

Supplementary Material to
**DFT Study on the Oxidative Addition of 4-Substituted Iodobenzenes on Pd(0)-Phosphine
 Complexes**

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Table S1. Cartesian coordinates of the minima and transition states for the Pd catalyzed oxidative addition of 4-substituted iodobenzenes.

1							
Pd	-0.00010	-0.00454	0.00142				
P	2.28214	0.00005	0.00027				
C	3.09676	1.59993	-0.45377	3a			
H	2.76583	1.90885	-1.46667	I	0.00000	0.00000	1.55731
H	2.78343	2.38538	0.26410	C	0.00000	0.00000	-0.55670
H	4.20450	1.51519	-0.44121	C	0.00000	1.22608	-1.24668
C	3.11606	-0.40235	1.60438	C	0.00000	-1.22608	-1.24668
H	2.79515	0.32499	2.37788	C	0.00000	1.21646	-2.65320
H	2.80597	-1.41457	1.93588	C	0.00000	-1.21646	-2.65320
H	4.22280	-0.37183	1.51156	C	0.00000	0.00000	-3.35831
C	3.10716	-1.18515	-1.15926	H	0.00000	2.17856	-0.69621
H	4.21428	-1.11948	-1.09393	H	0.00000	-2.17856	-0.69621
H	2.78828	-2.21971	-0.91718	H	0.00000	2.17393	-3.19827
H	2.78824	-0.96186	-2.19797	H	0.00000	-2.17393	-3.19827
P	-2.28255	0.00030	-0.00053	H	0.00000	0.00000	-4.45959
C	-3.10896	0.27471	-1.63511	3b			
H	-2.78883	1.25246	-2.04988	I	-2.65995	0.00000	0.00004
H	-2.79463	-0.51847	-2.34391	C	-0.54646	0.00000	-0.00008
H	-4.21610	0.26300	-1.54219	C	0.15894	-1.21705	0.00775
C	-3.10149	1.28486	1.05307	C	0.15895	1.21705	-0.00796
H	-4.20901	1.20960	1.00439	C	1.55968	-1.21951	0.00764
H	-2.77279	1.16309	2.10549	C	1.55969	1.21948	-0.00784
H	-2.78879	2.29249	0.71040	C	2.30388	-0.00002	-0.00004
C	-3.10832	-1.55121	0.58405	H	-0.38103	-2.17611	0.01506
H	-2.78925	-2.40084	-0.05372	H	-0.38100	2.17611	-0.01540
H	-2.78992	-1.76450	1.62504	H	2.07858	-2.18743	0.01627
H	-4.21547	-1.46503	0.55027	H	2.07862	2.18738	-0.01672
2				N	3.68240	0.00000	-0.00006
Pd	-1.30163	-0.00197	0.00049	C	4.41017	-1.25808	-0.01412
P	0.86102	-0.00132	0.00007	H	4.15823	-1.87661	-0.90566
C	1.67454	1.60339	-0.44139	H	5.49529	-1.04982	-0.04424
H	1.35069	1.91093	-1.45610	H	4.20438	-1.87367	0.89177
H	1.35449	2.38524	0.27662	C	4.41010	1.25811	0.01436
H	2.78196	1.51581	-0.42006	H	5.49522	1.04991	0.04457
C	1.69214	-0.41389	1.60267	H	4.20440	1.87386	-0.89146
H	1.37256	0.30843	2.38169	H	4.15797	1.87649	0.90595
H	1.38533	-1.43052	1.92353	3c			
H	2.79904	-0.37828	1.50129	I	-2.31838	-0.07973	-0.00002
C	1.69284	-1.17823	-1.16377	C	-0.21169	0.07586	0.00005
H	2.79905	-1.08667	-1.10426	C	0.57459	-1.08705	0.00007
H	1.39630	-2.21640	-0.91059	C	0.39538	1.34808	0.00006
H	1.36338	-0.96569	-2.20088	C	1.97796	-0.98802	0.00008
				C	1.79124	1.44697	0.00005

C	2.59682	0.28278	0.00004
H	0.10358	-2.08133	0.00009
H	-0.21717	2.26213	0.00008
H	2.57418	-1.91135	0.00013
H	2.28369	2.43160	0.00005
O	3.94070	0.48352	-0.00009
C	4.79188	-0.66063	-0.00007
H	4.63835	-1.28770	-0.90627
H	5.82971	-0.27699	-0.00072
H	4.63921	-1.28688	0.90688

3d

C	-2.98270	0.00459	-0.00596
C	-2.25435	-1.20715	-0.00524
C	-2.25363	1.21300	-0.00507
C	-0.85064	-1.21998	-0.00223
C	-0.84750	1.22406	-0.00223
C	-0.15366	0.00241	-0.00056
H	-2.79651	-2.16734	-0.00735
H	-2.79483	2.17342	-0.00738
H	-0.30558	-2.17573	-0.00271
H	-0.30219	2.17963	-0.00290
I	1.96026	-0.00100	0.00103
C	-4.49171	-0.00337	0.00737
H	-4.90724	1.01211	-0.14747
H	-4.90167	-0.66897	-0.78124
H	-4.88035	-0.38183	0.97807

3e

I	0.00000	0.00000	2.30334
C	0.00000	0.00000	0.19429
C	0.00000	1.22358	-0.50048
C	0.00000	-1.22358	-0.50048
C	0.00000	1.22452	-1.90501
C	0.00000	-1.22452	-1.90501
C	0.00000	0.00000	-2.59501
H	0.00000	2.17938	0.04389
H	0.00000	-2.17938	0.04389
H	0.00000	2.17516	-2.45854
H	0.00000	-2.17516	-2.45854
Cl	0.00000	0.00000	-4.35161

3f

C	-2.00425	0.00160	-0.03592
C	-1.30233	-1.21883	-0.02869
C	-1.30147	1.22131	-0.02856
C	0.10043	-1.22454	-0.01537
C	0.10142	1.22588	-0.01549
C	0.79344	0.00047	-0.00874
H	-1.84993	-2.17313	-0.03818
H	-1.84816	2.17606	-0.03770
H	0.64735	-2.17856	-0.01338
H	0.64895	2.17956	-0.01370
I	2.90130	-0.00028	0.00568
C	-3.51304	0.00024	0.00157
F	-4.04128	1.10327	-0.58884
F	-4.03874	-1.08417	-0.62520
F	-3.98802	-0.02195	1.27950

3g

I	0.00000	0.00000	2.17568
C	0.00000	0.00000	0.07159
C	0.00000	1.22660	-0.62123
C	0.00000	-1.22660	-0.62123
C	0.00000	1.22679	-2.02139
C	0.00000	-1.22679	-2.02139
C	0.00000	0.00000	-2.73009
H	0.00000	2.17964	-0.07272
H	0.00000	-2.17964	-0.07272
H	0.00000	2.17918	-2.57204
H	0.00000	-2.17918	-2.57204
C	0.00000	0.00000	-4.16416
N	0.00000	0.00000	-5.33916

3h

I	0.00000	0.00000	2.54393
C	0.00000	0.00000	0.44222
C	0.00000	1.22839	-0.25028
C	0.00000	-1.22839	-0.25028
C	-0.00221	1.22825	-1.65098
C	0.00221	-1.22825	-1.65098
C	0.00000	0.00000	-2.33140
H	0.00148	2.18090	0.29899
H	-0.00148	-2.18090	0.29899
H	-0.00382	2.16757	-2.22070
H	0.00382	-2.16757	-2.22070
N	0.00000	0.00000	-3.80949
O	0.05427	-1.09289	-4.38552
O	-0.05427	1.09289	-4.38552

4a

Pd	0.57684	-0.16801	0.02647
I	-2.75680	0.27740	-0.93060
P	0.53848	2.04543	0.76077
C	-1.36165	-0.90287	0.30455
C	-1.76566	-1.09465	1.67538
C	-0.60992	-1.95941	-0.37007
C	-1.38923	-2.24318	2.35905
H	-2.36010	-0.31459	2.17591
C	-0.30415	-3.15557	0.37139
H	-0.60786	-2.02105	-1.47082
C	-0.66124	-3.28773	1.70567
H	-1.66727	-2.35250	3.42022
H	0.19397	-3.98563	-0.15712
H	-0.41361	-4.20758	2.25903
C	0.31235	3.26885	-0.60543
H	1.14469	3.16559	-1.33114
H	-0.63528	3.04163	-1.13581
H	0.28099	4.31365	-0.22919
C	-0.81087	2.51900	1.93231
H	-0.71544	1.92104	2.86138
H	-0.77810	3.59913	2.18946
H	-1.79002	2.28674	1.46510
C	2.03834	2.69598	1.62574
H	1.91743	3.75889	1.92517
H	2.23168	2.08536	2.53119
H	2.91601	2.60996	0.95347

P	2.77999	-0.54305	-0.63506
C	3.11313	-2.04760	-1.65745
H	2.77665	-2.94484	-1.09890
H	2.52675	-1.98841	-2.59730
H	4.19062	-2.15596	-1.90571
C	3.97518	-0.75978	0.75804
H	3.96227	0.14604	1.39757
H	3.65747	-1.62246	1.37872
H	5.00953	-0.93454	0.39246
C	3.58647	0.78254	-1.64215
H	2.97950	0.97035	-2.55129
H	3.62343	1.72039	-1.05110
H	4.61881	0.50579	-1.94495

4b

Pd	-0.45436	0.55224	-0.08377
I	-0.85941	-2.79576	-0.95106
P	-2.25444	0.32041	1.38255
C	0.54414	-1.30223	-0.15193
C	1.24150	-1.67467	1.04804
C	1.22830	-0.44205	-1.10474
C	2.49682	-1.15976	1.33096
H	0.76264	-2.36289	1.76200
C	2.56694	-0.00008	-0.81392
H	0.91798	-0.43834	-2.16227
C	3.19154	-0.28720	0.41123
H	2.96335	-1.43158	2.28778
H	3.09214	0.56649	-1.59500
C	-3.86261	0.01347	0.52092
H	-4.07366	0.85136	-0.17441
H	-3.77174	-0.91592	-0.07822
H	-4.70695	-0.09332	1.23530
C	-2.20329	-1.08117	2.58974
H	-1.32936	-0.95284	3.26053
H	-3.12768	-1.14191	3.20330
H	-2.07617	-2.03078	2.03000
C	-2.67725	1.74609	2.48511
H	-3.55562	1.52822	3.12980
H	-1.80609	1.98372	3.12923
H	-2.90142	2.63611	1.86224
P	-0.50616	2.75301	-0.82367
C	0.51076	3.17441	-2.31189
H	1.56832	2.90903	-2.10698
H	0.16490	2.56615	-3.17290
H	0.45049	4.25143	-2.57812
C	0.11034	3.98100	0.41404
H	-0.49709	3.90376	1.33859
H	1.16012	3.73384	0.67397
H	0.06404	5.02240	0.02959
C	-2.15519	3.45852	-1.27909
H	-2.61226	2.83411	-2.07392
H	-2.82217	3.43157	-0.39299
H	-2.07725	4.50625	-1.64074
N	4.44985	0.22598	0.74435
C	5.22585	-0.40179	1.80222
H	5.49831	-1.46400	1.58250
H	6.16424	0.16725	1.94640

H	4.68343	-0.38603	2.77072
C	5.18416	0.95856	-0.26919
H	4.57338	1.79572	-0.67036
H	6.09722	1.39468	0.18025
H	5.49409	0.32575	-1.13931

4c

Pd	-0.58228	0.24958	-0.10506
I	1.31468	-2.53823	-0.92002
P	-1.73688	-1.06312	1.44216
C	1.39370	-0.47169	-0.17319
C	2.16960	-0.26150	1.01659
C	1.31411	0.60108	-1.15953
C	2.77452	0.96586	1.26500
H	2.26925	-1.07731	1.74918
C	2.01855	1.82553	-0.89773
H	1.06538	0.37160	-2.20825
C	2.69908	2.02542	0.30148
H	3.31508	1.10780	2.21175
H	2.04149	2.61826	-1.66219
C	-2.83239	-2.33354	0.66463
H	-3.57643	-1.82595	0.01757
H	-2.21365	-2.99341	0.02221
H	-3.36338	-2.95080	1.42054
C	-0.73987	-2.08810	2.61568
H	-0.11383	-1.42062	3.24240
H	-1.37943	-2.71308	3.27497
H	-0.06762	-2.74866	2.03012
C	-2.90050	-0.19914	2.59291
H	-3.41054	-0.90730	3.28046
H	-2.33676	0.54367	3.19365
H	-3.66689	0.34355	2.00256
P	-2.11809	1.81906	-0.87366
C	-1.72828	2.68692	-2.46119
H	-0.75058	3.20082	-2.35811
H	-1.63836	1.93744	-3.27414
H	-2.50507	3.43218	-2.73619
C	-2.37474	3.23864	0.28153
H	-2.73165	2.85489	1.25897
H	-1.40291	3.74721	0.44778
H	-3.10933	3.97215	-0.11426
C	-3.85212	1.24751	-1.17343
H	-3.84324	0.43740	-1.93096
H	-4.27215	0.84022	-0.23125
H	-4.50542	2.07153	-1.53194
O	3.29699	3.24806	0.47906
C	4.05211	3.46754	1.66113
H	3.42828	3.39479	2.58154
H	4.90816	2.76056	1.75417
H	4.45247	4.49782	1.58961

4d

Pd	-0.57027	-0.01703	-0.08989
I	2.76636	-0.68990	-0.89411
P	-0.61676	-2.02256	1.09801
C	1.37980	0.73278	0.05743
C	1.76419	1.19346	1.36820
C	0.65144	1.64324	-0.81976
C	1.38446	2.45373	1.80444

H	2.34555	0.52760	2.02494	H	-2.63753	-2.77301	2.95159
C	0.34708	2.96434	-0.33118	H	-2.47600	-0.97516	3.02300
H	0.66743	1.49209	-1.91167	H	-3.42923	-1.73763	1.70229
C	0.67063	3.37217	0.95799	P	-2.69422	0.60876	-0.86825
H	1.64679	2.76531	2.82987	C	-2.71582	1.71839	-2.34613
H	-0.13524	3.67600	-1.02320	H	-2.13590	2.63523	-2.11494
C	-0.57262	-3.52313	0.02067	H	-2.22081	1.20468	-3.19586
H	-1.43019	-3.49522	-0.68205	H	-3.74733	2.00514	-2.64266
H	0.36130	-3.50270	-0.57808	C	-3.66488	1.58734	0.36106
H	-0.60896	-4.46493	0.60903	H	-3.82180	0.97720	1.27339
C	0.77502	-2.34795	2.27050	H	-3.08008	2.48531	0.64806
H	0.78043	-1.56040	3.05152	H	-4.64978	1.90538	-0.04221
H	0.68838	-3.34259	2.75741	C	-3.88972	-0.71240	-1.36047
H	1.73330	-2.29482	1.71399	H	-3.43890	-1.32852	-2.16507
C	-2.09131	-2.34434	2.16845	H	-4.08738	-1.37052	-0.48987
H	-2.01366	-3.31792	2.69790	H	-4.85154	-0.28960	-1.72103
H	-2.18133	-1.53146	2.91762	Cl	1.20599	4.72744	1.05541
H	-3.00863	-2.34791	1.54500				
P	-2.76382	0.30072	-0.80102	4f			
C	-3.05475	1.53887	-2.14379	Pd	-0.44699	0.60649	-0.19869
H	-2.65281	2.52086	-1.82062	I	-1.74824	-2.61892	-0.77324
H	-2.50314	1.22473	-3.05370	P	-2.15770	0.96602	1.33686
H	-4.13256	1.64897	-2.38986	C	-0.02003	-1.43826	-0.14186
C	-3.86728	0.92397	0.54457	C	0.61539	-1.85858	1.08636
H	-3.88087	0.18630	1.37227	C	0.80927	-0.85471	-1.20003
H	-3.45418	1.87483	0.93903	C	1.96164	-1.61795	1.29911
H	-4.90525	1.09523	0.18760	H	0.01196	-2.35325	1.86275
C	-3.70011	-1.16648	-1.42759	C	2.21036	-0.68331	-0.95384
H	-3.17859	-1.58029	-2.31480	H	0.46568	-0.86490	-2.24709
H	-3.72001	-1.94843	-0.64143	C	2.77021	-1.02080	0.27297
H	-4.74350	-0.90737	-1.70721	H	2.41953	-1.89550	2.26086
C	0.31360	4.74502	1.47602	H	2.84581	-0.29019	-1.76227
H	-0.40370	4.68619	2.32514	C	-3.81073	1.22246	0.55660
H	1.20640	5.28825	1.85601	H	-3.75587	2.08122	-0.14316
H	-0.15383	5.36926	0.68757	H	-4.07132	0.31823	-0.03115
				H	-4.60501	1.41068	1.30999
4e				C	-2.49583	-0.37977	2.55549
Pd	-0.60235	-0.06353	-0.09813	H	-1.59034	-0.54323	3.17454
I	2.48769	-1.48140	-0.88964	H	-3.34989	-0.13078	3.22045
P	-1.01852	-1.89837	1.28036	H	-2.72042	-1.31826	2.00833
C	1.46531	0.27066	-0.06104	C	-1.99727	2.43882	2.44208
C	1.98124	0.76017	1.19282	H	-2.85818	2.52284	3.13895
C	0.89204	1.22428	-1.01209	H	-1.06174	2.35104	3.03095
C	1.87000	2.10135	1.52880	H	-1.94091	3.36068	1.82880
H	2.45078	0.05636	1.89706	P	0.15205	2.73918	-0.92778
C	0.85978	2.61911	-0.65320	C	1.16999	2.85123	-2.46645
H	0.84654	0.97882	-2.08562	H	2.10137	2.26674	-2.32251
C	1.30633	3.02345	0.59283	H	0.60761	2.40224	-3.31066
H	2.21693	2.46060	2.50914	H	1.43257	3.90058	-2.71881
H	0.50024	3.35757	-1.38601	C	1.21900	3.60273	0.30836
C	-1.23970	-3.48164	0.35353	H	0.65967	3.71604	1.25894
H	-2.07676	-3.37375	-0.36581	H	2.11132	2.97499	0.50926
H	-0.31580	-3.68752	-0.22496	H	1.54642	4.60292	-0.04700
H	-1.44595	-4.33550	1.03339	C	-1.18280	3.97403	-1.25604
C	0.29060	-2.34562	2.50655	H	-1.84664	3.58878	-2.05680
H	0.42270	-1.50337	3.21608	H	-1.79074	4.11036	-0.33882
H	0.03306	-3.26324	3.07704	H	-0.77156	4.95790	-1.56677
H	1.24867	-2.50649	1.97072	C	4.19881	-0.68890	0.56897
C	-2.53088	-1.84978	2.34299	F	4.31893	0.48403	1.27824

F	4.81449	-1.63934	1.32871
F	4.95273	-0.52526	-0.55181
4g			
Pd	-0.56716	-0.16795	-0.10450
I	2.88441	-0.48588	-0.82049
P	-0.32187	-2.10080	1.16545
C	1.28797	0.77531	-0.01686
C	1.56774	1.38947	1.26375
C	0.48461	1.52363	-0.98978
C	1.02448	2.61526	1.59552
H	2.20655	0.85796	1.98563
C	-0.01768	2.80848	-0.62957
H	0.53102	1.27097	-2.06152
C	0.22029	3.34739	0.64347
H	1.20617	3.04834	2.59066
H	-0.57595	3.39370	-1.37692
C	0.12431	-3.56397	0.13436
H	-0.66732	-3.73374	-0.62362
H	1.07232	-3.34875	-0.40019
H	0.24776	-4.48125	0.74836
C	1.00499	-2.09162	2.44798
H	0.77821	-1.31072	3.20182
H	1.09312	-3.07475	2.95678
H	1.97199	-1.84510	1.96352
C	-1.78485	-2.70451	2.11823
H	-1.55287	-3.63394	2.68032
H	-2.10294	-1.91982	2.83421
H	-2.62313	-2.90600	1.42102
P	-2.79828	-0.21647	-0.78865
C	-3.28844	1.02257	-2.06826
H	-3.09052	2.04071	-1.67555
H	-2.66777	0.87482	-2.97558
H	-4.36183	0.93996	-2.34181
C	-4.02395	0.10409	0.55432
H	-3.90622	-0.65749	1.35117
H	-3.82186	1.10029	0.99805
H	-5.06741	0.07814	0.17485
C	-3.39993	-1.80152	-1.52088
H	-2.75763	-2.07457	-2.38281
H	-3.32322	-2.60667	-0.76222
H	-4.45432	-1.72616	-1.86151
C	-0.32068	4.62042	0.99398
N	-0.76996	5.66866	1.29130
4h			
Pd	-0.14035	0.63547	-0.12444
I	-1.67089	-2.51072	-0.81063
P	-1.99329	1.02686	1.21720
C	0.09093	-1.44191	-0.09856
C	0.65460	-1.92809	1.14722
C	1.00806	-0.93352	-1.12403
C	2.00686	-1.81722	1.40429
H	-0.01491	-2.36833	1.90174
C	2.39699	-0.85623	-0.83405
H	0.68889	-0.86670	-2.17653
C	2.87963	-1.26814	0.40844
H	2.43486	-2.13978	2.36293
H	3.10594	-0.49928	-1.59452

C	-3.55164	1.13690	0.23774
H	-3.46162	1.95558	-0.50486
H	-3.69640	0.18484	-0.31283
H	-4.43224	1.32412	0.88806
C	-2.39182	-0.25387	2.48309
H	-1.55161	-0.32677	3.20315
H	-3.32372	-0.00902	3.03502
H	-2.51382	-1.23427	1.97867
C	-2.02307	2.58583	2.20456
H	-2.96547	2.67956	2.78470
H	-1.16516	2.59358	2.90695
H	-1.93058	3.45597	1.52404
P	0.53430	2.77652	-0.76811
C	1.84111	2.85324	-2.07151
H	2.75273	2.34517	-1.69656
H	1.48929	2.31328	-2.97413
H	2.09325	3.89980	-2.34486
C	1.26187	3.80747	0.57809
H	0.51557	3.94209	1.38612
H	2.13808	3.27664	1.00320
H	1.58356	4.80304	0.20562
C	-0.78468	3.86849	-1.45833
H	-1.26070	3.36622	-2.32503
H	-1.56207	4.03825	-0.68585
H	-0.37874	4.84999	-1.78279
N	4.29446	-1.13865	0.69407
O	5.03202	-0.60311	-0.15771
O	4.71284	-1.56502	1.78880

5TSa			
Pd	-0.41495	0.15670	0.20167
I	1.05708	-1.70254	-1.36845
P	-2.59166	-0.57927	0.62608
C	1.59626	-0.43816	0.48787
C	1.27076	-1.05501	1.73412
C	2.70529	0.44580	0.39337
C	1.94531	-0.62371	2.90230
H	0.55924	-1.89268	1.77973
C	3.37039	0.83099	1.56097
H	3.00166	0.85491	-0.58419
C	2.98006	0.31740	2.82308
H	1.67535	-1.07293	3.87222
H	4.19771	1.55647	1.49398
H	3.51521	0.63049	3.73330
C	-3.09257	-0.77323	2.39733
H	-2.39886	-1.48069	2.89583
H	-3.00781	0.20735	2.90926
H	-4.13321	-1.14939	2.49792
C	-3.99045	0.42556	-0.04987
H	-3.87702	0.51074	-1.14964
H	-4.97667	-0.03246	0.17881
H	-3.95408	1.44592	0.38185
C	-2.97345	-2.25240	-0.06701
H	-4.01956	-2.56378	0.14087
H	-2.80866	-2.23657	-1.16397
H	-2.27483	-2.99500	0.36986
P	-0.12296	2.30752	-0.65397
C	0.80451	2.42077	-2.25229
H	1.82136	1.99800	-2.12332

H	0.27976	1.81451	-3.01870
H	0.89221	3.46849	-2.61182
C	0.77806	3.53100	0.40182
H	0.21699	3.67033	1.34856
H	1.77747	3.12331	0.65655
H	0.90038	4.51361	-0.10208
C	-1.66524	3.24572	-1.06533
H	-2.26209	2.66613	-1.79830
H	-2.27181	3.36914	-0.14535
H	-1.44432	4.24881	-1.48988

5TSb

Pd	-0.83138	0.20169	0.23551
I	-0.73165	-1.53886	-1.95283
P	-2.39978	-0.55653	1.78869
C	0.94429	-0.59466	-0.63958
C	1.34380	-1.37745	0.47578
C	1.90309	0.22849	-1.28065
C	2.62234	-1.19995	1.04028
H	0.67241	-2.14778	0.88363
C	3.17455	0.38884	-0.72808
H	1.63496	0.77616	-2.19674
C	3.55776	-0.28833	0.47684
H	2.89398	-1.81115	1.91158
H	3.87706	1.06933	-1.22884
C	-1.76431	-0.99797	3.47335
H	-1.02408	-1.81893	3.38336
H	-1.24687	-0.11794	3.90732
H	-2.58095	-1.31262	4.15855
C	-3.79889	0.58161	2.21226
H	-4.32151	0.87607	1.27969
H	-4.53079	0.10728	2.90153
H	-3.39563	1.49928	2.68699
C	-3.32144	-2.09202	1.31839
H	-4.04343	-2.40285	2.10377
H	-3.86851	-1.91227	0.36997
H	-2.59607	-2.91193	1.13899
P	-0.73613	2.44150	-0.40431
C	-0.78106	2.76105	-2.22906
H	0.10650	2.30017	-2.70861
H	-1.68487	2.27982	-2.65556
H	-0.79749	3.84672	-2.46576
C	0.73716	3.43499	0.11748
H	0.80334	3.42496	1.22471
H	1.65687	2.95932	-0.27956
H	0.68357	4.48723	-0.23621
C	-2.12404	3.52002	0.18488
H	-3.09129	3.05953	-0.10140
H	-2.08653	3.58083	1.29185
H	-2.07128	4.54713	-0.23751
N	4.80607	-0.08475	1.04402
C	5.21275	-0.88423	2.18581
H	5.33483	-1.96800	1.94201
H	6.18013	-0.50865	2.56913
H	4.47362	-0.80841	3.01272
C	5.81630	0.66564	0.31781
H	6.10430	0.18506	-0.64814
H	5.47510	1.69923	0.09032
H	6.72583	0.74712	0.94173

5TSc

Pd	-0.61248	0.21595	0.21524
I	-0.33461	-2.00084	-1.51382
P	-2.25139	-0.16864	1.83217
C	1.21409	-0.62863	-0.45654
C	1.59854	-1.06625	0.83997
C	2.14478	0.07902	-1.26542
C	2.83614	-0.64419	1.38644
H	0.96820	-1.77049	1.40283
C	3.36748	0.47076	-0.72616
H	1.88220	0.35498	-2.29753
C	3.71621	0.13373	0.61254
H	3.10703	-0.97252	2.39999
H	4.07991	1.06462	-1.32004
C	-3.64504	1.04529	1.95157
H	-3.23728	2.04427	2.20715
H	-4.15126	1.11835	0.96780
H	-4.38814	0.74713	2.72222
C	-3.16681	-1.76319	1.62000
H	-2.44637	-2.60442	1.67998
H	-3.95674	-1.90034	2.38929
H	-3.63065	-1.78452	0.61265
C	-1.70863	-0.27502	3.60035
H	-2.56156	-0.47228	4.28470
H	-0.96226	-1.08886	3.70436
H	-1.22025	0.67757	3.89130
P	-0.68142	2.19909	-1.01713
C	-0.74826	1.98482	-2.85581
H	0.15000	1.43250	-3.19864
H	-1.63895	1.37747	-3.11659
H	-0.79931	2.95808	-3.38960
C	0.71968	3.39343	-0.82370
H	0.75868	3.73582	0.23083
H	1.67474	2.87609	-1.04718
H	0.61505	4.27559	-1.49117
C	-2.14056	3.30543	-0.73638
H	-3.07107	2.74006	-0.94701
H	-2.16080	3.61977	0.32694
H	-2.11315	4.21055	-1.38102
O	4.93489	0.57956	1.03407
C	5.33554	0.26521	2.36245
H	4.62635	0.67506	3.11686
H	5.43080	-0.83328	2.51848
H	6.32726	0.73415	2.51092

5TSd

Pd	-0.49255	0.21623	0.18322
I	0.21698	-2.04359	-1.37445
P	-2.49764	-0.12857	1.32730
C	1.44138	-0.63712	-0.01297
C	1.47438	-1.01852	1.35929
C	2.54743	0.04948	-0.58218
C	2.52690	-0.53918	2.17625
H	0.73012	-1.71812	1.76771
C	3.58103	0.48638	0.24746
H	2.56065	0.27398	-1.65924
C	3.58215	0.22302	1.64730

H	2.53377	-0.80808	3.24602
H	4.41038	1.06531	-0.19335
C	-2.46600	-0.01519	3.17479
H	-1.74628	-0.75825	3.57523
H	-2.11532	0.99447	3.47208
H	-3.46724	-0.19828	3.62045
C	-3.91730	0.98619	0.91665
H	-4.12380	0.92923	-0.17130
H	-4.83630	0.70802	1.47625
H	-3.64620	2.03244	1.16413
C	-3.25096	-1.79832	1.05857
H	-4.20861	-1.92041	1.60868
H	-3.43156	-1.94373	-0.02629
H	-2.53398	-2.57669	1.39079
P	-0.24387	2.17076	-1.06483
C	0.14430	1.91826	-2.85793
H	1.09204	1.35084	-2.95386
H	-0.66190	1.31442	-3.32207
H	0.24364	2.88063	-3.40449
C	1.08145	3.35661	-0.55482
H	0.85225	3.73853	0.46119
H	2.04853	2.81620	-0.50367
H	1.17468	4.21328	-1.25612
C	-1.71435	3.29151	-1.17106
H	-2.57489	2.72674	-1.58343
H	-1.98363	3.63721	-0.15229
H	-1.51963	4.17690	-1.81401
C	4.70919	0.72803	2.51569
H	4.59642	0.39383	3.56658
H	5.69893	0.37602	2.15161
H	4.75052	1.83963	2.51781

5TSe

Pd	-0.61093	0.25592	0.16808
I	-0.30014	-2.30154	-1.03438
P	-2.43449	0.31939	1.62990
C	1.19897	-0.77327	-0.17567
C	1.43411	-0.90606	1.22753
C	2.23730	-0.30335	-1.02609
C	2.62617	-0.38487	1.78186
H	0.73025	-1.45616	1.86911
C	3.42055	0.18527	-0.47038
H	2.08893	-0.27554	-2.11578
C	3.59530	0.16473	0.93507
H	2.80703	-0.45169	2.86534
H	4.20684	0.60352	-1.11666
C	-2.08379	0.15637	3.43997
H	-1.58275	-0.81474	3.62960
H	-1.39474	0.96689	3.75403
H	-3.01211	0.21122	4.04816
C	-3.52849	1.81180	1.60168
H	-3.93021	1.95231	0.57818
H	-4.37452	1.71419	2.31534
H	-2.93028	2.70650	1.86943
C	-3.65000	-1.04638	1.35189
H	-4.50789	-0.99026	2.05549
H	-4.02597	-0.99238	0.30967
H	-3.13604	-2.02119	1.47844
P	-0.46494	1.92290	-1.46151

C	-0.38566	1.30733	-3.20558
H	0.50573	0.66034	-3.33275
H	-1.28426	0.68984	-3.40907
H	-0.33839	2.13850	-3.94133
C	0.97942	3.07652	-1.38632
H	0.94246	3.63693	-0.42973
H	1.91903	2.48773	-1.39951
H	0.98535	3.79629	-2.23264
C	-1.87809	3.11268	-1.56914
H	-2.81739	2.54897	-1.74232
H	-1.97271	3.65844	-0.60871
H	-1.74212	3.84823	-2.39111
Cl	5.09238	0.79722	1.61660

5TSf

Pd	-0.89701	-0.29899	-0.10243
I	-1.00139	2.50854	0.36536
P	-2.52689	-1.01522	-1.62330
C	0.72828	1.00627	0.12812
C	1.12026	0.78021	-1.23188
C	1.70327	0.94230	1.16563
C	2.40693	0.26482	-1.49387
H	0.45690	1.05316	-2.06569
C	2.97930	0.46781	0.87719
H	1.43058	1.21386	2.19602
C	3.32934	0.09336	-0.45015
H	2.69782	0.03784	-2.53066
H	3.71577	0.36368	1.68915
C	-1.93894	-1.93615	-3.11558
H	-1.18973	-1.31980	-3.65319
H	-1.44192	-2.87273	-2.78948
H	-2.77264	-2.18521	-3.80616
C	-3.88771	-2.10798	-1.01170
H	-4.40896	-1.60519	-0.17194
H	-4.62437	-2.33185	-1.81271
H	-3.46022	-3.05992	-0.63771
C	-3.47823	0.38458	-2.37016
H	-4.23789	0.03275	-3.10053
H	-3.98356	0.95007	-1.56060
H	-2.77218	1.07328	-2.87742
P	-0.77773	-1.45029	1.92097
C	-1.02080	-0.40044	3.42457
H	-0.23449	0.38049	3.45863
H	-2.00301	0.10963	3.35399
H	-0.98133	-0.99557	4.36192
C	0.79205	-2.34325	2.31203
H	0.94882	-3.14587	1.56252
H	1.64365	-1.63739	2.23702
H	0.77379	-2.79026	3.32872
C	-2.03605	-2.77992	2.18269
H	-3.05219	-2.34423	2.10103
H	-1.92200	-3.54859	1.39168
H	-1.92741	-3.26526	3.17644
C	4.67977	-0.50628	-0.70735
F	5.67193	0.13692	-0.02678
F	5.02407	-0.49002	-2.02225
F	4.74676	-1.81597	-0.30934

5TSg

Pd	-0.54507	0.26385	0.15318
I	-0.08212	-2.44835	-0.69261
P	-2.45108	0.53286	1.49043
C	1.27794	-0.74446	-0.02886
C	1.45538	-0.67158	1.39764
C	2.35472	-0.37437	-0.89251
C	2.58772	-0.02035	1.91530
H	0.75456	-1.17441	2.08019
C	3.48284	0.23685	-0.36417
H	2.26360	-0.52568	-1.97803
C	3.60132	0.45212	1.04784
H	2.70916	0.08246	3.00472
H	4.28824	0.57752	-1.03265
C	-3.94583	1.32583	0.74902
H	-3.70687	2.36995	0.46479
H	-4.23929	0.77191	-0.16562
H	-4.79800	1.32960	1.46151
C	-3.13919	-1.07878	2.08209
H	-2.36539	-1.61364	2.66961
H	-4.04597	-0.93850	2.70831
H	-3.39473	-1.70618	1.20360
C	-2.25126	1.48588	3.06154
H	-3.19373	1.51990	3.64848
H	-1.45501	1.01546	3.67381
H	-1.93340	2.52074	2.81984
P	-0.39961	1.66273	-1.70418
C	-0.29062	0.79561	-3.33384
H	0.61568	0.15750	-3.36016
H	-1.17598	0.13906	-3.45553
H	-0.24830	1.51552	-4.17881
C	1.02712	2.83169	-1.78254
H	0.97155	3.53215	-0.92439
H	1.97470	2.26234	-1.69874
H	1.03330	3.41290	-2.72909
C	-1.82813	2.80330	-1.98203
H	-2.75975	2.21023	-2.07642
H	-1.92894	3.47753	-1.10741
H	-1.69168	3.41564	-2.89892
C	4.75775	1.09904	1.57750
N	5.71057	1.64215	2.00819

5TSh

Pd	0.71939	-0.28198	0.11039
I	0.52915	2.56158	-0.31204
P	2.50223	-0.95657	1.47349
C	-0.99515	0.89995	-0.04662
C	-1.29961	0.61078	1.33464
C	-2.02898	0.78343	-1.03165
C	-2.51480	-0.01312	1.65262
H	-0.61814	0.92467	2.13967
C	-3.23954	0.19819	-0.69393
H	-1.83971	1.10675	-2.06559
C	-3.46884	-0.23094	0.64288
H	-2.75448	-0.29667	2.68712
H	-4.02466	0.03795	-1.44555
C	3.40467	0.48633	2.19494
H	3.80959	1.10959	1.37167
H	2.69017	1.10699	2.77333
H	4.23718	0.17068	2.85935

C	2.03920	-1.93498	2.97070
H	1.58171	-2.89315	2.64955
H	2.91858	-2.14796	3.61498
H	1.28293	-1.37330	3.55602
C	3.88027	-1.95840	0.76108
H	4.66608	-2.16256	1.51907
H	3.48354	-2.92097	0.38158
H	4.33075	-1.40528	-0.08778
P	0.58758	-1.37950	-1.93608
C	0.63301	-0.26884	-3.41144
H	-0.21199	0.44705	-3.37237
H	1.57626	0.31414	-3.39354
H	0.57597	-0.84380	-4.36016
C	-0.91396	-2.40907	-2.23597
H	-0.93819	-3.23348	-1.49457
H	-1.81936	-1.78676	-2.08761
H	-0.92503	-2.83426	-3.26184
C	1.95317	-2.56417	-2.31475
H	2.92139	-2.02539	-2.29067
H	1.97165	-3.35651	-1.53965
H	1.82275	-3.03479	-3.31258
N	-4.72765	-0.86986	0.97783
O	-5.55738	-1.04871	0.06421
O	-4.92063	-1.22132	2.15815

6a

Pd	-0.16916	0.14249	0.02760
I	-0.10101	-2.55188	-0.04915
P	0.09167	2.40697	-0.08099
C	1.87027	0.04814	0.03483
C	2.56817	0.10760	1.26177
C	2.61818	-0.09422	-1.15475
C	3.97474	0.02867	1.29924
H	2.01266	0.21295	2.20914
C	4.02373	-0.17197	-1.12058
H	2.10137	-0.15080	-2.12735
C	4.70865	-0.10746	0.10693
H	4.49929	0.07366	2.26850
H	4.58766	-0.28652	-2.06158
H	5.80874	-0.16718	0.13424
C	1.74299	3.07685	-0.53096
H	2.49879	2.74976	0.20822
H	2.04313	2.69906	-1.52755
H	1.69684	4.18544	-0.55246
C	-0.98915	3.24180	-1.31608
H	-0.74348	2.84824	-2.32287
H	-2.05812	3.04387	-1.11059
H	-0.81357	4.33762	-1.30065
C	-0.25078	3.24563	1.51867
H	-0.14740	4.34608	1.41723
H	-1.26965	3.00013	1.87261
H	0.47888	2.87796	2.26830
P	-2.55383	0.16754	0.07204
C	-3.38816	-1.28931	0.83068
H	-3.13334	-2.20342	0.26097
H	-3.02997	-1.41962	1.87166
H	-4.48822	-1.14222	0.83229
C	-3.27720	0.20970	-1.62182
H	-4.38674	0.19362	-1.59220

H	-2.93509	1.11994	-2.15362
H	-2.91034	-0.67606	-2.17930
C	-3.42364	1.53642	0.95858
H	-3.15472	1.49391	2.03354
H	-3.13297	2.52759	0.56092
H	-4.52325	1.42210	0.86138

6b

Pd	-0.82854	0.14147	0.01644
I	-0.76590	-2.55852	-0.04601
P	-0.55002	2.39935	-0.11929
C	1.21430	0.05873	0.00519
C	1.93653	0.17248	1.21120
C	1.96507	-0.10843	-1.17673
C	3.34178	0.11457	1.24758
H	1.40093	0.31285	2.16611
C	3.36896	-0.16702	-1.16523
H	1.45117	-0.19767	-2.14897
H	3.84870	0.20726	2.21865
H	3.89913	-0.30101	-2.11881
C	1.08524	3.05793	-0.64076
H	1.86882	2.73586	0.07110
H	1.34275	2.66600	-1.64372
H	1.04144	4.16648	-0.67439
C	-1.67249	3.24308	-1.31168
H	-1.46386	2.85324	-2.32825
H	-2.73419	3.04734	-1.07042
H	-1.49387	4.33850	-1.29852
C	-0.82522	3.24670	1.48923
H	-0.69996	4.34463	1.38489
H	-1.83910	3.02296	1.87131
H	-0.08330	2.86223	2.21813
P	-3.21104	0.17361	0.10838
C	-4.03834	-1.28226	0.87785
H	-3.79717	-2.19552	0.30075
H	-3.66191	-1.41776	1.91172
H	-5.13776	-1.13164	0.89986
C	-3.97907	0.22969	-1.56594
H	-5.08760	0.21478	-1.50877
H	-3.64923	1.14324	-2.09983
H	-3.62842	-0.65248	-2.13941
C	-4.04862	1.54314	1.02585
H	-3.74513	1.49543	2.09136
H	-3.76427	2.53393	0.62268
H	-5.15151	1.43577	0.96373
C	4.09989	-0.07055	0.05505
N	5.48813	-0.15114	0.07896
C	6.22636	-0.15169	-1.17044
H	6.08148	0.78434	-1.76427
H	7.30661	-0.25581	-0.95552
H	5.93294	-1.00593	-1.81974
C	6.20013	0.11530	1.31473
H	5.87376	-0.56846	2.12892
H	7.28198	-0.05292	1.15565
H	6.06482	1.16218	1.68352

6c

Pd	0.61182	0.14274	-0.01271
I	0.50324	-2.55238	0.06437

P	0.38580	2.40923	0.09010
C	-1.42826	0.08572	0.09292
C	-2.20213	0.13554	-1.08269
C	-2.11488	-0.01684	1.32481
C	-3.61300	0.08426	-1.04956
H	-1.70951	0.21126	-2.06697
C	-3.51582	-0.06670	1.37940
H	-1.54992	-0.06443	2.27087
H	-4.17561	0.11944	-1.99406
H	-4.04564	-0.15212	2.34179
C	-1.23423	3.11184	0.60041
H	-2.02846	2.78152	-0.09578
H	-1.49225	2.75864	1.61748
H	-1.17106	4.21988	0.59817
C	1.52924	3.23780	1.27181
H	1.32304	2.85378	2.29104
H	2.58574	3.02523	1.02200
H	1.36727	4.33576	1.25694
C	0.67939	3.22865	-1.52949
H	0.61384	4.33235	-1.43212
H	1.67357	2.94991	-1.92637
H	-0.09261	2.87832	-2.24423
P	2.99202	0.12865	-0.16459
C	3.77252	-1.34401	-0.95029
H	3.51977	-2.25295	-0.37140
H	3.37755	-1.46814	-1.97868
H	4.87453	-1.21843	-0.98931
C	3.77625	0.16137	1.50256
H	4.88376	0.12880	1.43483
H	3.46611	1.07709	2.04468
H	3.41598	-0.71830	2.07382
C	3.85314	1.48157	-1.08425
H	3.53608	1.44907	-2.14636
H	3.60193	2.47708	-0.67092
H	4.95312	1.34213	-1.03609
C	-4.27935	-0.01457	0.19053
O	-5.63816	-0.06781	0.34007
C	-6.43770	-0.04492	-0.83482
H	-7.49126	-0.10754	-0.50016
H	-6.30252	0.89708	-1.41401
H	-6.22195	-0.90934	-1.50331

6d

Pd	0.39564	0.14121	-0.02355
I	0.28767	-2.55233	0.05136
P	0.16539	2.40855	0.07846
C	-1.64547	0.07951	-0.01373
C	-2.35542	0.13963	-1.23352
C	-2.39252	-0.03161	1.17739
C	-3.76166	0.09066	-1.25890
H	-1.80882	0.22487	-2.18820
C	-3.79950	-0.07871	1.14992
H	-1.87687	-0.08445	2.15095
H	-4.28852	0.13743	-2.22800
H	-4.35806	-0.16777	2.09786
C	-1.47400	3.10541	0.53064
H	-2.23884	2.78034	-0.20007
H	-1.77306	2.74303	1.53318
H	-1.41248	4.21346	0.54024

C	1.26221	3.23368	1.30601
H	1.01733	2.84563	2.31513
H	2.32782	3.02337	1.09573
H	1.09908	4.33142	1.28881
C	0.51536	3.23531	-1.52599
H	0.44272	4.33839	-1.42665
H	1.52399	2.96158	-1.88861
H	-0.23015	2.88525	-2.26843
P	2.78046	0.13228	-0.08186
C	3.59063	-1.33676	-0.84345
H	3.32186	-2.24737	-0.27445
H	3.22869	-1.46026	-1.88398
H	4.69294	-1.20771	-0.84681
C	3.51073	0.16499	1.60943
H	4.61992	0.13666	1.57605
H	3.18055	1.07883	2.14274
H	3.13582	-0.71677	2.16789
C	3.66746	1.48847	-0.97109
H	3.39233	1.45190	-2.04472
H	3.39433	2.48354	-0.57075
H	4.76567	1.35652	-0.88005
C	-4.51262	-0.01685	-0.06673
C	-6.02200	-0.08978	-0.10150
H	-6.45547	0.67162	-0.78418
H	-6.37162	-1.08079	-0.46741
H	-6.46168	0.06287	0.90512

6e

Pd	0.60558	0.14021	-0.02557
I	0.48569	-2.54998	0.04876
P	0.38972	2.41059	0.07485
C	-1.43399	0.08174	-0.01063
C	-2.14839	0.14055	-1.22761
C	-2.17395	-0.02645	1.18716
C	-3.55569	0.09846	-1.25797
H	-1.60803	0.21857	-2.18580
C	-3.58046	-0.06893	1.18120
H	-1.65338	-0.08305	2.15733
C	-4.25945	-0.00112	-0.04673
H	-4.10087	0.14299	-2.21330
H	-4.14575	-0.15545	2.12184
C	-1.24962	3.11065	0.52149
H	-2.01309	2.79051	-0.21282
H	-1.55376	2.74898	1.52286
H	-1.18476	4.21841	0.53272
C	1.48407	3.22943	1.30787
H	1.23421	2.84045	2.31537
H	2.54994	3.01711	1.10112
H	1.32327	4.32748	1.29149
C	0.74767	3.23544	-1.52827
H	0.68207	4.33878	-1.42738
H	1.75502	2.95575	-1.88977
H	0.00094	2.89141	-2.27226
P	2.98815	0.12230	-0.08087
C	3.79071	-1.34973	-0.84354
H	3.51727	-2.25980	-0.27598
H	3.42943	-1.46980	-1.88468
H	4.89351	-1.22542	-0.84537
C	3.71184	0.14905	1.61275

H	4.82095	0.11685	1.58218
H	3.38344	1.06308	2.14677
H	3.33221	-0.73266	2.16803
C	3.88247	1.47541	-0.96622
H	3.60989	1.44144	-2.04056
H	3.61437	2.47151	-0.56520
H	4.97959	1.33679	-0.87246
Cl	-6.02497	-0.04321	-0.06758

6f

Pd	1.00557	0.14072	-0.02287
I	0.84016	-2.54537	0.05622
P	0.82853	2.41557	0.07801
C	-1.03115	0.10843	0.00531
C	-1.74688	0.17045	-1.21257
C	-1.76854	0.02004	1.20749
C	-3.15089	0.14924	-1.23300
H	-1.20462	0.23746	-2.17009
C	-3.17244	-0.00100	1.19909
H	-1.24354	-0.03392	2.17503
C	-3.86958	0.06861	-0.02349
H	-3.69061	0.20080	-2.19156
H	-3.72994	-0.06854	2.14616
C	-0.79893	3.14133	0.52659
H	-1.56876	2.83247	-0.20595
H	-1.10650	2.78716	1.52963
H	-0.71683	4.24790	0.53551
C	1.93770	3.21361	1.31076
H	1.68722	2.82324	2.31754
H	2.99988	2.98930	1.09833
H	1.79062	4.31364	1.29985
C	1.19842	3.23496	-1.52484
H	1.15785	4.33925	-1.42140
H	2.19782	2.93367	-1.89099
H	0.44120	2.90939	-2.26649
P	3.38801	0.08315	-0.09525
C	4.15411	-1.39881	-0.87531
H	3.85623	-2.30891	-0.32020
H	3.79049	-1.49580	-1.91810
H	5.25979	-1.30373	-0.87546
C	4.11783	0.08404	1.59559
H	5.22607	0.03278	1.56092
H	3.80714	0.99992	2.13708
H	3.72464	-0.79479	2.14599
C	4.30544	1.42465	-0.97359
H	4.02352	1.40909	-2.04591
H	4.06465	2.42236	-0.55950
H	5.39965	1.25870	-0.89059
C	-5.37135	-0.00654	-0.04759
F	-5.93430	0.45654	1.10193
F	-5.82613	-1.28567	-0.20650
F	-5.90858	0.71415	-1.07159

6g

Pd	0.52094	0.14096	-0.02888
I	0.36990	-2.54498	0.05218
P	0.33243	2.41596	0.06918
C	-1.51256	0.08913	-0.01243
C	-2.22463	0.12650	-1.23533

C	-2.25324	0.00424	1.19039
C	-3.62505	0.08793	-1.26522
H	-1.67785	0.18446	-2.19069
C	-3.65319	-0.03307	1.18256
H	-1.72898	-0.03588	2.15881
H	-4.16598	0.11676	-2.22383
H	-4.21674	-0.09867	2.12616
C	-1.30522	3.12836	0.50069
H	-2.06431	2.81574	-0.24153
H	-1.62207	2.77079	1.49964
H	-1.23188	4.23550	0.51218
C	1.42301	3.21759	1.31551
H	1.16253	2.82464	2.31875
H	2.48872	2.99868	1.11519
H	1.27005	4.31679	1.30401
C	0.71335	3.23847	-1.52895
H	0.66414	4.34227	-1.42443
H	1.71860	2.94465	-1.88495
H	-0.03392	2.90847	-2.27867
P	2.90343	0.09839	-0.07978
C	3.68397	-1.37863	-0.85427
H	3.39213	-2.29022	-0.29847
H	3.32561	-1.48043	-1.89838
H	4.78871	-1.27356	-0.84991
C	3.61616	0.10107	1.61797
H	4.72481	0.05386	1.59309
H	3.29736	1.01562	2.15697
H	3.22133	-0.77960	2.16420
C	3.82110	1.44607	-0.94769
H	3.55854	1.42345	-2.02478
H	3.56333	2.44298	-0.54200
H	4.91514	1.29117	-0.84419
C	-4.35343	0.01354	-0.05046
C	-5.78487	-0.01316	-0.06888
N	-6.96114	-0.03009	-0.08406

6h

Pd	0.76166	0.14059	-0.02684
I	0.60234	-2.54466	0.04215
P	0.57795	2.41631	0.07886
C	-1.26929	0.08956	-0.00658
C	-1.98514	0.14717	-1.22845
C	-2.00693	-0.01299	1.19875
C	-3.38600	0.11382	-1.25437
H	-1.44059	0.21838	-2.18396
C	-3.40724	-0.04901	1.19395
H	-1.47941	-0.06849	2.16442
H	-3.94870	0.16012	-2.19738
H	-3.98699	-0.12896	2.12425
C	-1.05839	3.12709	0.51745
H	-1.81906	2.81845	-0.22480
H	-1.37289	2.76466	1.51546
H	-0.98489	4.23413	0.53388
C	1.67300	3.21382	1.32348
H	1.41705	2.81745	2.32651
H	2.73796	2.99642	1.11760
H	1.51920	4.31292	1.31591
C	0.95463	3.24134	-1.51880
H	0.90763	4.34496	-1.41135

H	1.95820	2.94661	-1.87871
H	0.20430	2.91447	-2.26679
P	3.14396	0.09427	-0.08130
C	3.92016	-1.38454	-0.85631
H	3.62719	-2.29535	-0.29982
H	3.56047	-1.48594	-1.89998
H	5.02510	-1.28166	-0.85310
C	3.85966	0.09702	1.61509
H	4.96817	0.04815	1.58793
H	3.54336	1.01232	2.15425
H	3.46469	-0.78281	2.16257
C	4.06030	1.44059	-0.95227
H	3.79135	1.42042	-2.02782
H	3.80757	2.43742	-0.54320
H	5.15448	1.28243	-0.85546
C	-4.08411	0.02040	-0.03719
N	-5.55348	-0.00345	-0.05210
O	-6.12768	0.08904	-1.14714
O	-6.14645	-0.11237	1.03124

7a

Pd	-0.55556	0.18366	-0.00755
I	2.03040	-1.47790	-0.02088
P	-2.78023	-0.25584	0.03367
C	1.49595	0.61632	0.00952
C	1.63840	1.35935	1.22050
C	1.21868	1.29012	-1.22267
C	1.57566	2.76184	1.17469
H	1.83686	0.83504	2.16720
C	1.15694	2.70654	-1.22762
H	1.19746	0.73406	-2.17162
C	1.35188	3.43602	-0.04569
H	1.70067	3.33374	2.10811
H	0.97139	3.22759	-2.18062
H	1.31761	4.53648	-0.06599
C	-3.47231	-0.67731	1.69764
H	-2.94229	-1.56597	2.09733
H	-3.29794	0.16997	2.39171
H	-4.56131	-0.89106	1.64655
C	-3.93011	1.07625	-0.53310
H	-3.68653	1.34675	-1.58079
H	-4.99172	0.75364	-0.47466
H	-3.78429	1.97709	0.09707
C	-3.33563	-1.69563	-0.98663
H	-4.42820	-1.87114	-0.88742
H	-3.09270	-1.50398	-2.05179
H	-2.78782	-2.60512	-0.66603

7b

Pd	0.82970	-0.58908	0.00105
I	1.11228	1.97327	0.02018
P	3.12670	-1.18796	-0.01340
C	-1.12114	-0.24277	0.00123
C	-1.84783	-0.25250	1.21469
C	-1.84600	-0.17948	-1.21174
C	-3.24562	-0.35536	1.21848
H	-1.31835	-0.19708	2.18079
C	-3.24374	-0.28029	-1.22343
H	-1.31486	-0.06765	-2.17188

C	-3.98336	-0.39251	-0.00533
H	-3.76997	-0.39474	2.18325
H	-3.76646	-0.26304	-2.18977
C	4.10264	-0.52661	1.40299
H	4.00975	0.57864	1.41627
H	3.68459	-0.92077	2.35168
H	5.17463	-0.80573	1.33034
C	3.52335	-2.99124	0.00775
H	3.06092	-3.47984	-0.87435
H	4.61885	-3.17211	-0.00908
H	3.09454	-3.45033	0.92210
C	4.05040	-0.56836	-1.48251
H	5.12594	-0.84010	-1.43964
H	3.60071	-0.99202	-2.40367
H	3.95125	0.53564	-1.52554
N	-5.36048	-0.50531	-0.01050
C	-6.09448	-0.38348	-1.25970
H	-5.75887	-1.13783	-2.00471
H	-7.16943	-0.55590	-1.06742
H	-5.98420	0.62413	-1.72536
C	-6.09647	-0.50351	1.24301
H	-5.72806	-1.29556	1.93056
H	-6.02820	0.47095	1.78221
H	-7.16357	-0.70863	1.03810

7c

Pd	0.57755	-0.59056	-0.04062
I	0.83720	1.96823	0.01817
P	2.88404	-1.15638	0.06695
C	-1.37647	-0.25921	-0.12687
C	-2.14553	-0.23538	1.05474
C	-2.03800	-0.30275	-1.37766
C	-3.54709	-0.36971	1.00647
H	-1.65605	-0.12237	2.03635
C	-3.43172	-0.43695	-1.43662
H	-1.46319	-0.24679	-2.31722
C	-4.19661	-0.47556	-0.24507
H	-4.12056	-0.37448	1.94461
H	-3.95785	-0.49861	-2.40242
C	3.75115	-0.51599	1.55959
H	3.64265	0.58757	1.58875
H	3.27418	-0.93459	2.46916
H	4.82936	-0.77982	1.55339
C	3.29167	-2.95643	0.07480
H	2.89049	-3.42830	-0.84550
H	4.38751	-3.12912	0.12179
H	2.80961	-3.43868	0.94985
C	3.89546	-0.49520	-1.32326
H	4.97016	-0.74632	-1.20423
H	3.52336	-0.91511	-2.27994
H	3.77675	0.60703	-1.35869
O	-5.54376	-0.59554	-0.40347
C	-6.36234	-0.59270	0.76265
H	-6.12602	-1.44603	1.43727
H	-6.26570	0.35804	1.33312
H	-7.40668	-0.69390	0.41047

7d

Pd	-0.35640	0.54268	-0.00562
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I	-0.46122	-2.03120	0.01578
P	-2.66887	1.13415	-0.00975
C	1.60769	0.29482	-0.00086
C	2.30378	0.42043	1.21902
C	2.32328	0.30846	-1.21806
C	3.69067	0.66522	1.21086
H	1.77057	0.33773	2.18079
C	3.70820	0.55077	-1.21118
H	1.80285	0.14111	-2.17559
C	4.41441	0.73754	0.00030
H	4.22493	0.78464	2.16864
H	4.25670	0.58204	-2.16819
C	-3.16818	2.28615	1.34295
H	-2.96066	1.80870	2.32246
H	-2.56918	3.21741	1.27691
H	-4.24702	2.54218	1.28493
C	-3.23589	2.00448	-1.53504
H	-3.05588	1.35267	-2.41409
H	-4.31500	2.26056	-1.48374
H	-2.64613	2.93506	-1.66510
C	-3.87291	-0.24715	0.15597
H	-4.91741	0.12831	0.14695
H	-3.72959	-0.95985	-0.68097
H	-3.68354	-0.78861	1.10479
C	5.90198	0.99848	-0.00939
H	6.43871	0.27519	-0.65890
H	6.12913	2.01244	-0.40636
H	6.33508	0.93368	1.00880

7e

Pd	0.70057	-0.07428	0.01095
I	-0.96211	2.63280	-0.03531
P	2.86064	-0.78454	0.03711
C	-1.31359	0.51532	0.02186
C	-1.79427	-0.08790	1.22497
C	-1.29161	-0.24086	-1.19683
C	-2.31446	-1.38948	1.19363
H	-1.79491	0.48243	2.16579
C	-1.82419	-1.55686	-1.20727
H	-1.03754	0.24114	-2.15271
C	-2.33749	-2.10315	-0.02506
H	-2.69395	-1.85471	2.11526
H	-1.84354	-2.13119	-2.14526
Cl	-2.99391	-3.73604	-0.04196
C	3.62300	-0.95210	1.71386
H	3.58257	0.02694	2.23365
H	3.03913	-1.68309	2.30943
H	4.67912	-1.29065	1.65161
C	3.18797	-2.44241	-0.71162
H	2.86404	-2.43085	-1.77227
H	4.26436	-2.71203	-0.65892
H	2.59000	-3.20776	-0.17652
C	4.08529	0.28625	-0.84118
H	5.11529	-0.12221	-0.76386
H	3.80285	0.36262	-1.91089
H	4.06099	1.30567	-0.40532

7f

Pd	-0.85288	0.45574	0.02873
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I	-1.39931	-2.67486	-0.04751
P	-2.00989	2.42017	0.03407
C	0.25897	-1.32022	0.03043
C	1.02078	-1.20456	1.23525
C	0.73624	-0.71607	-1.18095
C	2.26802	-0.57004	1.20657
H	0.64300	-1.64630	2.16903
C	2.00107	-0.07564	-1.17540
H	0.22651	-0.89776	-2.13880
C	2.76697	-0.02197	-0.00060
H	2.85606	-0.49139	2.13305
H	2.38304	0.36161	-2.10997
C	-2.48661	3.06279	1.70111
H	-3.11467	2.30970	2.21921
H	-1.57187	3.22666	2.30613
H	-3.04881	4.01746	1.62237
C	-1.16044	3.87852	-0.71727
H	-0.92773	3.65702	-1.77877
H	-1.78864	4.79315	-0.66207
H	-0.20392	4.05677	-0.18533
C	-3.63202	2.40854	-0.85330
H	-4.14368	3.39168	-0.77968
H	-3.46478	2.16195	-1.92149
H	-4.28222	1.62456	-0.41432
C	4.13814	0.59727	-0.02905
F	5.11406	-0.31724	-0.31019
F	4.24535	1.57077	-0.97297
F	4.47564	1.15801	1.16374

7g

Pd	-0.64000	-0.08457	0.01989
I	1.71165	-2.17508	-0.03785
P	-2.92137	0.01553	0.03606
C	1.44929	-0.05303	0.01682
C	1.73846	0.66500	1.22136
C	1.19811	0.66111	-1.20370
C	1.84233	2.05764	1.19121
H	1.91461	0.11632	2.15820
C	1.29835	2.07108	-1.20927
H	1.09086	0.12354	-2.15745
C	1.64008	2.76903	-0.02783
H	2.07567	2.61024	2.11337
H	1.12999	2.62269	-2.14619
C	-3.68952	0.33343	1.68712
H	-3.39150	-0.46893	2.39247
H	-3.31888	1.29991	2.08509
H	-4.79779	0.36627	1.62023
C	-3.67632	1.34003	-1.00635
H	-3.37133	1.19339	-2.06245
H	-4.78520	1.32985	-0.94076
H	-3.29745	2.32722	-0.67196
C	-3.82617	-1.49348	-0.53070
H	-4.92646	-1.34870	-0.48637
H	-3.53152	-1.72879	-1.57375
H	-3.54364	-2.35348	0.11025
C	1.75375	4.19476	-0.04806
N	1.84651	5.36769	-0.06200

7h

Pd	-0.62872	0.45651	0.03257
I	-1.18189	-2.68953	-0.05369
P	-1.67644	2.48974	0.05742
C	0.46122	-1.33251	0.01094
C	1.24082	-1.21912	1.20949
C	0.91177	-0.70979	-1.20516
C	2.46503	-0.54843	1.17973
H	0.88547	-1.68509	2.14022
C	2.14831	-0.02258	-1.20675
H	0.39554	-0.89760	-2.15835
C	2.91435	0.02650	-0.03254
H	3.08256	-0.45323	2.08296
H	2.52680	0.45054	-2.12302
C	-2.17071	3.11025	1.72648
H	-2.86745	2.38673	2.19660
H	-1.27070	3.19341	2.36893
H	-2.66531	4.10228	1.65800
C	-0.68295	3.89657	-0.60913
H	-0.42193	3.68907	-1.66676
H	-1.24096	4.85507	-0.54877
H	0.25952	3.98102	-0.03067
C	-3.25172	2.63036	-0.89572
H	-3.68124	3.65181	-0.81985
H	-3.05753	2.39428	-1.96175
H	-3.98509	1.89535	-0.50591
N	4.19086	0.74113	-0.04898
O	4.55185	1.27119	-1.11252
O	4.84759	0.78632	1.00414

8TSa

Pd	-0.46315	0.22838	-0.00915
I	1.42238	-1.79636	-0.00036
P	-2.74429	0.22755	0.00070
C	1.59579	0.45303	0.00342
C	1.82783	1.12053	1.23946
C	1.81691	1.12307	-1.23332
C	2.26894	2.45681	1.22138
H	1.69211	0.58703	2.19210
C	2.25774	2.45994	-1.21776
H	1.67322	0.59159	-2.18598
C	2.49145	3.12336	0.00131
H	2.44165	2.97846	2.17664
H	2.42113	2.98294	-2.17391
H	2.84332	4.16683	0.00103
C	-3.52195	-0.58569	1.46995
H	-3.25071	-1.66113	1.47182
H	-3.12599	-0.12897	2.39962
H	-4.62825	-0.48707	1.45615
C	-3.59818	1.86854	-0.03494
H	-3.24864	2.43951	-0.91909
H	-4.70293	1.76088	-0.08005
H	-3.32329	2.44066	0.87475
C	-3.56374	-0.66050	-1.39996
H	-4.66864	-0.67138	-1.28573
H	-3.30034	-0.16204	-2.35521
H	-3.18827	-1.70322	-1.44003

8TSb

Pd	0.82006	0.34355	-0.01247
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I	0.93048	-2.52969	0.00460
P	2.35461	2.00136	-0.00263
C	-0.73098	-1.07405	0.00117
C	-1.36558	-0.72810	-1.22627
C	-1.36068	-0.72053	1.22910
C	-2.59679	-0.05778	-1.21978
H	-0.91154	-1.02071	-2.18503
C	-2.59240	-0.05175	1.22358
H	-0.90249	-1.00713	2.18768
C	-3.25398	0.28385	0.00214
H	-3.04840	0.20279	-2.18636
H	-3.04128	0.21282	2.19038
C	3.57284	2.00148	-1.39725
H	4.10177	1.02694	-1.41868
H	3.03025	2.12263	-2.35702
H	4.31714	2.81967	-1.29191
C	1.73288	3.74481	-0.05010
H	1.08357	3.92395	0.83118
H	2.56484	4.48140	-0.04789
H	1.11884	3.88987	-0.96247
C	3.46908	2.05191	1.47465
H	4.22072	2.86650	1.39796
H	2.85649	2.20478	2.38638
H	3.99330	1.07907	1.56879
N	-4.47837	0.92644	0.00264
C	-5.04272	1.40288	-1.25001
H	-6.04905	1.81979	-1.05971
H	-4.42264	2.19799	-1.72876
H	-5.15770	0.57616	-1.98342
C	-5.02913	1.42722	1.25192
H	-4.39611	2.22088	1.71545
H	-6.03088	1.85499	1.06160
H	-5.15045	0.61279	1.99808

8TSc

Pd	-0.68751	-0.24719	0.01919
I	-0.30800	2.54254	-0.08895
P	-2.44714	-1.68042	0.00164
C	1.10169	0.81925	0.07565
C	1.68929	0.27755	-1.10059
C	1.64133	0.49345	1.35543
C	2.79467	-0.59207	-0.99751
H	1.31180	0.56607	-2.09376
C	2.74041	-0.36881	1.44152
H	1.20667	0.92975	2.26747
C	3.32289	-0.92008	0.27230
H	3.22786	-1.00751	-1.91843
H	3.16354	-0.64325	2.42118
C	-3.41457	-1.77578	-1.57177
H	-3.83480	-0.77575	-1.80208
H	-2.73784	-2.06390	-2.40237
H	-4.24120	-2.51439	-1.50051
C	-2.05272	-3.46220	0.31256
H	-1.56065	-3.56252	1.30149
H	-2.96380	-4.09751	0.29246
H	-1.34262	-3.81862	-0.46160
C	-3.77727	-1.36639	1.24987
H	-4.59993	-2.10843	1.16769
H	-3.34090	-1.41913	2.26808

H	-4.18564	-0.34627	1.10128
O	4.37838	-1.75503	0.47338
C	4.97070	-2.37528	-0.66403
H	5.40068	-1.62699	-1.36698
H	5.78723	-3.01604	-0.28115
H	4.24081	-3.01097	-1.21362

8TSd

Pd	-0.56078	0.18428	0.00182
I	0.77310	-2.32579	0.00234
P	-2.73267	0.84382	-0.00425
C	1.48347	-0.22606	0.00236
C	1.82202	0.39882	1.23607
C	1.86733	0.37583	-1.23084
C	2.54013	1.60982	1.21645
H	1.56743	-0.08278	2.19188
C	2.58461	1.58346	-1.20932
H	1.63889	-0.12164	-2.18517
C	2.93759	2.21779	0.00543
H	2.79853	2.08975	2.17491
H	2.87710	2.04475	-2.16732
C	-3.32073	1.74241	1.50263
H	-3.17971	1.09516	2.39219
H	-2.71091	2.65824	1.64228
H	-4.39256	2.02338	1.42196
C	-3.23162	2.00275	-1.35791
H	-3.03405	1.52548	-2.33951
H	-4.30760	2.27168	-1.29315
H	-2.61901	2.92509	-1.29383
C	-4.00010	-0.49469	-0.16815
H	-5.03411	-0.08857	-0.16895
H	-3.82376	-1.04834	-1.11301
H	-3.88675	-1.20839	0.67328
C	3.69227	3.52487	-0.00368
H	3.04262	4.35825	-0.35179
H	4.06335	3.79027	1.00636
H	4.56250	3.49033	-0.69242

8TSe

Pd	-0.65895	-0.23098	0.00373
I	0.17098	2.69883	-0.02492
P	-2.59086	-1.42468	0.02332
C	1.16851	0.78413	0.01175
C	1.44740	0.10664	-1.21756
C	1.73695	0.30879	1.23234
C	2.33805	-0.99169	-1.21913
H	1.07690	0.50440	-2.17370
C	2.62035	-0.78151	1.21111
H	1.51806	0.82150	2.18057
C	2.92152	-1.41056	-0.01468
H	2.57389	-1.50585	-2.16249
H	3.06774	-1.14790	2.14681
C	-4.07464	-0.58108	-0.69010
H	-4.24844	0.37116	-0.14877
H	-3.88028	-0.34072	-1.75529
H	-4.98381	-1.21531	-0.61827
C	-2.59412	-3.03904	-0.87876
H	-1.80303	-3.69263	-0.45810
H	-3.57633	-3.55146	-0.79523

H	-2.36307	-2.86139	-1.94878
C	-3.20039	-1.92195	1.69763
H	-4.15457	-2.48688	1.63211
H	-2.43490	-2.55238	2.19404
H	-3.35558	-1.01448	2.31588
Cl	4.02908	-2.77722	-0.02384

8TSf

Pd	-0.96879	0.31811	0.00053
I	-1.25729	-2.48592	0.00064
P	-2.40489	2.09107	0.00119
C	0.49800	-1.14347	-0.00030
C	1.13955	-0.84069	1.23749
C	1.14083	-0.84306	-1.23798
C	2.40609	-0.23592	1.22351
H	0.66125	-1.10671	2.19130
C	2.40736	-0.23839	-1.22383
H	0.66304	-1.10986	-2.19185
C	3.04345	0.05714	-0.00009
H	2.90042	0.00714	2.17620
H	2.90268	0.00297	-2.17643
C	-2.04789	3.43734	1.21833
H	-2.06552	3.01804	2.24497
H	-1.03362	3.84383	1.02868
H	-2.79269	4.25838	1.14660
C	-2.52785	3.02962	-1.58687
H	-2.84986	2.34175	-2.39507
H	-3.25383	3.86680	-1.50938
H	-1.52989	3.43277	-1.85413
C	-4.17852	1.71162	0.36025
H	-4.80884	2.62601	0.33397
H	-4.55540	0.98503	-0.38830
H	-4.25609	1.24360	1.36288
C	4.36254	0.78101	0.00019
F	5.11413	0.49089	-1.09489
F	4.19613	2.13848	0.00237
F	5.11536	0.48767	1.09363

8TSg

Pd	0.59281	-0.27175	-0.01054
I	0.05496	2.46391	0.00351
P	2.53041	-1.49435	-0.00218
C	-1.24531	0.66718	0.00220
C	-1.77742	0.19650	1.24115
C	-1.79204	0.21396	-1.23673
C	-2.82773	-0.72879	1.23279
H	-1.38186	0.57600	2.19456
C	-2.84288	-0.71075	-1.22880
H	-1.40759	0.60667	-2.18928
C	-3.37212	-1.18362	0.00189
H	-3.23287	-1.10772	2.18302
H	-3.26002	-1.07564	-2.17935
C	3.83762	-0.91696	-1.17355
H	3.44434	-0.95462	-2.20993
H	4.09239	0.13703	-0.94048
H	4.75467	-1.53999	-1.10646
C	3.43455	-1.52316	1.60954
H	2.78826	-1.98463	2.38377
H	4.38289	-2.09651	1.53523

H	3.65880	-0.48280	1.92144
C	2.40534	-3.29235	-0.41251
H	3.39498	-3.79386	-0.36031
H	1.70954	-3.78261	0.29863
H	1.99012	-3.40687	-1.43466
C	-4.44736	-2.12686	0.00162
N	-5.32970	-2.90524	0.00143

8TSh

Pd	0.78188	-0.29598	-0.00006
I	0.69758	2.47441	0.00050
P	2.50365	-1.81259	-0.00080
C	-0.87984	0.92646	-0.00119
C	-1.49266	0.56630	1.24005
C	-1.49584	0.56992	-1.24180
C	-2.68510	-0.16519	1.23171
H	-1.03879	0.87677	2.19238
C	-2.68836	-0.16132	-1.23250
H	-1.04401	0.88257	-2.19440
C	-3.27557	-0.51162	-0.00008
H	-3.16938	-0.47459	2.16816
H	-3.17530	-0.46770	-2.16857
C	4.20688	-1.09518	-0.00262
H	4.33543	-0.46856	-0.90870
H	4.32900	-0.44463	0.88722
H	4.98570	-1.88681	0.00977
C	2.56504	-2.96848	1.43895
H	1.61969	-3.54669	1.48551
H	3.42017	-3.67298	1.36148
H	2.65807	-2.38300	2.37639
C	2.56264	-2.97365	-1.43671
H	3.43313	-3.66051	-1.37289
H	1.62827	-3.57088	-1.46229
H	2.62521	-2.39154	-2.37874
N	-4.52385	-1.27642	0.00060
O	-5.02032	-1.58260	1.09676
O	-5.02172	-1.58236	-1.09501

9a

Pd	0.13490	-0.65019	0.00002
I	2.71579	-0.10411	0.00003
P	-1.99465	-1.41295	-0.00006
C	-0.64193	1.15438	0.00002
C	-0.88671	1.80881	1.22341
C	-0.88625	1.80895	-1.22339
C	-1.36840	3.13284	1.21568
H	-0.70166	1.29733	2.18061
C	-1.36793	3.13298	-1.21568
H	-0.70085	1.29756	-2.18057
C	-1.61222	3.79640	-0.00001
H	-1.55294	3.64543	2.17398
H	-1.55210	3.64569	-2.17399
H	-1.99133	4.83058	-0.00002
C	-1.95574	-3.24927	-0.00024
H	-1.41715	-3.60625	-0.90111
H	-1.41818	-3.60637	0.90120
H	-2.98686	-3.66071	-0.00087
C	-3.01967	-0.96153	1.45033
H	-2.48712	-1.24317	2.38052

H	-3.19206	0.13274	1.45170
H	-3.99551	-1.48839	1.40917
C	-3.01973	-0.96122	-1.45031
H	-3.99592	-1.48739	-1.40875
H	-3.19136	0.13317	-1.45192
H	-2.48755	-1.24341	-2.38055

9b

Pd	1.36566	0.27620	0.00074
I	2.04870	-2.27796	0.00739
P	1.04574	2.51161	-0.00778
C	-0.60140	0.13769	-0.00061
C	-1.30381	0.02338	-1.21429
C	-1.30920	0.05768	1.21253
C	-2.69357	-0.18314	-1.21813
H	-0.77351	0.07965	-2.17788
C	-2.69925	-0.14726	1.21612
H	-0.78278	0.13834	2.17647
C	-3.43364	-0.26364	-0.00119
H	-3.20232	-0.28434	-2.18668
H	-3.21137	-0.22478	2.18501
C	2.67998	3.35509	-0.01811
H	3.25451	3.05719	0.88210
H	3.24728	3.04918	-0.92018
H	2.54897	4.45763	-0.02232
C	0.15458	3.19746	-1.45626
H	0.64907	2.85868	-2.38839
H	-0.88898	2.82578	-1.45067
H	0.15145	4.30668	-1.41975
C	0.16718	3.21197	1.44154
H	0.16741	4.32083	1.39576
H	-0.87774	2.84423	1.44640
H	0.66708	2.87936	2.37301
N	-4.80670	-0.45484	-0.00251
C	-5.50586	-0.65866	1.25389
H	-5.34652	0.19248	1.95202
H	-6.59227	-0.72782	1.05860
H	-5.18834	-1.59019	1.78209
C	-5.48857	-0.75457	-1.24951
H	-6.56923	-0.88179	-1.05213
H	-5.37786	0.06908	-1.98971
H	-5.11440	-1.68991	-1.73084

9c

Pd	1.10293	0.36837	-0.02157
I	2.07548	-2.08323	-0.02345
P	0.50888	2.55175	-0.04602
C	-0.82355	-0.01418	0.10487
C	-1.57368	-0.23435	-1.06245
C	-1.44194	-0.13236	1.36743
C	-2.93733	-0.58541	-0.98006
H	-1.10744	-0.13966	-2.05533
C	-2.79854	-0.47947	1.45327
H	-0.86967	0.03884	2.29232
C	-3.55832	-0.70792	0.28230
H	-3.49874	-0.76039	-1.90888
H	-3.29233	-0.58282	2.43225
C	2.01960	3.58384	-0.22345
H	2.70444	3.37939	0.62422

H	2.53654	3.32169	-1.16853
H	1.75850	4.66284	-0.23371
C	-0.58755	3.07958	-1.41635
H	-0.13866	2.78184	-2.38483
H	-1.57116	2.58122	-1.31075
H	-0.72879	4.18014	-1.39562
C	-0.31569	3.17821	1.46663
H	-0.47486	4.27426	1.39535
H	-1.29514	2.67426	1.58486
H	0.31251	2.95143	2.35104
O	-4.86888	-1.03649	0.46959
C	-5.66221	-1.30856	-0.68041
H	-5.26025	-2.16448	-1.26786
H	-6.67101	-1.57250	-0.30910
H	-5.74622	-0.42068	-1.34734

9d

Pd	-0.71357	0.59689	0.00314
I	-2.44195	-1.39912	0.01005
P	0.57385	2.45979	-0.01291
C	0.96715	-0.42165	0.00289
C	1.58791	-0.76189	1.21944
C	1.51005	-0.87325	-1.21494
C	2.74756	-1.56012	1.20904
H	1.17248	-0.41620	2.17864
C	2.66862	-1.67277	-1.20498
H	1.03212	-0.61769	-2.17330
C	3.31159	-2.02674	0.00149
H	3.22105	-1.82715	2.16894
H	3.07914	-2.03008	-2.16445
C	-0.51833	3.93659	-0.03645
H	-1.16027	3.90651	-0.93995
H	-1.16829	3.92914	0.86183
H	0.08402	4.86945	-0.04564
C	1.66924	2.70694	1.43598
H	1.07150	2.65294	2.36771
H	2.43508	1.90669	1.45425
H	2.17161	3.69445	1.37381
C	1.68075	2.66364	-1.45966
H	2.19410	3.64658	-1.41919
H	2.43687	1.85366	-1.45436
H	1.08782	2.59169	-2.39324
C	4.57764	-2.85100	-0.00135
H	5.48114	-2.20297	-0.05360
H	4.67029	-3.46107	0.92034
H	4.61841	-3.53463	-0.87390

9e

Pd	-1.09166	0.37304	-0.00031
I	-2.06186	-2.07495	0.00011
P	-0.49698	2.56093	-0.00009
C	0.82708	-0.02892	-0.00008
C	1.50815	-0.20416	1.22078
C	1.50815	-0.20454	-1.22089
C	2.86835	-0.56486	1.22374
H	0.98796	-0.06577	2.18092
C	2.86834	-0.56528	-1.22375
H	0.98800	-0.06638	-2.18109
C	3.53601	-0.73999	0.00002

H	3.40372	-0.70926	2.17416
H	3.40368	-0.70999	-2.17414
C	-2.02284	3.58232	-0.00075
H	-2.62380	3.34740	-0.90239
H	-2.62539	3.34586	0.89943
H	-1.77036	4.66349	0.00034
C	0.46265	3.13342	1.45207
H	-0.08601	2.87523	2.37979
H	1.44611	2.62365	1.46569
H	0.61861	4.23116	1.40599
C	0.46497	3.13431	-1.45035
H	0.61919	4.23229	-1.40423
H	1.44921	2.62603	-1.46154
H	-0.08120	2.87512	-2.37926
Cl	5.24086	-1.18378	0.00008

9f

Pd	-1.55355	0.28075	-0.00010
I	-2.22458	-2.26616	0.00008
P	-1.22844	2.52690	-0.00027
C	0.39512	0.10280	0.00005
C	1.08966	0.00154	1.22274
C	1.08983	0.00194	-1.22259
C	2.47902	-0.20307	1.21964
H	0.55428	0.07305	2.18132
C	2.47919	-0.20268	-1.21937
H	0.55457	0.07376	-2.18121
C	3.17698	-0.30157	0.00017
H	3.01877	-0.29043	2.17493
H	3.01907	-0.28973	-2.17460
C	-2.86270	3.36546	0.00015
H	-3.43286	3.06317	-0.90128
H	-3.43228	3.06337	0.90202
H	-2.73149	4.46791	-0.00001
C	-0.33901	3.20779	1.44992
H	-0.83766	2.87186	2.38080
H	0.70383	2.83370	1.44754
H	-0.33079	4.31688	1.41230
C	-0.33988	3.20757	-1.45110
H	-0.33153	4.31667	-1.41362
H	0.70293	2.83338	-1.44937
H	-0.83918	2.87159	-2.38162
C	4.67560	-0.45131	0.00026
F	5.12899	-1.11872	1.09400
F	5.12921	-1.11797	-1.09385
F	5.30978	0.76027	0.00074

9g

Pd	0.99782	0.37984	-0.00271
I	1.98826	-2.05495	0.00191
P	0.36896	2.56487	-0.00085
C	-0.90172	-0.06611	-0.00093
C	-1.57568	-0.26565	-1.22523

C	-1.57820	-0.25302	1.22390
C	-2.91979	-0.66144	-1.22663
H	-1.05411	-0.11824	-2.18278
C	-2.92243	-0.64869	1.22650
H	-1.05848	-0.09588	2.18094
C	-3.60322	-0.85549	0.00026
H	-3.44725	-0.82435	-2.17869
H	-3.45196	-0.80170	2.17906
C	1.88047	3.60619	-0.02230
H	2.49774	3.37797	0.86997
H	2.47192	3.37927	-0.93218
H	1.61218	4.68346	-0.01784
C	-0.62165	3.11865	-1.43845
H	-0.08110	2.87244	-2.37414
H	-1.59532	2.59005	-1.43923
H	-0.79799	4.21310	-1.38876
C	-0.57991	3.11846	1.46486
H	-0.75533	4.21340	1.42217
H	-1.55467	2.59242	1.49107
H	-0.01453	2.86876	2.38482
C	-4.97957	-1.25271	0.00069
N	-6.11041	-1.57501	0.00082

9h

Pd	-1.25561	0.33387	0.00011
I	-2.18131	-2.12809	0.00012
P	-0.75450	2.54814	0.00000
C	0.66619	0.01093	-0.00000
C	1.35541	-0.12705	1.22643
C	1.35517	-0.12754	-1.22652
C	2.72967	-0.40099	1.22797
H	0.82334	-0.01860	2.18325
C	2.72943	-0.40148	-1.22822
H	0.82291	-0.01947	-2.18328
C	3.40149	-0.52914	-0.00017
H	3.28896	-0.51312	2.16718
H	3.28853	-0.51397	-2.16749
C	-2.33252	3.48410	-0.00041
H	-2.92019	3.21724	-0.90188
H	-2.92052	3.21746	0.90090
H	-2.13535	4.57674	-0.00051
C	0.17572	3.16449	1.45216
H	-0.34097	2.85281	2.38159
H	1.19640	2.73387	1.44620
H	0.24609	4.27151	1.42000
C	0.17631	3.16421	-1.45189
H	0.24686	4.27123	-1.41981
H	1.19691	2.73343	-1.44556
H	-0.34013	2.85253	-2.38146
N	4.84976	-0.79315	-0.00026
O	5.42133	-0.89559	-1.09436
O	5.42155	-0.89512	1.09377