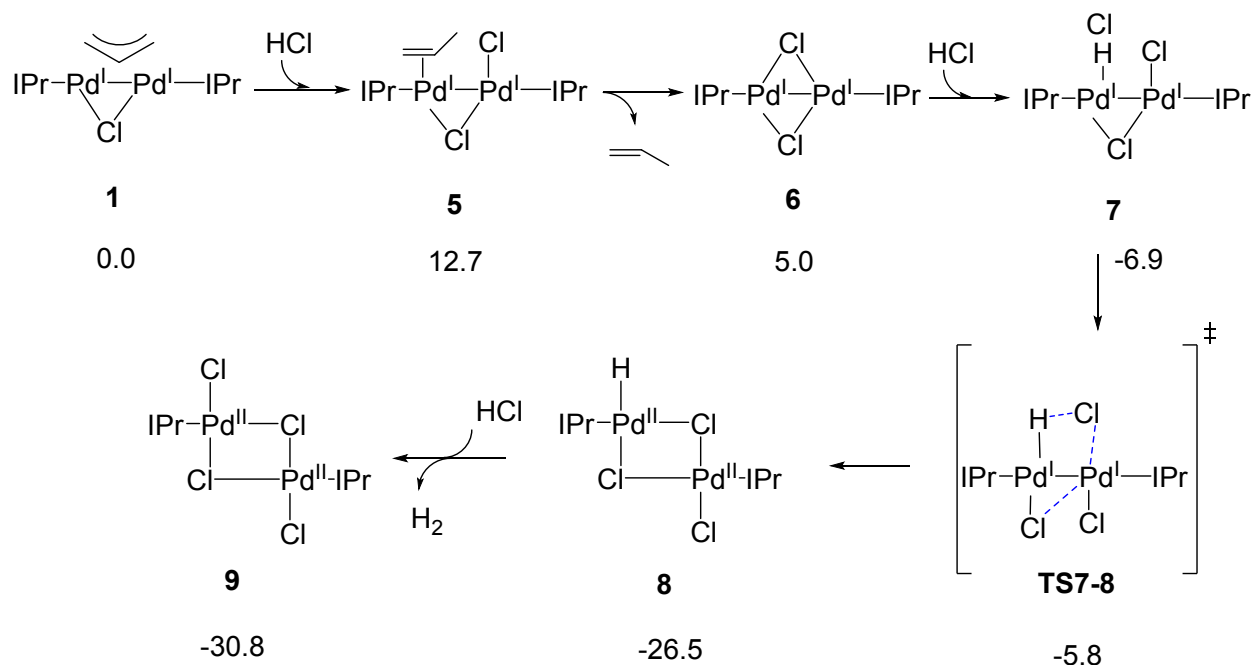


Figure S2. Direct protonation mechanism of **1** with 3 HCl molecules giving complex **9** in acetone. Free energies are in kcal.mol⁻¹.

141			
1			
Pd	-1.384010	0.403054	-0.087392
N	-3.708460	-1.544484	-0.170447
C	-5.093630	-1.642846	-0.284638
C	-5.569412	-0.363846	-0.375534
C	-3.281673	-0.233537	-0.191687
N	-4.457329	0.476694	-0.323745
C	-2.854861	-2.673074	0.087911
C	-2.851961	-3.212318	1.397507
C	-2.061028	-4.351675	1.629382
C	-1.282553	-4.907847	0.607467
C	-1.268505	-4.324192	-0.663917
C	-2.056610	-3.195271	-0.955206
C	-3.646952	-2.584001	2.536844
C	-2.005028	-2.564945	-2.339403
C	-4.537009	1.910097	-0.353403
C	-4.829475	2.547759	-1.584916
C	-4.918617	3.952150	-1.587865
C	-4.701140	4.690929	-0.418151
C	-4.396617	4.035075	0.780550
C	-4.314469	2.630742	0.845326
C	-0.608924	-1.980177	-2.612084
H	0.171850	-2.767197	-2.618296
H	-0.587814	-1.465716	-3.595243
H	-0.335773	-1.240230	-1.826055
C	-2.436336	-3.554292	-3.434550
H	-2.441184	-3.056787	-4.426209
H	-1.742010	-4.417515	-3.501362
H	-3.452951	-3.955118	-3.244982
C	-4.799599	-3.497880	2.987603
H	-4.416544	-4.460119	3.386461
H	-5.392684	-3.013476	3.790370
H	-5.486267	-3.734805	2.149592
C	-2.738300	-2.191493	3.714049
H	-3.328787	-1.667972	4.494480
H	-2.276086	-3.082007	4.188649
H	-1.922132	-1.523582	3.373598
H	-0.662071	-5.793633	0.811948
H	-2.037659	-4.795833	2.636016
H	-0.622865	-4.744639	-1.448876
H	-5.143529	4.476078	-2.528802
H	-4.220568	4.624312	1.693282
H	-4.097025	-1.645447	2.155481
H	-2.722149	-1.719349	-2.349971
Pd	1.271728	0.446595	-0.017802
N	4.174282	0.951000	0.668010
C	5.413688	0.329781	0.824216
C	5.248639	-0.971087	0.435107
C	3.218834	0.074242	0.196898
N	3.910080	-1.110048	0.067129
C	3.945954	2.359493	0.848728
C	3.157400	2.798216	1.943262
C	2.957705	4.184063	2.077315
C	3.519067	5.091820	1.168025
C	4.279531	4.628628	0.089487
C	4.499379	3.250432	-0.102466
C	2.571580	1.806146	2.939899
C	5.293996	2.764193	-1.311126
C	3.355176	-2.311533	-0.497096
C	3.363608	-2.448356	-1.905395
C	2.876375	-3.653949	-2.445018

S9

H	1.893444	-0.614780	-3.336148	C	2.985620	-4.862082	-1.685628
C	2.842349	-3.121937	1.881813	C	3.243322	-4.706347	-0.319112
H	2.773958	-2.029668	2.066626	C	3.626840	-3.457991	0.207588
C	4.153925	-3.638611	2.504404	C	3.740165	2.326543	0.712573
H	5.045599	-3.131704	2.087444	C	3.682907	2.734398	2.066205
H	4.269235	-4.728145	2.325402	C	3.336099	4.073631	2.330642
H	4.154047	-3.471797	3.601186	C	3.044829	4.959731	1.287296
C	1.630740	-3.769089	2.564691	C	3.065887	4.516608	-0.041967
H	1.675607	-4.877946	2.525308	C	3.407177	3.190002	-0.364259
H	0.685636	-3.429021	2.101502	C	3.624084	-1.316897	-3.031863
H	1.607681	-3.483144	3.635674	C	2.618424	-1.328117	-4.189584
C	-0.073131	2.175596	-1.024645	C	3.953619	-3.306770	1.686728
H	-0.142452	2.970426	-0.259830	C	5.392559	-3.773318	1.976013
H	2.038406	2.634316	-1.285039	C	3.999842	1.768305	3.201166
C	1.262742	1.881187	-1.499929	C	3.046251	1.922695	4.395632
H	1.356791	1.416215	-2.499677	C	3.418562	2.697888	-1.807957
C	-1.323576	1.775735	-1.632238	C	2.459586	3.463528	-2.726920
H	-2.168858	2.477815	-1.547114	C	5.067948	-1.236451	-3.564469
H	-1.267692	1.259850	-2.609955	C	2.948037	-4.030027	2.595155
154				C	-4.731009	-2.260372	3.647478
2				C	-0.272704	-3.370835	-1.919728
C	-0.508426	3.300270	-0.066729	C	5.464732	1.910134	3.655470
O	-0.947516	2.279650	0.837124	C	4.842471	2.703826	-2.396340
C	-0.358892	2.621876	2.090899	H	-3.562775	2.965921	2.535096
C	-0.502284	4.151121	2.206607	H	-4.442503	1.534669	3.181169
C	-0.619444	4.611629	0.729543	H	-3.224114	1.338628	1.862347
Pd	-1.403521	-0.050415	0.283754	H	-6.744634	2.578428	2.627621
C	-1.317708	-0.941388	2.152080	H	-5.902526	4.059848	2.109830
C	0.022873	-1.379168	1.871195	H	-7.053551	3.256614	0.994342
C	1.250721	-0.738417	2.283706	H	-4.465736	1.708121	-4.827384
Pd	1.324374	-0.153288	0.304155	H	-3.655921	0.115105	-4.996647
Cl	0.521022	0.444801	-1.943999	H	-4.874285	0.364291	-3.712797
C	-3.316640	-0.390284	-0.265488	H	-1.324502	1.067062	-4.783864
N	-4.231573	0.438991	-0.881775	H	-2.058884	2.695080	-4.819240
C	-5.389736	-0.243480	-1.256372	H	-0.922937	2.222385	-3.491264
C	-5.209061	-1.546648	-0.884369	H	-3.700257	5.672821	-1.661942
N	-3.950136	-1.617864	-0.289133	H	-2.845466	4.078363	-3.371915
C	-4.050665	1.851805	-1.084718	H	-4.751573	4.830548	0.434318
C	-3.433049	2.299186	-2.278961	H	-3.877629	-4.927733	2.925972
C	-3.323299	3.691643	-2.461105	H	-0.956436	-5.144516	-0.251727
C	-3.799219	4.588928	-1.496491	H	-2.531787	0.433826	-2.771555
C	-4.391716	4.115179	-0.319251	H	-5.559997	1.202606	0.987616
C	-4.532931	2.734143	-0.087622	H	3.028812	-5.132749	2.504707
C	-3.404927	-2.825207	0.270087	H	3.137901	-3.775730	3.657583
C	-3.978963	-3.322457	1.464980	H	1.905268	-3.743256	2.356154
C	-3.451866	-4.515456	1.998364	H	5.644278	-3.634659	3.047714
C	-2.379917	-5.164827	1.379123	H	5.513836	-4.849257	1.732190
C	-1.812783	-4.634822	0.211091	H	6.133514	-3.208711	1.376160
C	-2.311969	-3.459451	-0.379675	H	5.314055	-2.134651	-4.168763
C	-2.914584	1.317639	-3.325323	H	5.193708	-0.343886	-4.211424
C	-1.743022	1.870517	-4.145875	H	5.810399	-1.165378	-2.745889
C	-5.130938	2.202707	1.210086	H	2.721670	-0.395325	-4.779747
C	-6.269472	3.073897	1.756883	H	2.786940	-2.176577	-4.885184
C	-5.104978	-2.593786	2.192845	H	1.580489	-1.361325	-3.806947
C	-6.419977	-3.389406	2.124302	H	2.685453	-5.845311	-2.079050
C	-1.695177	-2.881412	-1.647072	H	2.878393	-3.900684	-3.622255
C	-2.600051	-3.098095	-2.873512	H	3.146081	-5.570208	0.354850
C	-4.045537	0.849851	-4.262458	H	3.290322	4.424497	3.372111
C	-4.024366	1.994489	2.261469	H	2.804277	5.213802	-0.850186
C	3.315782	-0.055802	0.129495	H	3.416673	-0.399390	-2.444945
N	4.168485	-1.090347	-0.194581	H	3.898881	-2.224088	1.922820
C	5.506367	-0.704637	-0.098596	H	-6.229249	0.259347	-1.744153
C	5.508302	0.607977	0.284467	H	-5.851298	-2.424930	-0.993169
N	4.169897	0.986521	0.411458	H	6.327147	-1.392244	-0.319203
C	3.736399	-2.371752	-0.692418	H	6.330285	1.306099	0.463299
C	3.469549	-2.497664	-2.080100	H	-1.971407	-6.089268	1.815475
C	3.097947	-3.768920	-2.553432	H	-5.269915	-1.627028	1.676220

H	-3.797608	-1.665750	3.696288	C	-3.286277	4.385531	-2.396509
H	-4.582515	-3.176147	4.256169	C	-2.165634	4.994970	-1.819953
H	-5.539466	-1.671010	4.126902	C	-1.653696	4.526676	-0.603256
H	-6.722548	-3.589526	1.076654	C	-2.250591	3.446057	0.073771
H	-7.243436	-2.834368	2.618903	C	-3.143553	-1.025732	3.366793
H	-6.320983	-4.370715	2.633408	C	-2.008326	-1.558524	4.248276
H	-1.608183	-1.783004	-1.466764	C	-5.215282	-2.171604	-1.173581
H	0.151869	-2.812736	-2.775446	C	-6.479468	-2.902801	-1.645700
H	-0.231336	-4.451352	-2.173368	C	-5.075287	2.557289	-2.446954
H	0.396698	-3.183554	-1.057055	C	-5.901911	3.442218	-3.387347
H	-2.155500	-2.607011	-3.763403	C	-1.695817	2.929760	1.394259
H	-3.613296	-2.673601	-2.729383	C	-2.620795	3.262673	2.578489
H	-2.712722	-4.179431	-3.100716	C	-4.265987	-0.430474	4.239033
H	2.778744	6.003932	1.512479	C	-4.057472	-2.318093	-2.180461
H	3.863094	0.743093	2.799485	C	3.312716	0.050413	-0.012834
H	5.658361	2.932017	4.043017	N	4.120638	1.067417	0.449596
H	6.172906	1.726336	2.824220	C	5.469317	0.712101	0.406076
H	5.696858	1.187804	4.464933	C	5.523857	-0.561409	-0.085393
H	3.207784	2.878654	4.935402	N	4.205770	-0.949456	-0.332794
H	3.210589	1.104147	5.125106	C	3.664842	2.330269	0.972866
H	1.986319	1.886963	4.075874	C	3.310848	2.406840	2.344058
H	3.048378	1.651396	-1.781131	C	2.954017	3.671717	2.845444
H	5.545580	2.090171	-1.801288	C	2.941235	4.803867	2.020940
H	5.245553	3.737251	-2.443733	C	3.280173	4.694688	0.667976
H	4.832536	2.293881	-3.427202	C	3.652096	3.454738	0.114217
H	2.781992	4.512878	-2.894758	C	3.852102	-2.270708	-0.780438
H	1.429337	3.462900	-2.323398	C	3.968986	-2.573586	-2.158144
H	2.422384	2.967511	-3.717000	C	3.720158	-3.901264	-2.557632
H	0.112025	-2.401994	1.462689	C	3.362324	-4.877913	-1.621710
H	2.096404	-1.393167	2.549298	C	3.222620	-4.541032	-0.268340
H	1.157878	0.133704	2.957716	C	3.456166	-3.229865	0.186911
H	-2.083703	-1.727276	2.225871	C	3.347636	1.179528	3.247618
H	-1.439777	-0.130946	2.898019	C	2.286130	1.208875	4.353998
H	0.714800	2.318946	2.087801	C	4.062283	3.351780	-1.348842
H	-0.884931	2.051718	2.880744	C	5.501148	3.861042	-1.551291
H	-1.410265	4.423267	2.780730	C	4.360740	-1.513593	-3.180362
H	0.370592	4.595474	2.723991	C	3.504211	-1.578504	-4.454284
H	0.176895	5.326112	0.443072	C	3.322039	-2.865902	1.660880
H	-1.597234	5.097016	0.542914	C	2.258897	-3.691239	2.394219
H	0.542380	3.091554	-0.366175	C	4.752495	0.976749	3.847852
H	-1.150217	3.256979	-0.964450	C	3.083176	4.069851	-2.289769
154				C	-4.574028	1.294534	-3.175366
TS2-3				C	-0.262292	3.369888	1.686634
C	-0.977981	-3.264333	-0.060593	C	5.858095	-1.604026	-3.529189
O	-0.564857	-2.217682	-0.962725	C	4.680739	-2.956092	2.381438
C	0.057828	-2.769515	-2.128368	H	-3.757153	-3.382718	-2.277748
C	-0.352222	-4.243070	-2.152431	H	-4.360393	-1.953176	-3.183487
C	-0.435982	-4.568496	-0.653172	H	-3.173260	-1.735571	-1.843255
Pd	-1.531080	-0.025350	-0.200906	H	-6.829872	-2.479591	-2.609104
C	-1.020302	1.096864	-2.627277	H	-6.295448	-3.983902	-1.815432
C	0.226573	1.442822	-2.118537	H	-7.303944	-2.811722	-0.909830
C	1.448964	0.667940	-2.202217	H	-4.730776	-1.215043	4.872480
Pd	1.342977	0.047867	-0.214345	H	-3.856269	0.352066	4.910344
Cl	0.452794	-0.579695	1.959863	H	-5.065317	0.036521	3.632640
C	-3.416623	0.461746	0.200563	H	-1.574982	-0.727200	4.839449
N	-4.388770	-0.277045	0.849593	H	-2.363427	-2.323659	4.970500
C	-5.526726	0.480543	1.132757	H	-1.190449	-1.983701	3.635294
C	-5.279261	1.741586	0.665754	H	-4.064361	-5.460635	2.005763
N	-4.002562	1.714801	0.101661	H	-3.176268	-3.779015	3.613038
C	-4.265959	-1.676065	1.154494	H	-5.020432	-4.731496	-0.179626
C	-3.686691	-2.063000	2.390037	H	-3.669262	4.759569	-3.356518
C	-3.626537	-3.441227	2.669246	H	-0.767362	5.009203	-0.168058
C	-4.119421	-4.388515	1.761652	H	-2.714830	-0.209751	2.746329
C	-4.662575	-3.978413	0.538260	H	-5.459460	-1.091277	-1.115249
C	-4.742376	-2.612257	0.205385	H	3.104128	5.169653	-2.146506
C	-3.380402	2.841120	-0.538443	H	3.351111	3.872271	-3.347506
C	-3.915929	3.290386	-1.773145	H	2.042971	3.724731	-2.132544

H	5.812862	3.749126	-2.610229	C	0.868083	0.509847	-2.425324
H	5.583374	4.934912	-1.283266	C	-0.480114	0.317679	-2.556801
H	6.223348	3.303045	-0.922780	C	0.044321	0.041226	-0.351829
H	5.032182	1.833582	4.496080	N	-0.965874	0.047058	-1.278608
H	4.777333	0.057179	4.468289	C	2.473491	0.577992	-0.503775
H	5.531182	0.873570	3.067284	C	3.518760	-0.340797	-0.758286
H	2.282554	0.239598	4.891508	C	4.786902	-0.038774	-0.224614
H	2.482581	2.002045	5.105534	C	4.997223	1.112344	0.539763
H	1.274904	1.347209	3.925922	C	3.938806	1.996023	0.788809
H	2.653254	5.781152	2.437460	C	2.654390	1.755419	0.269779
H	2.667739	3.768483	3.901980	C	3.319559	-1.603489	-1.587684
H	3.258548	5.588260	0.026509	C	1.518086	2.751123	0.488024
H	3.803746	-4.170957	-3.620728	C	-2.357494	-0.051876	-0.922760
H	2.928837	-5.314946	0.454798	C	-3.104526	1.148708	-0.832106
H	3.108968	0.303945	2.610091	C	-4.456032	1.042885	-0.451636
H	4.049566	2.275565	-1.616278	C	-5.026878	-0.202383	-0.162161
H	-6.399939	0.056400	1.635929	C	-4.258636	-1.370788	-0.252690
H	-5.881346	2.653957	0.703921	C	-2.905035	-1.325753	-0.636230
H	6.257573	1.392835	0.737917	Cl	1.106294	-2.525616	1.078441
H	6.368675	-1.230949	-0.266736	C	1.643425	3.550335	1.790398
H	-1.682005	5.843567	-2.327861	H	2.490256	4.267250	1.766103
H	-5.760618	2.209437	-1.646896	H	0.722347	4.144225	1.959447
H	-3.989336	0.638881	-2.500646	H	1.787260	2.882718	2.663605
H	-3.920127	1.568372	-4.029178	C	1.373176	3.692212	-0.723455
H	-5.429578	0.710793	-3.573935	H	0.514727	4.381524	-0.582654
H	-6.249772	4.367578	-2.885344	H	2.287382	4.307046	-0.857549
H	-6.793477	2.888302	-3.744086	H	1.203366	3.129769	-1.662950
H	-5.326633	3.739593	-4.288327	C	3.856659	-1.411762	-3.018727
H	-1.661141	1.814959	1.282236	H	4.950181	-1.221537	-3.007065
H	0.109772	2.837316	2.582166	H	3.678015	-2.322091	-3.626856
H	-0.179852	4.458705	1.889708	H	3.380957	-0.557256	-3.540219
H	0.427677	3.111814	0.859021	C	3.957275	-2.838376	-0.932399
H	-2.229623	2.798170	3.507031	H	3.685239	-3.749711	-1.502605
H	-3.652477	2.889174	2.428051	H	5.065480	-2.777251	-0.921597
H	-2.675377	4.359937	2.743230	H	3.588284	-2.959402	0.103800
H	3.177830	-5.912143	-1.950527	H	5.995190	1.322311	0.953888
H	4.180302	-0.525816	-2.708702	H	5.620560	-0.733740	-0.401584
H	6.095703	-2.582886	-3.995177	H	4.116329	2.894409	1.396534
H	6.497666	-1.495592	-2.631687	H	-5.067888	1.954001	-0.371665
H	6.142574	-0.806883	-4.246393	H	-4.716750	-2.342226	-0.018193
H	3.713801	-2.492119	-5.047832	H	2.228873	-1.796944	-1.634784
H	3.721085	-0.708093	-5.105797	H	0.583015	2.160965	0.571402
H	2.422286	-1.565757	-4.217974	H	1.636972	0.757329	-3.161292
H	2.971828	-1.814045	1.702036	H	-1.134153	0.349254	-3.432015
H	5.449796	-2.317747	1.903965	H	-6.083337	-0.263154	0.140949
H	5.058464	-4.000166	2.385625	C	-2.495291	2.509201	-1.159034
H	4.579162	-2.625143	3.435503	H	-1.393664	2.387612	-1.185204
H	2.548217	-4.757483	2.503487	C	-2.801301	3.580360	-0.100654
H	1.284715	-3.629685	1.873177	H	-2.465540	3.267907	0.907372
H	2.108591	-3.281390	3.412399	H	-3.884704	3.811202	-0.042556
H	0.298457	2.440644	-1.648700	H	-2.279019	4.525539	-0.353746
H	2.368260	1.250468	-2.386076	C	-2.944436	2.982395	-2.554304
H	1.393464	-0.225009	-2.853667	H	-2.688653	2.244937	-3.340396
H	-1.841295	1.823160	-2.601823	H	-2.460224	3.945083	-2.817419
H	-1.160374	0.180942	-3.224212	H	-4.043449	3.133026	-2.585415
H	1.162473	-2.653516	-2.048399	C	-2.074738	-2.592766	-0.780518
H	-0.291981	-2.197179	-3.013225	H	-1.018214	-2.329788	-0.568927
H	-1.344690	-4.361825	-2.635578	C	-2.444359	-3.680344	0.234188
H	0.376870	-4.874746	-2.697728	H	-1.701677	-4.500322	0.186057
H	0.577847	-4.781107	-0.259398	H	-3.446101	-4.120166	0.044236
H	-1.085550	-5.436348	-0.424794	H	-2.424295	-3.279576	1.267148
H	-0.581105	-3.023216	0.946385	C	-2.152831	-3.117891	-2.226278
H	-2.086244	-3.259823	-0.005127	H	-1.507560	-4.011743	-2.347227
75				H	-1.814806	-2.355584	-2.957307
3				H	-3.192020	-3.403652	-2.493234
Pd	-0.141298	-0.559170	1.560065	C	-1.521324	-0.232433	3.158548
N	1.170348	0.339030	-1.073832	H	-2.495154	-0.730706	3.004793

C	-0.448923	-0.965168	3.710488
H	-0.598563	-2.006277	4.031549
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68			
4			
Pd	0.031760	0.790876	1.320309
Cl	0.069418	-1.314055	2.254669
N	-1.118728	-0.528471	-1.117078
C	-0.718888	-1.073151	-2.336069
C	0.649861	-1.021791	-2.361184
C	-0.033673	-0.133063	-0.389987
N	1.052753	-0.446188	-1.156661
C	-2.485867	-0.336278	-0.701288
C	-3.066739	0.940818	-0.889888
C	-4.401921	1.108153	-0.479607
C	-5.118512	0.047219	0.087770
C	-4.512112	-1.202358	0.265099
C	-3.176598	-1.424712	-0.118833
C	-2.272181	2.112774	-1.453519
C	-2.523290	-2.787524	0.069458
C	2.421569	-0.207721	-0.770049
C	3.242262	-1.324210	-0.493741
C	4.591513	-1.070465	-0.176525
C	5.082609	0.235718	-0.106047
C	4.229952	1.325168	-0.334641
C	2.879606	1.133082	-0.670816
Cl	0.249143	2.310224	3.052264
C	-2.802847	-3.387754	1.455084
H	-3.875774	-3.633672	1.595198
H	-2.231647	-4.329839	1.579402
H	-2.486893	-2.691286	2.255398
C	-2.948098	-3.751942	-1.053796
H	-2.443586	-4.732913	-0.937775
H	-4.043658	-3.928356	-1.031491
H	-2.696401	-3.356627	-2.058631
C	-3.022821	2.860359	-2.566204
H	-3.936650	3.359465	-2.184057
H	-2.376980	3.650050	-3.000733
H	-3.327182	2.175247	-3.382618
C	-1.853753	3.065196	-0.321050
H	-1.184962	3.867747	-0.692546
H	-2.734828	3.537511	0.159440
H	-1.315737	2.523950	0.496132
H	-6.161656	0.199009	0.403906
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H	4.621544	2.347072	-0.240168
H	-1.343367	1.707120	-1.904798
H	-1.425835	-2.639558	0.006163
H	-1.444642	-1.431015	-3.070936
H	1.373438	-1.333047	-3.119462
H	6.137451	0.413005	0.152468
C	2.714353	-2.753909	-0.485287
H	1.619957	-2.715835	-0.657126
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H	4.438597	-3.677695	-1.489930
H	3.155152	-3.141106	-2.612168
H	2.920325	-4.617279	-1.618805
C	2.919143	-3.409897	0.891101
H	3.995250	-3.519518	1.137721
H	2.469601	-4.423834	0.901048
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C	1.945388	2.315003	-0.914576

H	0.962625	2.035010	-0.453307
C	1.693443	2.538343	-2.416090
H	1.312063	1.626346	-2.916546
H	2.634189	2.834665	-2.925148
H	0.952074	3.348648	-2.572101
C	2.375301	3.605461	-0.213877
H	3.308336	4.023815	-0.644857
H	2.520619	3.443696	0.872309
H	1.586562	4.374831	-0.333964

143			
5			
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C	0.834851	-0.416085	-3.031905
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C	-1.175736	0.946446	-2.100877
C	3.232366	-0.186871	0.132299
C	5.068352	-1.415551	0.751575
C	5.263098	-0.133734	1.188949
C	-3.067898	-0.039827	-0.085035
C	-5.341795	0.244015	-0.064521
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H	5.681012	-2.314259	0.857467
H	6.088761	0.327232	1.737908
H	-6.279427	0.795572	-0.166374
H	-5.752768	-1.875752	0.540907
H	1.459925	-0.318683	-3.940288
H	-1.845040	0.214170	-2.592226
H	-1.573790	1.972529	-2.200487
H	0.690782	1.775818	-2.905376
H	0.136003	-1.268928	-3.105181
C	-3.122315	-2.498001	0.574104
C	-2.331276	-5.122937	1.082166
C	-3.259465	-3.008617	1.888750
C	-2.575519	-3.264105	-0.489249
C	-2.179960	-4.582754	-0.201761
C	-2.856428	-4.339817	2.113127
H	-1.752124	-5.202588	-1.001318
H	-2.951203	-4.761937	3.124420
H	-2.023738	-6.161115	1.280724
C	-3.969531	2.211419	-0.730467
C	-3.725022	4.851180	-1.571523
C	-4.243747	2.520103	-2.085987
C	-3.581557	3.189432	0.219377
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C	-4.118105	3.864949	-2.483488
H	-3.145785	5.295823	0.468041
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H	-3.620848	5.895230	-1.904366
C	3.204757	-2.595028	-0.445933
C	1.923379	-4.843208	-1.483195
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C	2.946528	-4.223780	-2.205572
C	1.535032	-4.332361	-0.237903
H	3.243348	-4.621483	-3.189144
H	0.716047	-4.810851	0.314558
H	1.413905	-5.726339	-1.898412
C	3.988980	1.999450	1.111619
C	3.819395	4.704081	1.722323
C	4.597276	2.931180	0.238502
C	3.264721	2.383215	2.267173

C	3.204565	3.759672	2.552823	H	6.332155	4.333645	-1.617960
C	4.499120	4.295323	0.570121	H	7.021718	2.835690	-2.295008
H	2.644339	4.098608	3.434527	H	7.262898	3.228189	-0.559408
H	4.955001	5.047372	-0.090348	C	4.228766	2.578656	-2.213121
H	3.751876	5.774988	1.968141	H	3.895076	3.625775	-2.364897
C	-2.455570	-2.690234	-1.897173	H	3.325157	1.971129	-1.979629
H	-2.097760	-1.647294	-1.769642	H	4.666294	2.208182	-3.163228
C	-1.426423	-3.419695	-2.767403	C	2.553283	1.359790	3.146464
H	-1.746049	-4.454106	-3.012579	H	2.112366	0.606613	2.458522
H	-0.435575	-3.475776	-2.274650	C	3.531686	0.643655	4.097089
H	-1.306320	-2.889933	-3.734221	H	3.999359	1.367888	4.796689
C	-3.818983	-2.638793	-2.614126	H	4.343625	0.118821	3.557690
H	-4.218089	-3.662474	-2.771987	H	2.990884	-0.112164	4.702567
H	-3.713552	-2.157433	-3.608598	C	1.385281	1.956287	3.938834
H	-4.575380	-2.066270	-2.043322	H	0.807180	1.141799	4.415662
C	-3.845396	-2.196132	3.039374	H	0.686318	2.492996	3.270348
H	-3.907566	-1.141235	2.705062	H	1.734073	2.643664	4.738776
C	-5.257645	-2.691193	3.404997	H	-5.228500	-3.737962	3.773311
H	-5.955666	-2.665144	2.544523	Cl	0.673446	2.246572	0.230951
H	-5.691557	-2.063590	4.210036	H	1.655129	-0.870288	-2.251458
C	-2.935367	-2.209103	4.277929				
H	-1.936914	-1.808468	4.020880	134			
H	-2.827384	-3.227677	4.705222	6			
H	-3.368237	-1.562695	5.068369	Pd	-1.268404	0.066686	0.144506
C	-4.679396	1.457091	-3.089980	Pd	1.349047	0.145223	0.253487
H	-4.434933	0.466824	-2.653407	Cl	0.054031	1.405685	-1.413200
C	-6.202493	1.508330	-3.315031	N	4.150138	-0.955847	0.561906
H	-6.500522	2.483665	-3.752671	N	4.192207	1.038954	-0.281478
H	-6.765953	1.383438	-2.369781	N	-4.246130	0.690471	0.360105
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C	-3.937427	1.558024	-4.432413	C	3.328683	0.085599	0.201231
H	-4.215630	2.475813	-4.990232	C	5.487592	-0.661916	0.303754
H	-4.198382	0.694211	-5.077702	C	5.514309	0.602232	-0.227848
H	-2.839642	1.564210	-4.289712	C	-3.218578	-0.074319	-0.137079
C	-3.353189	2.836035	1.682263	C	-5.220669	-0.751632	-1.014829
H	-2.982550	1.791554	1.725958	C	-5.476498	0.292774	-0.166808
C	-2.269316	3.686100	2.354416	H	6.290549	-1.373258	0.516848
H	-2.580127	4.743662	2.490293	H	6.345855	1.225922	-0.567268
H	-1.329129	3.660126	1.768947	H	-5.884896	-1.356300	-1.638499
H	-2.046283	3.270489	3.356691	H	-6.412596	0.782636	0.115533
C	-4.681357	2.898035	2.460340	C	-4.060738	1.718436	1.349393
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H	-5.448274	2.227589	2.021737	C	-4.361216	1.408199	2.697400
C	4.748433	-2.526387	-2.577422	C	-4.183896	2.427697	3.651715
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C	6.092296	-3.192536	-2.221470	H	-4.403464	2.222191	4.709597
H	6.010279	-4.297593	-2.223367	H	-3.014045	4.951301	1.659191
H	6.443360	-2.878309	-1.218151	H	-3.578558	4.474518	4.036011
H	6.875103	-2.902312	-2.952155	C	-3.121026	-1.925819	-1.769865
C	4.894172	-0.999882	-2.660578	C	-1.757855	-3.795194	-3.311531
H	3.919562	-0.492808	-2.791396	C	-2.662946	-3.113890	-1.143645
H	5.539378	-0.737914	-3.523351	C	-2.871813	-1.629260	-3.129428
H	5.370682	-0.573430	-1.757686	C	-2.189308	-2.597957	-3.891181
C	1.746887	-2.650187	1.672337	C	-1.982614	-4.043024	-1.949837
H	1.696922	-1.544061	1.571329	H	-1.981386	-2.398938	-4.953406
C	0.357068	-3.107416	2.111145	H	-1.611551	-4.974633	-1.500139
H	-0.407479	-2.870280	1.349789	H	-1.220773	-4.537833	-3.921198
H	0.062901	-2.565565	3.028598	C	3.628040	-2.188880	1.088983
H	0.323880	-4.195413	2.328328	C	2.475347	-2.497461	2.119472
C	2.780739	-2.995211	2.762883	C	3.661140	-2.393166	2.489942
H	3.792235	-2.607039	2.538548	C	3.039206	-3.108814	0.189879
H	2.855645	-4.095035	2.894621	C	2.460657	-4.268606	0.739816
H	2.465110	-2.557275	3.731264	C	3.074448	-3.571590	2.984110
C	5.252198	2.492836	-1.065178	H	1.982457	-5.000257	0.070987
H	5.533451	1.425562	-0.957140	H	3.070893	-3.761545	4.066871
C	6.536018	3.266112	-1.395775	H	2.008077	-5.405671	2.529635
				C	3.729494	2.263610	-0.878178

6

Pd	-1.268404	0.066686	0.144506
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C	-3.121026	-1.925819	-1.769865
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H	1.982457	-5.000257	0.070987
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H	2.008077	-5.405671	2.529635
C	3.729494	2.263610	-0.878178

C	2.779408	4.598889	-2.048337	H	5.396287	-1.123964	5.258772
C	3.557010	2.295309	-2.282883	C	3.834971	1.077613	-3.155991
C	3.399531	3.352982	-0.039095	H	3.967290	0.209327	-2.479100
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C	3.088630	3.493791	-2.850709	H	5.075685	2.114016	-4.643415
H	2.648157	5.388126	-0.035216	H	5.356443	0.345411	-4.555236
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H	2.402502	5.523757	-2.510982	C	2.649670	0.742137	-4.075890
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C	-3.504341	-0.789334	3.543186	H	2.840126	-0.211902	-4.609410
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H	-2.728005	-0.771955	2.752955	H	4.009883	2.317178	1.728223
H	-3.759070	-1.847356	3.761266	C	4.240740	4.417158	2.114187
C	-5.840355	-0.029734	4.206912	H	3.728505	5.388050	1.952571
H	-5.470155	0.379499	5.169438	H	5.264890	4.502967	1.697770
H	-6.159416	-1.073467	4.402482	H	4.324994	4.270929	3.210345
H	-6.735599	0.554629	3.912474	C	2.047567	3.120608	2.062372
C	-3.237718	3.264659	-0.522536	H	2.084867	2.982020	3.162207
H	-2.871373	2.312820	-0.960063	H	1.522324	2.243550	1.619863
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H	-4.269531	3.839311	-2.367525	Cl	0.000477	-1.132780	1.849294
H	-4.915861	4.633726	-0.892640		136		
H	-5.298771	2.915532	-1.228604		7		
C	-2.107641	4.284327	-0.705680	Pd	1.579098	-0.156021	-1.051905
H	-1.202173	3.981486	-0.144078	Pd	-0.895253	-0.182603	-0.114501
H	-2.406044	5.304671	-0.385505	Cl	-0.393026	-0.618245	-2.395455
H	-1.826284	4.343455	-1.775865	N	-3.791996	0.594652	0.060010
C	-2.904550	-3.365840	0.340498	N	-3.562647	-1.524852	-0.364551
H	-2.838377	-2.377988	0.841647	N	3.840171	-0.005671	0.987237
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H	-5.102580	-3.255109	0.179288	C	-5.075597	0.075151	-0.103975
H	-4.505675	-4.046585	1.670806	C	-4.930632	-1.259071	-0.360941
C	-1.834145	-4.250809	0.989742	C	2.852336	0.597056	0.244669
H	-1.871690	-5.296960	0.619212	C	4.222161	2.163839	1.200248
H	-1.994237	-4.286288	2.086041	C	4.685817	0.931839	1.572418
H	-0.818674	-3.842770	0.818162	H	-5.963194	0.707230	-0.021385
C	-3.292744	-0.308627	-3.762260	H	-5.666927	-2.047297	-0.534605
H	-3.689883	0.340795	-2.956044	H	4.593573	3.169547	1.411144
C	-2.092666	0.428592	-4.380111	H	5.538631	0.631874	2.186787
H	-1.658414	-0.136386	-5.230824	C	4.042464	-1.425131	1.117829
H	-1.295965	0.592391	-3.627309	C	4.520168	-4.142820	1.420950
H	-2.409917	1.418785	-4.767442	C	4.715381	-2.111305	0.079652
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H	-3.293792	5.798936	1.035391	H	-6.464976	1.512410	2.158901
C	-3.013661	-2.836032	-0.625896	H	-6.069373	2.734576	3.402184
C	-2.060749	-5.395064	-1.127596	H	-6.163149	1.001865	3.849933
C	-2.998904	-3.301077	-1.963076	C	-3.508615	-2.461777	-3.130432
C	-2.556011	-3.610583	0.469338	H	-3.520051	-1.401978	-2.800434
C	-2.078727	-4.901664	0.181961	C	-4.948621	-2.859942	-3.509089
C	-2.513589	-4.602886	-2.186834	H	-4.983573	-3.916647	-3.846294
H	-1.698735	-5.528004	0.999953	H	-5.325151	-2.225989	-4.338157
H	-2.479842	-4.995085	-3.213562	H	-5.652322	-2.759931	-2.659889
H	-1.675027	-6.406613	-1.325732	C	-2.596069	-2.546486	-4.364531
C	2.854340	-1.298563	3.391303	H	-2.645081	-3.546631	-4.842211
H	2.525287	-0.330218	2.962306	H	-1.543815	-2.336473	-4.096039
C	1.582654	-2.029898	3.841837	H	-2.916493	-1.806071	-5.125428
H	1.813274	-2.989207	4.350299	C	-2.588528	-3.075426	1.896254
H	0.926032	-2.235735	2.977639	H	-2.287696	-2.007892	1.854002
H	1.012761	-1.400412	4.554153	C	-4.007530	-3.143921	2.493722
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H	4.142350	-1.942131	5.049219	H	-4.748239	-2.583528	1.889838
H	3.247950	-0.418757	5.359416	H	-4.013572	-2.710336	3.515013
H	4.677065	-0.419770	4.276084	C	-1.582137	-3.766551	2.822345
C	5.159024	-1.410693	-1.198977	H	-1.511645	-3.210781	3.778196
H	5.086339	-0.316979	-1.023712	H	-0.574270	-3.789894	2.365221
C	6.621834	-1.715024	-1.557863	H	-1.884131	-4.807305	3.065204
H	6.934227	-1.119984	-2.440222	Cl	-0.805361	0.177725	2.176094
H	6.770059	-2.783809	-1.814906	H	1.389359	-1.892920	-0.265336
H	7.304548	-1.472960	-0.718610	Cl	1.163408	-3.254344	-0.000894
C	4.210100	-1.745681	-2.362055	136			
H	3.163295	-1.434082	-2.118747	TS7-8			
H	4.180995	-2.835803	-2.562892	Pd	-1.313654	0.014618	0.033994
H	4.517529	-1.222340	-3.290026	Pd	1.335978	-0.220382	0.182325
C	1.109906	3.396398	1.968862	Cl	0.025552	0.402081	2.103775
H	1.334608	2.318740	2.112755	N	4.177037	0.497904	-0.474419
C	1.996792	4.218104	2.924765	N	3.987224	-1.576489	0.142656
H	1.802546	5.304093	2.801225	N	-4.339289	0.042817	-0.595840
H	3.077118	4.048607	2.754902	N	-3.546748	1.958336	0.040511
H	1.776735	3.950539	3.978456	C	3.266851	-0.427583	-0.036119
C	-0.367106	3.594002	2.323439	C	5.451300	-0.066204	-0.562028
H	-0.658861	4.664172	2.309598	C	5.329160	-1.374917	-0.173095
H	-0.562994	3.212954	3.344644	C	-3.195272	0.645844	-0.153289
H	-1.025620	3.037338	1.632942	C	-4.886593	2.170722	-0.275104
C	3.695072	2.518418	-2.396640	C	-5.387419	0.958800	-0.674569
H	4.136195	1.752977	-1.726991	H	6.317475	0.513675	-0.891779
C	3.014208	1.765586	-3.551638	H	6.069340	-2.174223	-0.079168
H	2.536463	2.463036	-4.270173	H	-5.355509	3.154783	-0.187496
H	2.220725	1.088164	-3.162963	H	-6.387073	0.660441	-1.001843
H	3.749462	1.149660	-4.107847	C	-4.464984	-1.367367	-0.869004
C	4.844731	3.410494	-2.892595	C	-4.780224	-4.071036	-1.394732
H	4.484722	4.186848	-3.598881	C	-4.983245	-2.195061	0.151850
H	5.604634	2.802927	-3.425312	C	-4.038030	-1.860690	-2.126071
H	5.346771	3.928870	-2.050895	C	-4.214885	-3.233934	-2.365546
C	-2.762931	2.307119	-2.083723	C	-5.148355	-3.559908	-0.147245
H	-2.676384	1.205112	-2.020844	H	-3.887424	-3.661131	-3.323438
C	-1.406723	2.818331	-2.587647	H	-5.542925	-4.236040	0.625694
H	-0.599789	2.578699	-1.867752	H	-4.903206	-5.144290	-1.604600
H	-1.408806	3.914933	-2.753691	C	-2.618719	2.916010	0.588067
H	-1.150710	2.330226	-3.548617	C	-0.715568	4.604593	1.698233
C	-3.901644	2.627564	-3.068718	C	-1.606601	3.439769	-0.256178
H	-4.867669	2.203227	-2.726396	C	-2.707886	3.216575	1.968633
H	-3.677475	2.205422	-4.069881	C	-1.733583	4.080697	2.502753
H	-4.037963	3.723295	-3.183688	C	-0.651707	4.286918	0.335803
C	-4.338941	1.541325	2.762417	H	-1.762075	4.330370	3.572974
H	-4.163260	0.498451	2.429275	H	0.165497	4.691483	-0.276873
C	-3.501169	1.744816	4.035021	H	0.047881	5.261811	2.141664
H	-2.426851	1.598120	3.813550	C	3.833022	1.863197	-0.771211
H	-3.799441	1.007401	4.807937	C	3.207211	4.510050	-1.341825
H	-3.645087	2.756361	4.468003	C	3.733583	2.256969	-2.125601
C	-5.841455	1.705325	3.054926	C	3.583552	2.746725	0.310923

C	3.267157	4.079019	-0.009084	H	1.793614	1.069637	-3.724757
C	3.433255	3.608007	-2.386763	H	2.887036	0.513530	-5.033160
H	3.064052	4.791672	0.802654	H	2.645370	2.264084	-4.765170
H	3.355083	3.950076	-3.429602	C	5.263316	1.526013	-3.996374
H	2.965748	5.560277	-1.567085	H	6.126513	1.461808	-3.303377
C	3.406478	-2.763794	0.721230	H	5.280910	2.535966	-4.456283
C	2.221111	-4.987105	1.878934	H	5.417573	0.783149	-4.805387
C	3.532051	-2.942377	2.118841	C	4.217143	-1.914854	3.012584
C	2.678812	-3.647512	-0.113507	H	4.670459	-1.140644	2.360565
C	2.089080	-4.765143	0.502465	C	5.359181	-2.531898	3.835692
C	2.931564	-4.085547	2.678332	H	4.985791	-3.304888	4.538821
H	1.488482	-5.458698	-0.100851	H	5.868338	-1.753233	4.440047
H	2.999682	-4.254629	3.763669	H	6.116810	-3.011686	3.183302
H	1.737209	-5.862256	2.337935	C	3.186010	-1.202381	3.906340
C	-3.400347	-0.941005	-3.161031	H	2.725577	-1.907597	4.628554
H	-2.828594	-0.175850	-2.594827	H	2.366707	-0.765395	3.302013
C	-2.388871	-1.661396	-4.060765	H	3.668964	-0.388814	4.486894
H	-2.882960	-2.375402	-4.752164	C	2.539728	-3.393162	-1.609934
H	-1.639947	-2.211973	-3.458481	H	2.497927	-2.292620	-1.747436
H	-1.846471	-0.923036	-4.684863	C	3.774068	-3.915047	-2.370234
C	-4.467862	-0.209640	-3.996307	H	3.869169	-5.015022	-2.256043
H	-5.080849	-0.933898	-4.572095	H	4.714912	-3.456243	-2.004456
H	-3.989656	0.484064	-4.718457	H	3.686712	-3.690805	-3.453519
H	-5.154476	0.384773	-3.361211	C	1.240559	-3.955842	-2.200042
C	-5.297530	-1.665577	1.544951	H	1.108454	-3.583521	-3.235993
H	-4.970109	-0.606935	1.585328	H	0.360009	-3.645747	-1.601367
C	-6.807895	-1.690495	1.833680	H	1.258187	-5.064878	-2.250642
H	-7.020846	-1.279194	2.841922	Cl	0.245703	-0.384103	-1.934794
H	-7.203996	-2.726767	1.803006	H	-1.934237	-1.428725	0.232051
H	-7.376867	-1.093172	1.091971	Cl	-1.340060	-3.250782	0.561933
C	-4.494056	-2.423208	2.617047		136		
H	-3.416672	-2.462361	2.357707	8			
H	-4.846954	-3.470100	2.721048	Pd	1.598497	-0.395790	0.493450
H	-4.611997	-1.931562	3.604606	Cl	0.666521	-1.066550	-1.724851
C	-1.573561	3.126139	-1.748539	N	3.737406	1.576491	-0.201624
H	-1.898977	2.071283	-1.871152	C	5.033839	1.652274	-0.708158
C	-2.578046	4.012979	-2.509210	C	5.431613	0.367092	-0.958852
H	-2.301569	5.084115	-2.419359	C	3.309464	0.278009	-0.131564
H	-3.609771	3.896052	-2.122256	N	4.364165	-0.458250	-0.611381
H	-2.589324	3.750326	-3.586976	C	2.985755	2.728024	0.223372
C	-0.172550	3.226308	-2.359225	C	3.275817	3.279966	1.492910
H	0.197549	4.271783	-2.389107	C	2.624675	4.478150	1.842919
H	-0.187719	2.853476	-3.402382	C	1.720393	5.085917	0.964434
H	0.559224	2.613739	-1.797636	C	1.414434	4.484501	-0.263495
C	-3.762002	2.571577	2.863542	C	2.028996	3.282999	-0.660680

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Pd	1.598497	-0.395790	0.493450
Cl	0.666521	-1.066550	-1.724851
N	3.737406	1.576491	-0.201624
C	5.033839	1.652274	-0.708158
C	5.431613	0.367092	-0.958852
C	3.309464	0.278009	-0.131564
N	4.364165	-0.458250	-0.611381
C	2.985755	2.728024	0.223372
C	3.275817	3.279966	1.492910
C	2.624675	4.478150	1.842919
C	1.720393	5.085917	0.964434
C	1.414434	4.484501	-0.263495
C	2.028996	3.282999	-0.660680
C	4.223623	2.600930	2.473992
C	1.679726	2.621596	-1.987141
C	4.380150	-1.896908	-0.698613
C	4.176917	-2.503992	-1.962779
C	4.217866	-3.909295	-2.015062
C	4.441415	-4.671604	-0.862046
C	4.630250	-4.042300	0.373316
C	4.604951	-2.639546	0.485149
C	0.180595	2.695446	-2.302818
H	-0.157322	3.729854	-2.520586
H	-0.056602	2.068244	-3.183406
H	-0.426228	2.303168	-1.463146
C	2.534455	3.199277	-3.130023
H	2.302218	2.682355	-4.083498
H	2.332162	4.281942	-3.270283
H	3.619908	3.081431	-2.933590
C	5.448260	3.477049	2.784034
H	5.152870	4.427104	3.275849
H	6.145174	2.949252	3.466734
H	6.004378	3.737848	1.860815
C	3.479197	2.182870	3.754046
H	4.158016	1.629973	4.435529

H	3.090090	3.063080	4.306396	H	5.111275	-0.859599	-4.895472
H	2.621277	1.524100	3.511470	H	5.686456	-2.459437	-4.322862
H	1.230658	6.030229	1.248966	C	4.840247	-1.976929	1.836592
H	2.829846	4.937133	2.822021	H	4.660035	-0.890407	1.716447
H	0.671156	4.946276	-0.927659	C	3.846455	-2.476033	2.897119
H	4.057880	-4.415523	-2.977780	H	3.983519	-1.917224	3.845647
H	4.799360	-4.650129	1.274842	H	3.987609	-3.553695	3.119723
H	4.591544	1.669456	1.998071	H	2.803458	-2.322380	2.554836
H	1.920743	1.543328	-1.895650	C	6.300804	-2.155340	2.287676
Pd	-1.460066	-0.537585	-0.688687	H	6.478566	-1.633733	3.250747
Cl	-2.406376	0.017612	-2.740607	H	7.009273	-1.745945	1.539021
N	-4.083607	-1.066936	0.607097	H	6.550806	-3.226675	2.434016
C	-5.287032	-0.455690	0.950139	H	-1.928498	5.963954	-0.539705
C	-5.139992	0.878761	0.690868	C	-4.735998	2.561773	-2.188218
C	-3.198822	-0.146520	0.110369	H	-4.783734	1.463391	-2.045903
N	-3.855129	1.053128	0.177907	C	-6.133052	3.159928	-1.937873
C	-3.763240	-2.441114	0.915181	H	-6.124591	4.260583	-2.082011
C	-3.498526	-2.765687	2.270950	H	-6.496622	2.965732	-0.909023
C	-3.186807	-4.105678	2.562187	H	-6.873045	2.731781	-2.644715
C	-3.130708	-5.071465	1.549997	C	-4.296347	2.799922	-3.641348
C	-3.390484	-4.716198	0.221992	H	-4.298192	3.878007	-3.904957
C	-3.713761	-3.391641	-0.129791	H	-4.994589	2.290636	-4.336063
C	-3.569305	-1.732459	3.392396	H	-3.282921	2.389759	-3.812340
C	-4.040580	-3.034179	-1.572066	C	-1.916237	2.058089	2.098856
C	-3.280375	2.354283	-0.069701	H	-1.982514	0.983673	1.839633
C	-3.724491	3.102841	-1.185625	C	-2.875671	2.312039	3.277204
C	-3.217022	4.408820	-1.330042	H	-3.925670	2.073828	3.011688
C	-2.309330	4.939149	-0.408239	H	-2.841188	3.374645	3.596785
C	-1.877187	4.168131	0.677632	H	-2.594409	1.682965	4.146891
C	-2.349193	2.858508	0.876166	C	-0.456109	2.300653	2.498575
Cl	-0.482302	-1.249128	1.376614	H	-0.279715	3.330960	2.870274
C	-3.004468	-3.587295	-2.561045	H	0.230678	2.113054	1.649277
H	-3.016778	-4.696460	-2.603636	H	-0.172046	1.600326	3.308856
H	-3.216255	-3.206890	-3.579610	H	2.114326	0.056506	1.877347
H	-1.983207	-3.254721	-2.288746	136			
C	-5.468701	-3.490509	-1.922789	9			
H	-5.726628	-3.192716	-2.959732	Pd	-1.517257	-0.502742	-0.650853
H	-5.569399	-4.593785	-1.849058	Cl	-0.673013	-1.170703	1.474776
H	-6.218889	-3.040195	-1.240656	N	-3.845758	1.270434	-0.018651
C	-4.894486	-1.862303	4.168080	C	-5.154291	1.209576	0.458925
H	-4.960776	-2.850939	4.667822	C	-5.390835	-0.091032	0.809451
H	-4.968849	-1.079744	4.950977	C	-3.264360	0.032901	0.027818
H	-5.777844	-1.767533	3.506429	N	-4.216523	-0.795739	0.556880
C	-2.375757	-1.803912	4.357828	C	-3.180997	2.513594	-0.334753
H	-2.438199	-0.976926	5.094726	C	-3.535070	3.201615	-1.519814
H	-2.364400	-2.752178	4.933444	C	-2.938763	4.458624	-1.737829
H	-1.416975	-1.711412	3.813518	C	-2.035847	5.001485	-0.818099
H	-2.875539	-6.112608	1.799885	C	-1.695449	4.289936	0.338567
H	-2.970354	-4.393379	3.601525	C	-2.255004	3.028320	0.610085
H	-3.340478	-5.480607	-0.567193	C	-4.543408	2.650793	-2.520270
H	-3.540917	5.016401	-2.187792	C	-1.907441	2.294600	1.900052
H	-1.153407	4.586755	1.389469	C	-3.986405	-2.159676	0.972787
H	-3.546133	-0.725915	2.927339	C	-3.782663	-2.399341	2.356284
H	-4.006748	-1.931757	-1.671974	C	-3.553917	-3.730096	2.749765
H	5.543881	2.610396	-0.838218	C	-3.519691	-4.767042	1.809652
H	6.370444	-0.037686	-1.344314	C	-3.718432	-4.494601	0.451771
H	-6.126882	-1.028204	1.350908	C	-3.956777	-3.183103	-0.001930
H	-5.818847	1.723213	0.831537	Cl	-2.298075	-0.038822	-2.789536
H	4.461709	-5.770149	-0.927245	C	-0.445040	2.476234	2.323217
C	3.950398	-1.685447	-3.228990	H	-0.226304	3.510956	2.659099
H	3.575504	-0.688981	-2.915177	H	-0.200424	1.791693	3.157772
C	2.888506	-2.295940	-4.156403	H	0.250682	2.230008	1.497283
H	1.946241	-2.493311	-3.611244	C	-2.877401	2.693330	3.028529
H	3.239670	-3.241464	-4.619233	H	-2.655899	2.113858	3.948283
H	2.662195	-1.592721	-4.982883	H	-2.781946	3.772262	3.271594
C	5.273858	-1.483454	-3.992755	H	-3.934244	2.501925	2.751697
H	6.047577	-0.988294	-3.374013	C	-5.905516	3.354873	-2.372059

H	-5.817699	4.439310	-2.591923	H	-1.701910	-1.332776	3.914051
H	-6.645550	2.925156	-3.077842	H	-2.741378	-2.259596	5.051193
H	-6.319872	3.260061	-1.348312	H	-2.740237	-0.476706	5.099501
C	-4.036734	2.746994	-3.967822	C	-5.195888	-1.298855	4.128698
H	-4.741271	2.230904	-4.651036	H	-6.048366	-1.213846	3.426272
H	-3.958298	3.799505	-4.310906	H	-5.260844	-0.457981	4.849266
H	-3.046654	2.262389	-4.065895	H	-5.328189	-2.243824	4.695279
H	-1.586397	5.988700	-1.007761	C	-4.210801	-2.911379	-1.477368
H	-3.189569	5.019080	-2.650401	H	-4.126959	-1.820390	-1.647736
H	-0.975674	4.716423	1.050081	C	-3.157900	-3.570597	-2.380028
H	-3.384502	-3.953933	3.813166	H	-3.305709	-3.248530	-3.429477
H	-3.685196	-5.315389	-0.279672	H	-3.218218	-4.678442	-2.352574
H	-4.673141	1.572646	-2.297689	H	-2.136054	-3.265419	-2.079540
H	-2.039811	1.210266	1.718362	C	-5.640516	-3.334773	-1.860762
Pd	1.517334	-0.502850	0.650871	H	-5.842017	-3.099286	-2.925797
Cl	2.298167	-0.039550	2.789663	H	-6.399161	-2.810444	-1.244173
N	4.216599	-0.795961	-0.556753	H	-5.789555	-4.425676	-1.718260
C	5.391049	-0.091414	-0.809088	H	1.586639	5.988339	1.008448
C	5.154625	1.209196	-0.458461	C	4.543319	2.650075	2.520861
C	3.264483	0.032737	-0.027733	H	4.672928	1.571936	2.298149
N	3.846048	1.270198	0.018949	C	5.905536	3.354008	2.372936
C	3.986106	-2.159698	-0.973105	H	5.817792	4.438421	2.592950
C	3.781917	-2.398787	-2.356626	H	6.320027	3.259329	1.349229
C	3.552550	-3.729313	-2.750509	H	6.645426	2.924112	3.078761
C	3.518188	-4.766573	-1.810747	C	4.036468	2.746113	3.968364
C	3.717477	-4.494701	-0.452825	H	3.958150	3.798574	4.311628
C	3.956441	-3.183453	0.001261	H	4.740840	2.229802	4.651580
C	3.836770	-1.287160	-3.401375	H	3.046293	2.261658	4.066231
C	4.211122	-2.912295	1.476687	C	1.908036	2.294728	-1.899924
C	3.181299	2.513335	0.335101	H	2.040137	1.210339	-1.718339
C	3.535199	3.201143	1.520319	C	2.878411	2.693444	-3.028044
C	2.938913	4.458146	1.738437	H	3.935130	2.501745	-2.750943
C	2.036124	5.001164	0.818676	H	2.783277	3.772445	-3.270930
C	1.695849	4.289794	-0.338137	H	2.657037	2.114208	-3.947975
C	2.255409	3.028212	-0.609770	C	0.445781	2.476694	-2.323497
Cl	0.673028	-1.170620	-1.474792	H	0.227301	3.511506	-2.659263
C	3.158352	-3.571413	2.379558	H	-0.250232	2.230401	-1.497829
H	3.218395	-4.679271	2.351890	H	0.201315	1.792332	-3.158247
H	3.306580	-3.249570	3.429018				
H	2.136472	-3.265966	2.079466				
C	5.640834	-3.336354	1.859361				
H	5.842857	-3.101368	2.924407				
H	5.789380	-4.427258	1.716354				
H	6.399436	-2.812069	1.242677				
C	5.195281	-1.298295	-4.128890				
H	5.327124	-2.243170	-4.695736				
H	5.260464	-0.457267	-4.849260				
H	6.047906	-1.213786	-3.426588				
C	2.685870	-1.348614	-4.417861				
H	2.739801	-0.474683	-5.098963				
H	2.740389	-2.257585	-5.051449				
H	1.701327	-1.330914	-3.913773				
H	3.327405	-5.798865	-2.141501				
H	3.382761	-3.952707	-3.813945				
H	3.684177	-5.315730	0.278341				
H	3.189608	5.018460	2.651125				
H	0.976134	4.716385	-1.049650				
H	3.743988	-0.318193	-2.870046				
H	4.127787	-1.821328	1.647413				
H	-5.784637	2.100341	0.513827				
H	-6.276237	-0.581501	1.220886				
H	6.276415	-0.581944	-1.220532				
H	5.785172	2.099836	-0.513084				
H	-3.329379	-5.799522	2.140088				
C	-3.837252	-1.288058	3.401404				
H	-3.743904	-0.318961	2.870408				
C	-2.686516	-1.350357	4.418026				

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Pd	-0.013995	0.205046	-1.926751
C	1.864885	2.558587	0.412594
H	0.906170	2.186201	-0.009506
C	2.844437	1.395902	0.300883
C	4.206774	1.598251	0.015085
H	4.582339	2.621462	-0.126865
C	5.092230	0.517748	-0.097327
C	4.627998	-0.794260	0.050793
H	5.327250	-1.635137	-0.064816
C	3.273361	-1.054484	0.332475
C	2.735549	-2.479411	0.370558
H	1.811966	-2.473996	0.985913
C	2.408314	0.056785	0.470217
N	1.037805	-0.182502	0.836485
C	-0.035048	-0.121888	-0.033297
C	0.627763	-0.459955	2.141336
H	1.341520	-0.544648	2.965630
C	-0.735112	-0.573994	2.109120
H	-1.462227	-0.757305	2.904389
N	-1.122654	-0.373032	0.785712
H	6.155362	0.701854	-0.315607
C	2.329612	-2.903792	-1.054424
H	3.221232	-2.949712	-1.714050
H	1.615098	-2.174042	-1.494279
H	1.850986	-3.904709	-1.046794
C	3.700147	-3.486623	1.009473
H	4.613915	-3.632378	0.397129

H	3.212386	-4.478182	1.099630	N	0.914819	-1.564942	0.541720
H	4.018768	-3.165854	2.022068	C	-0.102764	-0.723985	0.118875
C	2.266642	3.774948	-0.428900	C	0.424751	-2.786460	1.006597
H	3.172793	4.281054	-0.035048	H	1.085860	-3.573592	1.380072
H	1.448186	4.523031	-0.422652	C	-0.937374	-2.733608	0.883694
H	2.459207	3.489752	-1.482539	H	-1.712233	-3.456928	1.151037
C	1.621387	2.960941	1.878887	N	-1.241764	-1.485716	0.340864
H	2.555107	3.335039	2.348799	H	6.084227	-0.305671	0.669170
H	1.251867	2.111554	2.486256	C	2.203587	-1.400122	-2.767267
H	0.862751	3.769075	1.937463	H	3.117563	-0.902326	-3.154339
C	-2.488759	-0.275589	0.349470	H	1.528802	-0.612226	-2.362836
C	-5.136491	-0.003233	-0.487631	H	1.694294	-1.899780	-3.617028
C	-3.215967	-1.444856	0.017473	C	3.488257	-3.526586	-2.209884
C	-3.060669	1.021126	0.287957	H	4.417449	-3.115543	-2.656221
C	-4.395295	1.132163	-0.142341	H	2.972161	-4.095082	-3.009890
C	-4.550691	-1.271107	-0.401980	H	3.782094	-4.241195	-1.414352
H	-4.858514	2.128075	-0.211539	C	2.211665	1.562357	3.180048
H	-5.135661	-2.163848	-0.674630	H	3.156941	1.555913	3.762034
H	-6.178307	0.099557	-0.827441	H	1.419033	1.952054	3.850705
C	-2.695249	-2.879209	0.121586	H	2.324225	2.274718	2.337750
H	-3.376956	-3.463267	-0.533980	C	1.658682	-0.829709	3.824204
C	-2.883313	-3.435143	1.547017	H	2.620152	-0.985632	4.357309
H	-2.644689	-4.518465	1.574121	H	1.307165	-1.816454	3.462793
H	-3.924279	-3.301391	1.903343	H	0.916150	-0.456638	4.560320
H	-2.206346	-2.930131	2.265586	C	-2.570686	-0.969348	0.172414
C	-1.270211	-3.140234	-0.390753	C	-5.139949	0.094169	-0.094766
H	-1.136180	-4.225819	-0.575160	C	-3.301341	-1.249778	-1.008784
H	-0.500414	-2.838010	0.345343	C	-3.103862	-0.180386	1.224098
H	-1.057472	-2.589920	-1.329206	C	-4.398150	0.347401	1.064310
C	-2.269970	2.273686	0.647414	C	-4.594694	-0.698517	-1.111145
H	-1.307136	1.950473	1.090781	H	-4.828193	0.971631	1.862381
C	-2.987829	3.128547	1.703962	H	-5.179256	-0.896234	-2.023877
H	-2.349120	3.984543	2.004191	H	-6.150050	0.516821	-0.208186
H	-3.222237	2.539627	2.613801	C	-2.820674	-2.131428	-2.162158
H	-3.940339	3.548625	1.319739	H	-3.481202	-1.851063	-3.011341
C	-1.932220	3.084232	-0.615402	C	-3.091975	-3.621256	-1.875212
H	-1.310965	3.967929	-0.360433	H	-2.875490	-4.234477	-2.774477
H	-2.851528	3.444842	-1.122338	H	-4.147292	-3.796079	-1.584208
H	-1.360478	2.445893	-1.327619	H	-2.443380	-3.994122	-1.056882
79				C	-1.377462	-1.911080	-2.641283
IPrPd(THF)				H	-1.256022	-2.332904	-3.660278
O	0.262611	3.058805	-1.336336	H	-0.641374	-2.416961	-1.987601
C	1.537842	3.739601	-1.426068	H	-1.104997	-0.836556	-2.661357
C	1.196408	5.230672	-1.387452	C	-2.308933	0.127340	2.488156
C	-0.204011	5.261279	-2.018135	H	-1.392024	-0.495113	2.470085
C	-0.832480	3.995226	-1.438458	C	-3.082846	-0.244951	3.763133
H	2.023206	3.440867	-2.381193	H	-2.447329	-0.086394	4.658576
H	2.175307	3.397754	-0.586388	H	-3.400711	-1.307326	3.751187
H	1.152489	5.591250	-0.338682	H	-3.992457	0.377583	3.891208
H	1.938446	5.848407	-1.929270	C	-1.852054	1.596349	2.500412
H	-0.134812	5.189334	-3.123599	H	-1.236744	1.806705	3.400033
H	-0.779821	6.173560	-1.768789	H	-2.720170	2.288637	2.509303
H	-1.613831	3.533572	-2.073407	H	-1.235217	1.802525	1.593898
H	-1.257740	4.168083	-0.424287	27			
Pd	0.054936	1.051458	-0.588075	Pd(THF) ₂			
C	1.823739	0.171192	2.666781	O	-0.060972	0.231791	1.705650
H	0.840666	0.291761	2.164900	C	0.833331	0.375720	2.830291
C	2.775047	-0.362826	1.602999	C	0.104700	1.316725	3.790559
C	4.148111	-0.058012	1.619906	C	-0.690036	2.207835	2.824161
H	4.548963	0.581399	2.419639	C	-1.124633	1.207385	1.752360
C	5.011781	-0.551997	0.632683	H	1.795013	0.803478	2.468277
C	4.513095	-1.345490	-0.407144	H	1.029631	-0.633458	3.243233
H	5.194806	-1.705494	-1.191679	H	-0.585739	0.744938	4.445140
C	3.146145	-1.676207	-0.473377	H	0.801192	1.882479	4.439337
C	2.571911	-2.420518	-1.671827	H	-0.030750	2.985350	2.384917
H	1.628665	-2.904008	-1.343065	H	-1.549438	2.717706	3.301184
C	2.301957	-1.191267	0.553796	H	-1.233987	1.643782	0.739890

H	-2.072582	0.688382	2.018604
Pd	0.158323	-1.216177	0.189935
H	1.167196	-4.251404	-0.249183
C	0.462507	-4.085903	-1.087937
O	0.377695	-2.664119	-1.325796
C	0.458651	-2.361802	-2.735569
C	0.291159	-3.711532	-3.434706
C	0.922023	-4.677888	-2.420913

H	-0.542128	-4.457126	-0.784971
H	-0.333140	-1.624412	-2.973964
H	1.448797	-1.898128	-2.944019
H	0.777890	-3.736918	-4.428958
H	-0.784906	-3.945833	-3.573651
H	2.029041	-4.649413	-2.497243
H	0.596940	-5.728158	-2.552609