

Theoretical Study of Pd(0)-Catalyzed Carbohalogenation of Alkenes: Mechanism and Origins of Reactivities and Selectivities in Alkyl Halide Reductive Elimination from Pd(II) Species

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1. The full citation of Gaussian 09.

Gaussian 09, Revision A.2, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2009**.

2. BP86 absolute calculation energies, energies in solvent, enthalpies, and free energies.

Geometry	E _(elec)	E _(THF)	H _(correction)	G _(correction)	IF [*]
1	-1757.815288	-1757.825584	0.762777	0.655156	-
1d	-1050.298196	-1050.303042	0.241024	0.174537	-
2a	-474.327788	-474.338884	0.191799	0.137205	-
2b	-476.281008	-476.292296	0.192012	0.138440	-
2c	-923.100324	-923.103773	0.192394	0.140118	-
3a	-1417.254525	-1417.274632	0.574844	0.470990	-
3b	-1419.205085	-1419.225611	0.575075	0.472555	-
3c	-1866.021731	-1866.042001	0.575720	0.475299	-
3d	-1063.494863	-1063.511970	0.313139	0.234673	-
4b-ts	-1419.198739	-1419.216855	0.574246	0.474115	-84.8
4c-ts	-1866.003796	-1866.023029	0.574443	0.474884	-156.9
5a	-1417.281906	-1417.303801	0.575444	0.472624	-
5b	-1419.232864	-1419.256742	0.575941	0.475676	-
5c	-1866.041239	-1866.065255	0.576209	0.477867	-
5d	-1063.529148	-1063.548085	0.314863	0.234573	-
6a	-1417.273217	-1417.290298	0.576684	0.480830	-
6b	-1419.229575	-1419.247321	0.576759	0.481623	-
6c	-1866.041485	-1866.059066	0.577413	0.484952	-
6d	-1063.548958	-1063.562931	0.314919	0.240343	-
7a-ts	-1417.253131	-1417.270121	0.574643	0.478470	-248.8
7b-ts	-1419.206867	-1419.224545	0.574832	0.480946	-254.7
7c-ts	-1866.016917	-1866.034515	0.575216	0.483040	-263.1
7d-ts	-1063.526515	-1063.540002	0.313316	0.240804	-270.8
8a	-1417.302721	-1417.323850	0.576448	0.476669	-
8b	-1419.254287	-1419.277269	0.576823	0.479199	-
8c	-1866.063510	-1866.086758	0.577111	0.481449	-
8d	-1063.548276	-1063.566817	0.315487	0.238107	-
9a-ts	-1417.268938	-1417.283705	0.574769	0.476805	-99.3
9b-ts	-1419.215470	-1419.230437	0.574611	0.476010	-131.3
9c-ts	-1866.023275	-1866.038505	0.574616	0.477675	-205.8

9d-ts	-1063.511046	-1063.523084	0.313813	0.237277	-104.0
10a	-1417.281790	-1417.297716	0.577031	0.474930	-
10b	-1419.233167	-1419.248486	0.576769	0.475950	-
10c	-1866.045666	-1866.061559	0.577866	0.478204	-
10d	-1063.526365	-1063.538848	0.315681	0.237441	-
11a	-474.363425	-474.373572	0.193466	0.142612	-
11b	-476.316752	-476.327098	0.193766	0.143603	-
11c	-923.132740	-923.136238	0.194177	0.145303	-
12	-942.891847	-942.900177	0.381957	0.315756	-
12d	-589.132641	-589.138737	0.121066	0.077846	-
13-ts	-2232.140076	-2232.161367	0.956561	0.811201	-20.5
15d-ts	-1524.622458	-1524.636451	0.432738	0.336432	-70.9
16d	-1524.691408	-1524.706352	0.435486	0.340645	-
17d	-1063.564343	-1063.578873	0.315538	0.241763	-
18d	-1524.705685	-1524.719091	0.436587	0.345718	-
19	-435.010506	-435.022033	0.162974	0.111706	-
19d-ts	-1524.638162	-1524.650749	0.433457	0.339228	-163.8
20	-1378.001781	-1378.024194	0.548393	0.452189	-
21	-1377.987911	-1378.010380	0.546327	0.451185	-
22-ts	-1377.956606	-1377.974458	0.546459	0.449666	-100.9
23	-1377.972510	-1377.990735	0.548528	0.449592	-
24	-435.052279	-435.065353	0.164962	0.116841	-
25-ts	-1377.983463	-1378.001844	0.543072	0.448858	-592.0
26	-1377.992265	-1378.010577	0.544970	0.450231	-
27	-422.973748	-422.976638	0.149309	0.107893	-
28	-955.010666	-955.026113	0.392794	0.317512	-
P(tBu)₃	-814.864597	-814.870491	0.379080	0.318129	
PMe₃	-461.106101	-461.107784	0.117667	0.080311	
PH₃-8	-945.581220	-945.597501	0.225542	0.158770	-
PH₃-9-ts	-945.550571	-945.562118	0.223551	0.157264	-117.7
PH₃-17	-945.596238	-945.611411	0.225011	0.161329	-
PH₃-18	-1288.776290	-1288.790326	0.256365	0.184619	-
PH₃	-343.153783	-343.154621	0.027283	0.002356	
P(<i>i</i>Pr)₃-8	-1299.396078	-1299.417161	0.490770	0.397024	-

P(<i>i</i>Pr)₃-9-ts	-1299.361764	-1299.376294	0.488709	0.395858	-92.7
P(<i>i</i>Pr)₃-17	-1299.405769	-1299.422278	0.490707	0.399966	-
P(<i>i</i>Pr)₃-18	-1996.370952	-1996.388719	0.788285	0.666797	-
P(<i>i</i>Pr)₃	-696.956319	-696.961936	0.292252	0.236093	-
P(OMe)₃-8	-1289.243802	-1289.263706	0.334305	0.248245	-
P(OMe)₃-9-ts	-1289.209017	-1289.224964	0.331913	0.245597	-111.2
P(OMe)₃-17	-1289.249221	-1289.268480	0.334087	0.250632	-
P(OMe)₃-18	-1976.080972	-1976.100522	0.473636	0.362663	-
P(OMe)₃	-686.798999	-686.807092	0.136040	0.087734	-
Q-Phos[*]-8	-1770.001957	-1770.038186	0.615731	0.507570	-
Q-Phos[*]-9-ts	-1769.966284	-1769.996825	0.613798	0.504028	-94.5
Q-Phos[*]-17	-1770.000004	-1770.032743	0.615835	0.509115	-

* IF: The imaginary frequencies for the transition states.

3. BP86 geometries for all the optimized compounds and transition states.

1				H	2.95806000	-3.27938000	-1.90212500
Pd	0.00047200	-0.00389200	0.05705600	H	1.68731800	-2.03273200	-2.05290900
P	2.32526700	-0.00110800	0.00662800	H	3.38661000	-1.66075900	-2.49767300
C	3.01996200	-1.80656300	-0.30767200	C	4.51885600	-2.03584300	-0.00824300
C	2.98759200	1.15932300	-1.42768800	H	4.76083700	-1.90931400	1.06019800
C	3.07115400	0.64610100	1.69981600	H	4.78407000	-3.07895000	-0.27598300
P	-2.32535100	-0.00154500	0.00674000	H	5.17813500	-1.37022400	-0.59016200
C	-3.07406200	-0.75096800	1.65593500	C	2.07369700	0.93423800	-2.66120500
C	-2.99379100	-1.06669700	-1.49653200	H	2.31741700	1.69439000	-3.43106300
C	-3.01107900	1.82416700	-0.19328900	H	2.20033000	-0.05616800	-3.12335800
C	-2.73873000	2.30361600	-1.64056300	H	1.00947400	1.04314600	-2.37931900
H	-2.94646300	3.39090700	-1.69583500	C	2.77244500	2.63547500	-1.01272800
H	-1.68260900	2.14963400	-1.92620100	H	2.95942500	3.28009700	-1.89474000
H	-3.38527700	1.81341800	-2.38655300	H	1.73394300	2.81454700	-0.68102000
C	-2.08174100	-0.76791000	-2.71602100	H	3.46201700	2.96629100	-0.21895800
H	-2.33190300	-1.47598400	-3.53206200	C	4.46428600	0.97171900	-1.84139700
H	-2.20357700	0.25064000	-3.11381600	H	4.65824000	-0.02494400	-2.27182800
H	-1.01742700	-0.90071400	-2.44519800	H	4.71652800	1.71526700	-2.62475800
C	-4.50794600	2.04122800	0.12420000	H	5.16579100	1.12638700	-1.00458400
H	-4.74774100	1.85043600	1.18359400	C	2.20355300	1.84829600	2.15878000
H	-4.76929000	3.09990000	-0.07816200	H	2.49706300	2.12791600	3.19098400
H	-5.17158800	1.41525600	-0.49541800	H	2.32566400	2.74133200	1.52793200
C	-2.15265300	2.74128200	0.71792700	H	1.13140700	1.57599900	2.15678500
H	-1.07521500	2.57765100	0.52643400	C	4.55879800	1.06482800	1.68421500
H	-2.39703600	3.79947300	0.49368500	H	4.74683100	1.93295600	1.03008600
H	-2.33269100	2.58157300	1.79152600	H	4.86026400	1.36294600	2.70909800
C	-4.47076900	-0.84945500	-1.89492200	H	5.22863600	0.24741500	1.36926600
H	-4.66244200	0.17228800	-2.26320400	C	2.87510900	-0.44586600	2.78040200
H	-4.72670100	-1.54285200	-2.72179700	H	3.54212400	-1.31273700	2.64430100
H	-5.17080900	-1.05263600	-1.06735700	H	3.11097700	-0.00732500	3.77055400
C	-2.78178500	-2.56684600	-1.17598100	H	1.82929200	-0.80077500	2.81078600
H	-2.96986300	-3.15358000	-2.09724500				
H	-1.74364500	-2.76876900	-0.85647400	1d			
H	-3.47200700	-2.94643600	-0.40493900	Pd	-0.00005800	0.00111600	-0.00230000
C	-4.56451100	-1.15832800	1.61703300	P	2.28393400	-0.00013800	0.00036800
H	-4.75946000	-1.98193500	0.90975200	C	3.13685300	-0.09775200	1.65531600
H	-4.86575700	-1.51910400	2.62163400	C	3.13616500	-1.38611700	-0.90977700
H	-5.22992700	-0.31829500	1.35657100	C	3.13729200	1.48172500	-0.74234500
C	-2.21360500	-1.98570100	2.03485000	P	-2.28395000	0.00013500	0.00030900
H	-2.50374400	-2.32690600	3.04925900	C	-3.13695500	1.59327200	0.45822400
H	-2.34752100	-2.83665300	1.35028800	C	-3.13264500	-1.19294600	1.15445700
H	-1.13909200	-1.72272000	2.04372100	C	-3.14037400	-0.40346200	-1.60581500
C	-2.86986800	0.26905700	2.80306100	H	-4.24186700	-0.38038400	-1.49866800
H	-3.53201900	1.14660200	2.72303000	H	-2.82973400	-1.40654000	-1.94507200
H	-3.10700800	-0.22973100	3.76396100	H	-2.83536100	0.32433600	-2.37719300
H	-1.82208700	0.61571300	2.85413900	H	-4.23472200	-1.11714500	1.08298100
C	2.16783200	-2.78092700	0.54879300	H	-2.82305500	-2.22316800	0.90841300
H	1.08927000	-2.60943600	0.37136500	H	-2.82082300	-0.98440300	2.19226000
H	2.41459200	-3.82279400	0.25982900	H	-4.23872200	1.49034200	0.43104200
H	2.35095300	-2.68591400	1.62953000	H	-2.82926600	2.38855900	-0.24227900
C	2.74512200	-2.19849000	-1.78054900	H	-2.82582500	1.89673800	1.47251900

H	2.83016400	1.59141700	-1.79657000
H	2.82567400	2.39243600	-0.20266400
H	4.23904600	1.38779100	-0.69202800
H	2.83204900	0.76168700	2.27669200
H	4.23857700	-0.09679900	1.54787700
H	2.82374700	-1.01952300	2.17508400
H	4.23798400	-1.29908500	-0.84895800
H	2.82889800	-1.37308100	-1.96953800
H	2.82413800	-2.35279100	-0.47862800

2a

C	1.20991800	0.56888600	0.00033100
C	2.39278500	1.31459200	0.05151600
C	-0.05501700	1.20531300	-0.00368900
C	2.33840600	2.72081100	0.10094600
H	3.35805000	0.79891700	0.05360700
C	-0.09713300	2.61666700	0.04375500
C	1.09249600	3.36363900	0.09605200
H	3.26775400	3.29896900	0.14153800
H	-1.05925900	3.13694000	0.03534200
H	1.03398100	4.45740200	0.13159700
I	1.31397500	-1.57564700	-0.07695000
O	-1.15877300	0.40114100	-0.05643600
C	-2.46481400	1.02295200	-0.02647700
H	-2.53958200	1.64568000	0.89115000
H	-2.58990300	1.67707200	-0.91101300
C	-3.50906800	-0.07064800	-0.00668100
C	-4.47923500	-0.09394700	-0.94399800
H	-4.51122200	0.63640000	-1.76170500
H	-5.27703000	-0.84575700	-0.92281200
C	-3.41418600	-1.06942500	1.12224400
H	-2.44886600	-1.60682200	1.08576300
H	-3.45816200	-0.56239400	2.10652700
H	-4.23117400	-1.80928700	1.07587000

2b

C	1.44575600	-0.00932000	-0.02084900
C	2.74865200	0.49248500	0.02950500
C	0.31972100	0.84874600	-0.00340000
C	2.96095400	1.88254700	0.10096300
H	3.59363600	-0.20274500	0.01388200
C	0.54803500	2.24095400	0.06770400
C	1.85834900	2.74848800	0.11967800
H	3.98279100	2.27448500	0.14042800
H	-0.29762000	2.93432200	0.07901900
H	2.00767300	3.83273400	0.17373700
Br	1.16843000	-1.93854000	-0.11632200
O	-0.91358400	0.26435900	-0.05956300
C	-2.07684200	1.12319600	-0.00727600
H	-2.03003700	1.72564000	0.92563900
H	-2.07514400	1.81162200	-0.87461600
C	-3.31182000	0.25090000	-0.00836900
C	-4.26754600	0.43659400	-0.94231800
H	-4.15700900	1.17750800	-1.74341300
H	-5.19579400	-0.14694700	-0.93615100
C	-3.41315900	-0.77359100	1.09697000
H	-2.57758800	-1.49473700	1.03713100

H	-3.34646800	-0.29261800	2.09291400
H	-4.36342600	-1.33122300	1.04353700

2c

C	-1.58366900	0.63865400	-0.07415100
C	-2.94618800	0.32105500	-0.02417100
C	-0.59447700	-0.37725200	-0.00871500
C	-3.35439800	-1.02003800	0.09365800
H	-3.68123700	1.13065800	-0.07750300
C	-1.01707800	-1.71841100	0.11026500
C	-2.38701400	-2.03311700	0.16038100
H	-4.42173400	-1.26210300	0.13205200
H	-0.27852200	-2.52344000	0.16047100
H	-2.69008300	-3.08221500	0.25154100
Cl	-1.08561900	2.31605000	-0.22165800
O	0.70904300	0.02842000	-0.07081300
C	1.73997100	-0.98109300	0.02819000
H	1.61049600	-1.52547500	0.98872900
H	1.64072400	-1.70404900	-0.80461700
C	3.08548100	-0.29181900	-0.00946300
C	4.00920300	-0.66609500	-0.91878300
H	3.79850300	-1.43170100	-1.67534900
H	5.01044500	-0.21950600	-0.93545000
C	3.32534100	0.77251100	1.03514300
H	2.59403500	1.59427400	0.92786800
H	3.19555000	0.36367200	2.05678600
H	4.34197900	1.19330700	0.95603800

3a

Pd	-0.27092300	-0.40344100	0.36854900
C	1.70148800	-0.90434700	0.90381800
C	0.98192800	-1.60872000	1.92264100
C	2.44009900	0.28487500	1.24328000
C	1.00163200	-1.12844300	3.26246500
H	0.60113600	-2.61391700	1.71356200
C	2.42553500	0.73849900	2.57381800
C	1.71799200	0.02755700	3.57322000
H	0.47325600	-1.68949800	4.04138800
H	2.96415000	1.65033900	2.84786600
H	1.74305200	0.40050200	4.60360200
P	-2.41407600	0.30414400	-0.18395200
C	-3.01677200	1.70470200	1.04600500
C	-2.38504500	1.04991600	-1.99406200
C	-3.71029700	-1.15928500	-0.13804500
I	2.26884000	-1.99123400	-0.93994300
O	3.14247300	0.87189900	0.22915600
C	3.92893000	2.04551100	0.53152700
H	3.26748200	2.86210500	0.88131200
H	4.64273000	1.79376600	1.34568200
C	4.67790100	2.44720100	-0.71952900
C	4.56739800	3.70326700	-1.19972700
H	3.90488500	4.44353300	-0.73472800
H	5.13939600	4.03438100	-2.07471200
C	5.55971400	1.39009800	-1.34088100
H	6.31233900	1.02375400	-0.61478100
H	4.95997000	0.51167100	-1.64266800
H	6.09077800	1.77732400	-2.22698500

C	-4.00505400	-1.52016400	1.33858700	H	-4.90781500	0.70609700	-1.64859800
H	-4.57058000	-2.47272600	1.36097700	C	-4.95892100	2.24141100	-0.12248700
H	-3.07344800	-1.66947200	1.91348200	C	-4.92183100	3.57906300	-0.29478900
H	-4.62363200	-0.76554300	1.85169300	H	-4.31032000	4.04408200	-1.07774500
C	-5.04974100	-0.90102300	-0.86361000	H	-5.50622800	4.25496400	0.34086700
H	-4.92018600	-0.75440700	-1.94872700	C	-5.76925900	1.55987600	0.95454200
H	-5.70588300	-1.78529000	-0.73345900	H	-6.50632500	0.85956700	0.51398100
H	-5.59146200	-0.02871500	-0.46163400	H	-5.11450900	0.95659900	1.60970100
C	-3.02531800	-2.41085200	-0.74883000	H	-6.31340000	2.29234900	1.57470000
H	-2.84421000	-2.32823700	-1.83068800	C	3.73677100	-1.13362500	-1.92057300
H	-2.05506400	-2.60832400	-0.25734600	H	4.40009300	-1.99650400	-2.12863700
H	-3.68255600	-3.28924400	-0.58926000	H	2.73670100	-1.37604400	-2.32219500
C	-2.63304700	1.26977800	2.48513600	H	4.14562600	-0.27228600	-2.47390700
H	-2.83384500	2.11449200	3.17472500	C	5.11211900	-0.51855400	0.09289500
H	-3.21035600	0.40549600	2.84552500	H	5.18445900	-0.46848700	1.19199900
H	-1.56031500	1.01175800	2.54943400	H	5.83170300	-1.29231200	-0.24303900
C	-4.52382000	2.04603600	1.00087700	H	5.45212300	0.44637000	-0.31842800
H	-5.15726000	1.20616000	1.33309300	C	3.30567100	-2.27987500	0.22351200
H	-4.72233800	2.89057000	1.69147600	H	3.29528400	-2.28363900	1.32335000
H	-4.86257800	2.35499700	-0.00187700	H	2.30498800	-2.59253700	-0.12561600
C	-2.20408700	2.99238300	0.76449300	H	4.04495300	-3.03809000	-0.10480700
H	-1.11734400	2.79206800	0.76005200	C	1.81375000	1.48942400	-2.52996800
H	-2.48164200	3.47921800	-0.18449300	H	1.74688700	2.39103000	-3.17187600
H	-2.40755100	3.72006400	1.57509200	H	2.40679300	0.74067900	-3.07563100
C	-2.28044800	-0.11027700	-3.01479300	H	0.79618800	1.07978400	-2.39226700
H	-3.21102800	-0.69401300	-3.10641700	C	3.86795500	2.43175700	-1.39499700
H	-2.06829900	0.32052000	-4.01344300	H	4.51636900	1.70398500	-1.91170600
H	-1.45033600	-0.79512600	-2.76605100	H	3.81666600	3.33191600	-2.04031800
C	-3.57958600	1.94885300	-2.38391600	H	4.36544300	2.72762000	-0.45625200
H	-3.63350000	2.86830600	-1.77718200	C	1.55325200	3.04634000	-0.62772000
H	-3.46188500	2.26546100	-3.43998200	H	0.52625200	2.70364000	-0.40736800
H	-4.54793000	1.42733800	-2.30326900	H	1.96894600	3.52635500	0.27337500
C	-1.06407000	1.85181700	-2.14132300	H	1.48396500	3.82967400	-1.40851500
H	-0.95711500	2.17095700	-3.19765800	C	2.74773300	-0.23919400	2.79198100
H	-1.02598600	2.75700100	-1.51752900	H	3.72965900	-0.71993800	2.65006000
H	-0.18952500	1.22477500	-1.88322600	H	2.70171600	0.09969400	3.84590200
				H	1.95386100	-0.99411800	2.64965500
3b				C	3.67759200	1.99671000	2.10096500
Pd	0.16779300	-0.62474600	-0.12683700	H	3.50930300	2.95276800	1.57750500
C	-1.82694900	-1.35759200	-0.11069000	H	3.74099400	2.23004000	3.18298900
C	-1.08465400	-2.42596700	-0.71198500	H	4.66084600	1.60460600	1.79161200
C	-2.62654800	-0.48379300	-0.93407800	C	1.18945200	1.62155800	2.33875300
C	-1.14560400	-2.61611200	-2.12443200	H	1.25502300	1.83397300	3.42480200
H	-0.67707100	-3.21650700	-0.07257300	H	0.95097700	2.56913400	1.83313400
C	-2.64677400	-0.69443600	-2.32390300	H	0.34542800	0.92505200	2.17475500
C	-1.92219000	-1.76278400	-2.90720800				
H	-0.60113900	-3.45372900	-2.57413600	3c			
H	-3.23454400	-0.03414200	-2.96793700	Pd	0.06811800	-0.72180800	0.22529900
H	-1.97954000	-1.90922800	-3.99183300	C	-1.95407300	-1.41562300	0.64854800
P	2.27280600	0.36188700	0.03816600	C	-1.17104100	-2.58546100	0.37379100
C	2.43669500	1.89479400	-1.16730300	C	-2.80696600	-0.86977700	-0.38181100
C	2.52877700	0.98854400	1.87379200	C	-1.24458800	-3.19465100	-0.91476900
C	3.69659100	-0.90863800	-0.38918500	H	-0.72073200	-3.12797900	1.21269400
Br	-2.32843400	-1.51705700	1.82038400	C	-2.84669300	-1.49463200	-1.63952200
O	-3.35426900	0.46754800	-0.27893000	C	-2.07859900	-2.65696200	-1.89489200
C	-4.20006000	1.33487000	-1.06561000	H	-0.66480000	-4.10391900	-1.10699300
H	-3.58297200	1.92158100	-1.77403000	H	-3.48331600	-1.09069200	-2.43162400

H	-2.14521100	-3.12915500	-2.88157700	C	0.52523200	-0.64820600	0.99015300
P	2.10452300	0.35974400	-0.03499500	C	-0.34300800	-1.04303500	2.05426600
C	1.98956600	1.73852600	-1.42150900	C	1.46573900	0.42076400	1.18922100
C	2.63687400	1.21211100	1.64212600	C	-0.27982000	-0.37052200	3.30348200
C	3.49559500	-0.91867500	-0.54929700	H	-0.92613400	-1.96506600	1.96038400
Cl	-2.31925800	-0.98983500	2.34414600	C	1.49912700	1.06863400	2.43742800
O	-3.56967700	0.20237500	-0.01599200	C	0.63613600	0.66759700	3.48382100
C	-4.48642600	0.74481700	-0.99153200	H	-0.93553700	-0.69118300	4.12062400
H	-3.92518600	1.11711600	-1.87084100	H	2.19444500	1.89588300	2.60721900
H	-5.16884500	-0.06711800	-1.32517400	H	0.69793700	1.18734400	4.44681400
C	-5.27542600	1.85666100	-0.33707800	P	-3.23231700	0.87572800	-0.66189200
C	-5.32550400	3.07756900	-0.90923100	C	-3.86803700	2.44553700	0.11369900
H	-4.76278100	3.31195500	-1.82111200	C	-3.27406400	1.33839900	-2.46755800
H	-5.93497700	3.88426400	-0.48479000	C	-4.73999600	-0.21241400	-0.54620300
C	-6.01498700	1.49826300	0.93027800	I	0.88676500	-2.07186000	-0.68501100
H	-6.70488700	0.64800400	0.76099900	O	2.28933400	0.71249300	0.13924500
H	-5.30653200	1.17713800	1.71553500	C	3.25918100	1.77021100	0.30918900
H	-6.60077200	2.35221700	1.31082000	H	2.74048100	2.72558300	0.52065300
C	3.27480900	-1.32658700	-2.02671600	H	3.90773500	1.51918300	1.17648900
H	3.93377700	-2.18787000	-2.25444200	C	4.08422600	1.86737500	-0.95453400
H	2.23251100	-1.64408600	-2.20969400	C	4.20337000	3.04998700	-1.59307500
H	3.53423700	-0.52496900	-2.73750000	H	3.67470400	3.94780800	-1.25022500
C	4.95553800	-0.43905100	-0.37951800	H	4.83791300	3.16052900	-2.48050200
H	5.22102700	-0.25648500	0.67540100	C	4.77568500	0.60233800	-1.40450100
H	5.63728800	-1.23126600	-0.74994800	H	5.43262300	0.20301300	-0.60659800
H	5.17660800	0.47666500	-0.95293500	H	4.03457500	-0.18730300	-1.62670800
C	3.28380400	-2.21066600	0.28322200	H	5.38806700	0.77591500	-2.30561900
H	3.49442200	-2.07944400	1.35507700	H	-5.63408100	0.28677500	-0.96574900
H	2.24462600	-2.57414700	0.18364600	H	-4.92881300	-0.46769200	0.51049700
H	3.97007900	-2.99390000	-0.09726200	H	-4.55742300	-1.15139100	-1.09630300
C	1.16590400	1.15354200	-2.59933300	H	-3.04385800	0.45016500	-3.08040200
H	0.91682300	1.97476300	-3.30136900	H	-4.26274000	1.73763800	-2.76268400
H	1.70662300	0.38525400	-3.17187500	H	-2.50164000	2.09998700	-2.67109700
H	0.22387800	0.70294600	-2.23522800	H	-4.81808400	2.77319900	-0.34939700
C	3.33427000	2.28242900	-1.95335400	H	-4.02624200	2.28266100	1.19345700
H	3.92929400	1.50691700	-2.46440400	H	-3.11425500	3.24306600	-0.00195400
H	3.13278500	3.07881700	-2.69797000				
H	3.95727200	2.72513000	-1.15828300	4b-ts			
C	1.15368400	2.91946500	-0.86973800	Pd	0.02508800	-0.57165700	0.14127300
H	0.19291600	2.57352800	-0.44723900	C	-1.82679100	-1.43700400	0.14925100
H	1.68728300	3.50775900	-0.10519600	C	-1.46333800	-2.78714100	-0.07463200
H	0.92295700	3.60834800	-1.70653000	C	-2.85594100	-0.82094100	-0.63285400
C	3.07369600	0.11525700	2.64405400	C	-2.02790300	-3.50139700	-1.15236600
H	4.04782000	-0.33680200	2.39549700	H	-0.77538500	-3.27773500	0.62163400
H	3.17640000	0.57807500	3.64549100	C	-3.40476600	-1.55564400	-1.70298100
H	2.31504200	-0.68423100	2.72147300	C	-2.99068700	-2.88030400	-1.95865100
C	3.75809000	2.27086300	1.53791300	H	-1.72708200	-4.53909900	-1.33511600
H	3.44739200	3.15724600	0.95943600	H	-4.16389000	-1.10144000	-2.34679200
H	4.01430000	2.62578100	2.55652600	H	-3.44738400	-3.42641100	-2.79198400
H	4.68236000	1.87343900	1.08634600	P	2.18093600	0.28644500	-0.16678900
C	1.37143100	1.86123200	2.26507300	C	3.04565000	-0.53155900	-1.72094700
H	1.63236300	2.25102600	3.26979300	C	2.09171700	2.21790300	-0.46015100
H	0.97471000	2.70268900	1.67847700	C	3.29442500	-0.05192800	1.40740700
H	0.56302200	1.11631000	2.38316000	Br	-1.66879300	-0.71893400	2.24868600
				O	-3.24063300	0.44290600	-0.28086800
3d				C	-4.29033800	1.06563700	-1.05395400
Pd	-1.27501600	0.03057900	0.13671200	H	-3.93687000	1.18129000	-2.10235300

H	-5.19125700	0.42170400	-1.05570700	H	4.14186700	-3.64030100	1.96527500
C	-4.59788200	2.41735700	-0.44965900	P	-2.04594600	0.22835200	0.11274900
C	-5.86806600	2.73816100	-0.12729900	C	-2.20580600	0.41649100	2.05305700
H	-6.69170300	2.02279600	-0.24034300	C	-2.41015400	1.96878100	-0.70969500
H	-6.12720600	3.73054900	0.26048100	C	-3.40042600	-1.03982400	-0.50484600
C	-3.43303200	3.36360400	-0.28399400	Cl	1.55296400	-0.67102400	-2.38456400
H	-2.68259100	2.93555700	0.40533400	O	3.24511900	0.45188300	0.01973100
H	-2.91764600	3.53381200	-1.24987700	C	4.37540900	1.06983800	0.67213200
H	-3.75980700	4.33948900	0.11359800	H	4.21480400	1.03511200	1.77251600
C	3.00129000	-1.49978300	1.88219900	H	5.30115800	0.51031100	0.43474800
H	3.49408900	-1.65949300	2.86221100	C	4.47657100	2.50320600	0.20106500
H	1.91515700	-1.65891300	2.01341400	C	5.63848400	2.96888600	-0.30200600
H	3.37932200	-2.27100700	1.19473100	H	6.51342200	2.32040500	-0.43169400
C	2.82282400	0.87022100	2.55833100	H	5.75325900	4.01720900	-0.60236200
H	3.09390700	1.92676000	2.40067800	C	3.24225500	3.35631000	0.37133300
H	1.73223800	0.79822100	2.71794700	H	2.40104000	2.93768100	-0.21079600
H	3.31930000	0.54383900	3.49354300	H	2.91712000	3.37813200	1.43041700
C	4.81732900	0.12949600	1.21670800	H	3.41968000	4.39344700	0.03948200
H	5.32446900	-0.04557100	2.18694900	C	-2.86447000	-2.46887400	-0.22508600
H	5.24218200	-0.59135300	0.49837200	H	-3.55271100	-3.20412000	-0.68802700
H	5.08817200	1.14573200	0.88447500	H	-1.86125700	-2.60577900	-0.66986400
C	1.03544400	2.78955600	0.52242900	H	-2.79529900	-2.70985600	0.84576000
H	1.33355600	2.71908600	1.57845100	C	-3.51984100	-0.93192000	-2.04548500
H	0.87981200	3.86262200	0.29131900	H	-4.02582700	-0.01036000	-2.37625200
H	0.06800600	2.26620400	0.41048400	H	-2.53267100	-0.99335000	-2.53700700
C	1.52887600	2.48625500	-1.87788800	H	-4.12787800	-1.78355400	-2.40969600
H	0.59436500	1.92428800	-2.05624200	C	-4.80621100	-0.88847200	0.11780600
H	1.29185100	3.56536300	-1.96222300	H	-5.48929900	-1.62448000	-0.35194900
H	2.24500900	2.24954800	-2.68154100	H	-4.81004500	-1.09259300	1.20148200
C	3.41741300	2.99568800	-0.29683400	H	-5.23878900	0.11256200	-0.04475700
H	3.24087100	4.06368200	-0.53750600	C	-1.85350000	1.93180000	-2.15702700
H	3.80386000	2.96001200	0.73564200	H	-2.40018300	1.24484300	-2.81915600
H	4.21055400	2.63397600	-0.97221100	H	-1.93706000	2.94749800	-2.59305200
C	1.96865000	-0.66521800	-2.82997500	H	-0.78892200	1.63767900	-2.16961000
H	1.63568300	0.30108000	-3.23637400	C	-1.58780200	3.05238200	0.02850100
H	2.39090300	-1.25166100	-3.67050200	H	-0.52190600	2.77241300	0.10444200
H	1.07753900	-1.19947600	-2.44981100	H	-1.64387200	3.99230400	-0.55527500
C	3.45840500	-1.98045300	-1.36280600	H	-1.97259000	3.27440200	1.03722200
H	3.75608800	-2.50156800	-2.29418400	C	-3.89316100	2.40279600	-0.73681700
H	4.32013200	-2.02585900	-0.67765900	H	-3.96221300	3.42046500	-1.17121500
H	2.61907900	-2.54478700	-0.91871400	H	-4.51401500	1.74357200	-1.36612700
C	4.27970700	0.20901900	-2.28417500	H	-4.34550600	2.44285700	0.26832400
H	4.69944700	-0.37887700	-3.12541700	C	-0.88079400	1.04221900	2.56761200
H	4.02955600	1.20585800	-2.68381300	H	-0.73187100	2.08255100	2.24367100
H	5.08247400	0.33161000	-1.53766000	H	-0.89074100	1.03646800	3.67611000
4c-ts				H	-0.00635200	0.45348200	2.22973700
Pd	0.11557500	-0.58378000	-0.39430900	C	-2.27621900	-0.99155000	2.69297500
C	1.92988200	-1.49268300	-0.42717400	H	-2.16531600	-0.88350300	3.79002300
C	1.71641200	-2.88478800	-0.33061600	H	-3.23750300	-1.49983200	2.51385000
C	3.02211500	-0.87678200	0.25962100	H	-1.45661600	-1.64218100	2.33873400
C	2.49176000	-3.66020200	0.55325300	C	-3.40085300	1.25274400	2.56386300
H	0.95284200	-3.35089800	-0.96211600	H	-3.40369700	1.23807800	3.67255800
C	3.78817400	-1.67149000	1.13692500	H	-3.33891700	2.31025800	2.25747400
C	3.52072300	-3.04819700	1.28354900	H	-4.37281900	0.85459400	2.22784400
H	2.30006700	-4.73500200	0.64684700	5a			
H	4.60475200	-1.22361400	1.71150700	Pd	0.07789100	-0.78505600	-0.04655300

C	0.88394600	0.09153100	1.55435500	H	-1.59872400	-1.15158600	-3.70100200
C	0.61351000	-0.34879900	2.85690700	H	-0.53023300	-1.19343000	-2.28821100
C	1.84128000	1.12040100	1.35233000	C	-3.73595200	0.22167700	-2.61158100
C	1.24228000	0.24898600	3.97122200	H	-4.33623700	-0.63887600	-2.27433000
H	-0.07709200	-1.18077100	3.01969100	H	-4.25992500	1.14516900	-2.31366600
C	2.46051700	1.72397900	2.46847100	H	-3.72569900	0.19364300	-3.71973100
C	2.15820500	1.28935800	3.77199700				
H	1.01649700	-0.11542100	4.98004100	5b			
H	3.18652900	2.53054800	2.32660600	Pd	0.10778500	-0.25430600	-0.91284700
H	2.65533700	1.76477800	4.62540000	C	0.99391000	-1.50717500	0.35259900
P	-2.02464800	0.24332600	-0.17086400	C	0.66353500	-2.86551400	0.43315300
C	-2.29904900	2.06684900	0.45799800	C	2.10105100	-1.00872000	1.08808500
C	-2.27637300	0.17581800	-2.10684600	C	1.39966600	-3.73967400	1.26397100
C	-3.34028400	-0.92981600	0.67561300	H	-0.15800900	-3.26652100	-0.16762900
I	2.11592900	-2.42293700	-0.37074400	C	2.82874600	-1.88280800	1.92455100
O	2.10059300	1.48271600	0.04742000	C	2.47557700	-3.24254200	2.00993400
C	3.18208000	2.40942500	-0.19752200	H	1.12866400	-4.80084700	1.30816500
H	2.92896800	3.40697800	0.21430600	H	3.67543300	-1.50895800	2.50917300
H	4.09404300	2.03507700	0.31494500	H	3.05669400	-3.90774100	2.65898600
C	3.41578100	2.48441400	-1.69074500	P	-1.83777700	0.26878900	0.24251600
C	3.29836600	3.66508700	-2.33472900	C	-1.98480400	0.11214500	2.17933900
H	2.99842900	4.58123900	-1.81086300	C	-2.02585000	2.14656300	-0.27086300
H	3.50810000	3.75682600	-3.40739900	C	-3.27961800	-0.75747900	-0.59134400
C	3.82582400	1.19937000	-2.36939000	Br	1.81051900	-0.49966800	-2.69078800
H	4.78472100	0.82697200	-1.95748900	O	2.38815400	0.33071200	0.94325800
H	3.08513000	0.39929600	-2.18686200	C	3.61161300	0.82856800	1.53063800
H	3.94642000	1.33614100	-3.45773700	H	3.53440400	0.81436200	2.63637000
C	-4.77146000	-0.35095300	0.75908500	H	4.44866600	0.16582300	1.22440300
H	-5.44207400	-1.12859600	1.17590700	C	3.84666100	2.23398900	1.02064900
H	-4.83855100	0.52180700	1.42956200	C	3.90773200	3.26645200	1.88835600
H	-5.17451600	-0.06267100	-0.22594500	H	3.75684100	3.12433600	2.96584700
C	-3.39837400	-2.28675800	-0.07047700	H	4.12105900	4.28800700	1.55077100
H	-2.39693100	-2.74116900	-0.17558700	C	4.05066100	2.37772000	-0.46861200
H	-4.01153200	-2.98323100	0.53434500	H	4.95377800	1.82437500	-0.79429700
H	-3.87176300	-2.22112800	-1.06344000	H	3.20605700	1.93865300	-1.03069500
C	-2.83179600	-1.26706800	2.10009000	H	4.16890000	3.43496000	-0.76193700
H	-1.87391400	-1.81175900	2.04679300	C	-4.66482500	-0.61202100	0.08013900
H	-2.69159500	-0.38703700	2.74386100	H	-5.40476700	-1.18422700	-0.51405600
H	-3.57339100	-1.92849500	2.59019100	H	-4.68828000	-1.02344200	1.10238900
C	-3.55406900	2.75928400	-0.12261800	H	-5.01416200	0.43332400	0.11905200
H	-4.48921000	2.22057900	0.09783100	C	-3.41038900	-0.36077400	-2.08367400
H	-3.63707400	3.76663300	0.33195400	H	-2.44591000	-0.44278600	-2.61662600
H	-3.48568700	2.90519200	-1.21370800	H	-4.11108100	-1.06945500	-2.56690100
C	-1.05169400	2.91097100	0.09331700	H	-3.82044800	0.65065900	-2.23456800
H	-0.97019400	3.11934700	-0.98300100	C	-2.85671100	-2.24932500	-0.59774800
H	-1.13394800	3.88630500	0.61256600	H	-1.92536000	-2.38226000	-1.17553600
H	-0.11734600	2.42869900	0.41606000	H	-2.70594400	-2.67313300	0.40569900
C	-2.39206300	2.06074000	2.00462100	H	-3.65343800	-2.83866400	-1.09317600
H	-1.52114500	1.56777100	2.46966700	C	-3.13748200	0.94284800	2.79256900
H	-2.40141800	3.11292600	2.35005900	H	-4.12440300	0.68830100	2.37416600
H	-3.31595600	1.59077800	2.37909400	H	-3.17524700	0.73438200	3.88026100
C	-1.48855500	1.33488600	-2.76558000	H	-2.98189600	2.02833000	2.68000800
H	-0.44660000	1.38602300	-2.40452900	C	-0.64539900	0.55687800	2.81815700
H	-1.45721900	1.15490600	-3.85812800	H	-0.40899500	1.61737400	2.65267200
H	-1.96873300	2.31535300	-2.61478200	H	-0.71969500	0.39893500	3.91244800
C	-1.60104800	-1.13645200	-2.59279600	H	0.19708100	-0.04397000	2.44462300
H	-2.10613700	-2.04976700	-2.25033600	C	-2.17862400	-1.37456200	2.57158700

H	-1.38135000	-2.01878100	2.16318300	C	2.69847000	-0.43337600	3.01686600
H	-2.12268700	-1.44341000	3.67571100	H	3.72824600	-0.24042900	2.67604900
H	-3.16028200	-1.77793100	2.27413200	H	2.61403900	-0.04268600	4.05036100
C	-1.12392400	3.02128200	0.63399900	H	2.54965800	-1.52426900	3.07298800
H	-0.08587400	2.64787800	0.67070700	C	0.22247900	-0.08408100	2.69441500
H	-1.09648900	4.04344000	0.20797200	H	0.00415300	-1.16120300	2.69364100
H	-1.50902500	3.11130700	1.66241900	H	0.17053100	0.26464300	3.74509200
C	-1.45207400	2.28295600	-1.70865900	H	-0.57102400	0.42527700	2.12774000
H	-2.03551700	1.75304700	-2.47441400	C	1.78531900	1.79853600	2.29200600
H	-1.43660800	3.35568400	-1.98647300	H	1.04932900	2.34995200	1.68278600
H	-0.39694000	1.93399000	-1.76682400	H	1.59822700	2.06054700	3.35171800
C	-3.46352000	2.70903700	-0.23526800	H	2.79906500	2.15467000	2.04736700
H	-4.13535700	2.21069000	-0.95305900	C	0.92437400	-2.86692000	1.02955300
H	-3.91989900	2.64477700	0.76610700	H	-0.10413800	-2.48973700	0.89237800
H	-3.43034400	3.78136000	-0.51366800	H	0.92223500	-3.94519500	0.77600600
5c				H	1.19697900	-2.78653400	2.09434800
Pd	-0.11840600	0.05353300	-1.14895800	C	1.52501600	-2.53913700	-1.35231900
C	-1.10050000	1.53457900	-0.24909300	H	2.20029400	-2.14932700	-2.12666400
C	-0.74439200	2.87973200	-0.40786400	H	1.52387100	-3.64407500	-1.43890300
C	-2.28875300	1.20299400	0.45333700	H	0.48797100	-2.21313200	-1.59204700
C	-1.53241200	3.90868800	0.15400100	C	3.35201500	-2.68890000	0.39171900
H	0.14337700	3.14622500	-0.98825600	H	4.10762800	-2.31206100	-0.31721300
C	-3.06769700	2.23313700	1.02438200	H	3.69133400	-2.45301700	1.41409600
C	-2.68823600	3.57960400	0.87317200	H	3.33998500	-3.79314300	0.29537600
H	-1.23713700	4.95495600	0.01376500	5d			
H	-3.97347400	1.98899200	1.58863800	Pd	-0.88023700	0.44604500	-0.31057400
H	-3.30959500	4.36571500	1.31756500	C	0.34970700	0.72535100	1.22773900
P	1.70378100	-0.21684300	0.26012500	C	-0.04474400	1.50839100	2.32136700
C	1.62818300	0.26464700	2.14430200	C	1.57831000	0.01799200	1.26715100
C	1.93343700	-2.15262700	0.09690100	C	0.76655700	1.58758700	3.47522600
C	3.24155600	0.66827000	-0.56713100	H	-1.00434800	2.03672600	2.29618000
Cl	-1.60506900	-0.07732500	-2.92095800	C	2.38639900	0.10119800	2.42167600
O	-2.60035000	-0.13422800	0.55430400	C	1.97771400	0.88448800	3.51800200
C	-3.91039300	-0.49198000	1.05071600	H	0.43695600	2.18911800	4.32998200
H	-3.97214100	-0.28982000	2.13896000	H	3.33422900	-0.44429000	2.47328400
H	-4.66973600	0.12882600	0.52983900	H	2.61635200	0.93434700	4.40735200
C	-4.14335500	-1.95773000	0.75386400	P	0.09233700	2.23875000	-1.29314000
C	-4.33456200	-2.83104500	1.76545400	C	1.93104800	2.26854000	-1.47467700
H	-4.29527600	-2.51499300	2.81548200	C	-0.51356300	2.41840000	-3.03762800
H	-4.54490800	-3.89092600	1.57677800	C	-0.28605800	3.88301600	-0.53337300
C	-4.18657800	-2.34133300	-0.70607100	I	-2.43512300	-1.59452700	0.21285000
H	-5.03481500	-1.84218400	-1.21554300	O	1.90395700	-0.71398200	0.14753100
H	-3.27450300	-2.00548100	-1.23310300	C	3.05632300	-1.58342400	0.21368000
H	-4.29962400	-3.43138300	-0.83588000	H	3.98055500	-0.98554100	0.34414500
C	4.54054900	0.65199200	0.27083800	H	2.94290700	-2.25525700	1.09145200
H	5.34975500	1.11714400	-0.32655600	C	3.11124200	-2.38957000	-1.06575200
H	4.45379700	1.23661700	1.20148200	C	4.20944800	-2.33739600	-1.84920400
H	4.87124700	-0.36729200	0.53128700	H	5.06371700	-1.69364700	-1.60473400
C	3.53120500	0.02054400	-1.94372000	H	4.29592200	-2.94674000	-2.75691400
H	2.63116600	-0.00135800	-2.58422400	C	1.91192200	-3.25774000	-1.36303900
H	4.28776700	0.64059500	-2.46329000	H	1.75542500	-4.00196100	-0.55745500
H	3.94481400	-0.99773000	-1.86866000	H	0.98694600	-2.65412300	-1.40818500
C	2.83868300	2.13256400	-0.87619200	H	2.03125900	-3.79957900	-2.31666600
H	1.98168900	2.15642600	-1.57159700	H	2.25249400	3.16400100	-2.03714800
H	2.57860800	2.71958600	0.01663500	H	2.39454500	2.27650000	-0.47447700
H	3.69309300	2.63530200	-1.37122100	H	2.26311000	1.35817700	-1.99954000

H	0.17528500	4.70279200	-1.11389700	H	-1.25028000	4.57149500	0.11734800
H	0.10342100	3.90208700	0.49835300	H	-0.95656400	4.15814500	1.83342000
H	-1.37839700	4.03206400	-0.49641200	H	0.27059300	5.04154800	0.91073600
H	-0.07382300	3.31409500	-3.51419300	C	-2.39024100	3.13069400	-1.72494900
H	-1.61308000	2.50810600	-3.04581800	H	-1.55020500	3.82054000	-1.90283100
H	-0.23357200	1.52457200	-3.62015500	H	-3.02049900	3.15440200	-2.63603500
6a				H	-3.00204300	3.52727700	-0.89806600
Pd	0.41805500	-0.83415000	-0.05295400	C	-1.07718400	1.19419200	-2.68253300
C	2.17750500	0.00000500	-0.59843900	H	-0.12505900	1.74239500	-2.76270300
C	2.38858000	0.17830700	-1.98183600	H	-0.85998300	0.11348500	-2.60419600
C	3.25836400	0.21865100	0.27296100	H	-1.63920000	1.35575500	-3.62365400
C	3.62709600	0.64171600	-2.46933500	C	-3.23374200	0.79577000	-1.51520700
H	1.58071800	-0.03206800	-2.69254400	H	-3.99517200	1.13102000	-0.79251600
C	4.49223500	0.70811300	-0.19961200	H	-3.68368100	0.89017800	-2.52348300
C	4.67262000	0.93032600	-1.57458000	H	-3.02297400	-0.27262800	-1.34986800
H	3.76486500	0.78063800	-3.54823900	6b			
H	5.29660400	0.89460000	0.52131200	Pd	0.62323400	-0.78727600	-0.23944100
H	5.63264600	1.30659300	-1.94607800	C	2.01163900	0.64922500	-0.52590500
P	-0.88836900	1.35052900	0.12853300	C	2.17263500	1.14602500	-1.83728800
C	-1.95167800	1.66394300	-1.49274500	C	2.96441700	1.01699200	0.44077700
C	-2.10507200	1.28187700	1.66972900	C	3.21950400	2.03627800	-2.15137300
C	0.24855700	2.94077400	0.41904600	H	1.47246600	0.84819200	-2.62724500
I	-1.70493500	-2.59900600	-0.66690700	C	4.00040600	1.92476100	0.14616500
C	1.63370100	-2.08905400	1.41931900	C	4.12182600	2.44364300	-1.15332600
C	1.60499700	-2.71377200	0.15812200	H	3.31907300	2.41260500	-3.17653600
H	2.47926600	-2.65120900	-0.50103200	H	4.70084800	2.20326900	0.94204100
H	0.88947700	-3.51328600	-0.05508500	H	4.92827200	3.14774600	-1.38818900
O	3.13278000	-0.02886800	1.63797100	P	-1.34734500	0.73628300	0.14978900
C	2.92989500	-1.42810000	1.92903500	C	-2.48153400	0.78378000	-1.45602300
H	3.80246900	-1.99135500	1.53958900	C	-2.41113400	0.05612000	1.65420900
H	2.94458800	-1.47731000	3.03085500	C	-0.87901400	2.59741600	0.61180100
C	0.66106900	-2.49178000	2.51239500	Br	-0.73818800	-2.92764500	-0.98791100
H	0.35450100	-1.62440100	3.12565100	C	2.17997500	-1.85860100	1.07046400
H	-0.23782100	-2.98167500	2.10554100	C	2.35862200	-2.19366300	-0.28267000
H	1.16678800	-3.20462600	3.19785900	H	3.17031100	-1.73037000	-0.85645500
C	-2.79776500	-0.09697700	1.75047200	H	1.91886600	-3.10647800	-0.69686600
H	-2.07408600	-0.90910900	1.92081300	O	2.89411400	0.50134300	1.73436000
H	-3.49780300	-0.07644900	2.60966600	C	3.17217400	-0.91468100	1.77769300
H	-3.37339700	-0.35909900	0.85189000	H	4.18943800	-1.08048100	1.36743600
C	-1.28272200	1.43176900	2.97361800	H	3.18462900	-1.15315100	2.85449800
H	-1.92612800	1.13243300	3.82383200	C	1.38752100	-2.74797800	2.00914000
H	-0.39128100	0.78035100	2.98251500	H	0.82864900	-2.15393400	2.75552700
H	-0.95857300	2.46715200	3.16087300	H	0.68543600	-3.39891100	1.46535900
C	-3.20817400	2.36948100	1.65060100	H	2.09659800	-3.38729900	2.57683600
H	-3.94598200	2.20467900	0.84986200	C	-2.53630600	-1.48280100	1.57642800
H	-3.75877300	2.31236700	2.61091300	H	-1.55705600	-1.98192000	1.64434200
H	-2.82124200	3.39443100	1.55699900	H	-3.15244300	-1.81606700	2.43564000
C	1.28823500	2.62603200	1.53067000	H	-3.01597800	-1.84158600	0.65562100
H	2.20382600	3.21885200	1.34345100	C	-1.67364500	0.36703300	2.98015100
H	0.92103200	2.90914900	2.52977000	H	-2.14515100	-0.22961400	3.78527100
H	1.58647900	1.56943200	1.56863800	H	-0.60545800	0.08925400	2.93954800
C	1.02877800	3.24735400	-0.88437500	H	-1.74931600	1.42500800	3.27532300
H	1.63377800	2.39320000	-1.22121500	C	-3.84251000	0.64636200	1.72829500
H	0.37745300	3.56891800	-1.71209400	H	-4.47398800	0.32189600	0.88595500
H	1.72402500	4.08413300	-0.67699100	H	-4.32036100	0.26661600	2.65339200
C	-0.48905700	4.23755500	0.83852300	H	-3.86821200	1.74506000	1.77527900

C	0.23162200	2.59916600	1.69776500	H	-2.83093500	-2.42924700	0.15192100
H	0.79382700	3.55006400	1.62660200	C	-1.75521700	-0.53265100	2.85630100
H	-0.18297800	2.54671200	2.71592600	H	-2.17328000	-1.30295300	3.53341200
H	0.95381800	1.77971700	1.58589900	H	-0.66474800	-0.69681900	2.79592100
C	-0.30301800	3.29718200	-0.64505500	H	-1.94062800	0.44585900	3.32676900
H	0.56628100	2.76297500	-1.05637200	C	-3.93230600	-0.27088300	1.61349000
H	-1.04705500	3.43414900	-1.44519600	H	-4.51707200	-0.50589600	0.70973900
H	0.04010700	4.30744000	-0.34809700	H	-4.37209300	-0.85976400	2.44312200
C	-2.04370500	3.46817200	1.14810400	H	-4.08123400	0.79212600	1.85317000
H	-2.90064200	3.53899500	0.46103100	C	-0.10078900	2.13289600	1.98758500
H	-2.40767100	3.12779400	2.13104700	H	0.19004700	3.17640700	2.21888500
H	-1.65227800	4.49486000	1.29430700	H	-0.42672500	1.67148500	2.93047600
C	-3.44582200	1.99000100	-1.54956100	H	0.79715200	1.60630700	1.64187400
H	-2.93426600	2.96231600	-1.62145200	C	-0.74017800	3.14469700	-0.19271300
H	-4.04491000	1.87346600	-2.47445500	H	0.18487400	2.79951000	-0.67843600
H	-4.15568000	2.02842100	-0.70648200	H	-1.49921900	3.33912000	-0.96662600
C	-1.51064700	0.79564800	-2.66464700	H	-0.51310700	4.11710100	0.28676100
H	-0.85284900	1.67968400	-2.68347500	C	-2.47739200	2.77478600	1.58045100
H	-0.88314400	-0.11461700	-2.66963600	H	-3.35138800	2.83573400	0.91397900
H	-2.10454400	0.79942300	-3.59997000	H	-2.76886900	2.23431400	2.49564600
C	-3.33794700	-0.49942300	-1.58480400	H	-2.22777200	3.80946900	1.89000800
H	-4.14891800	-0.54985500	-0.84024800	C	-3.66863800	1.63395600	-1.37968000
H	-3.81877800	-0.48066700	-2.58318500	H	-3.27727900	2.65689100	-1.26829100
H	-2.73218200	-1.41737600	-1.52560600	H	-4.24103400	1.61015000	-2.32815100
6c				H	-4.38493500	1.44183200	-0.56367800
Pd	0.67105500	-0.84173600	-0.48525900	C	-1.59883200	0.87714400	-2.62802200
C	1.92026100	0.74238200	-0.41494600	H	-1.03781500	1.81285600	-2.47436300
C	2.02508900	1.55641300	-1.56380400	H	-0.87966200	0.05177100	-2.78098900
C	2.84869700	0.95099900	0.62223200	H	-2.18583400	0.98796700	-3.56124700
C	2.98482300	2.58594600	-1.64219100	C	-3.26887800	-0.78290800	-1.83048600
H	1.34731000	1.39577300	-2.41146100	H	-4.08111400	-1.04487600	-1.13273100
C	3.79615400	1.99164900	0.56865100	H	-3.73322500	-0.64946000	-2.82792500
C	3.85683900	2.81931600	-0.56468800	H	-2.56135000	-1.62401600	-1.89965200
H	3.04004100	3.20661900	-2.54462700	6d			
H	4.47669600	2.13045800	1.41671100	Pd	-0.10237900	-0.25960800	-0.22021000
H	4.59386100	3.62922300	-0.61204800	C	1.89386700	0.01221400	-0.49891600
P	-1.44880800	0.36668100	0.14018300	C	2.32266300	0.90250300	-1.50787000
C	-2.56783300	0.54936000	-1.46310000	C	2.87896100	-0.60732900	0.29545500
C	-2.44335900	-0.67993600	1.47697300	C	3.68759400	1.20526500	-1.68400300
C	-1.21717000	2.16877800	0.91244800	H	1.58250400	1.37977900	-2.16406800
Cl	-0.47193300	-2.78299300	-1.47860700	C	4.24494300	-0.29331900	0.14743700
C	2.34010500	-2.05522800	0.54210500	C	4.64729400	0.62814400	-0.83299700
C	2.50295500	-2.05405200	-0.85317400	H	3.99365500	1.89718100	-2.47781200
H	3.26482800	-1.41287600	-1.31276700	H	4.97338900	-0.79119600	0.79774000
H	2.10788100	-2.87300300	-1.46338800	H	5.70940600	0.87359300	-0.94774400
O	2.84379000	0.12922100	1.74981700	P	-0.14389600	1.87732300	0.73354800
C	3.26947200	-1.21371000	1.43689700	C	-0.74261600	3.21408300	-0.39483800
H	4.27722500	-1.16170100	0.97623200	C	-1.26899300	1.99062000	2.19743900
H	3.35774800	-1.70626300	2.42002300	C	1.43837500	2.56075100	1.40861000
C	1.64199100	-3.19118900	1.26433400	I	-2.87318300	-0.16147900	-0.46759400
H	1.06718800	-2.82192700	2.13379700	C	0.32680800	-2.42154800	0.38567200
H	0.97130500	-3.75400000	0.59736900	C	-0.18289300	-2.39606400	-0.91843700
H	2.41319200	-3.88394300	1.66320800	H	0.50272200	-2.48271100	-1.77143900
C	-2.39439300	-2.18547900	1.12973900	H	-1.24521400	-2.56739300	-1.11886600
H	-1.36423100	-2.57281100	1.12639500	O	2.54725400	-1.58652800	1.22937300
H	-2.96806700	-2.72839600	1.90750500	C	1.81643600	-2.66786200	0.60262100

H	2.31134300	-2.92120900	-0.35424500
H	1.93231900	-3.51967900	1.29777500
C	-0.54925200	-2.65443100	1.60230700
H	-0.17099300	-2.09482100	2.47659300
H	-1.59794800	-2.37174100	1.42094900
H	-0.51483800	-3.73205900	1.86756100
H	-2.28804200	1.70173000	1.89375200
H	-1.74297200	2.93867300	-0.76827800
H	-0.05780000	3.30931600	-1.25477100
H	-1.26686400	3.02016800	2.60008500
H	-0.79218500	4.18200200	0.13626900
H	-0.92435700	1.29393100	2.98021100
H	1.84863700	1.86408200	2.15848200
H	2.18267500	2.67300700	0.60412700
H	1.25399200	3.54192800	1.88274000

7a-ts

Pd	-0.41018000	-0.80031500	0.08287200
C	-2.27543400	0.15591500	-0.38518000
C	-2.35944700	0.20824500	-1.80032300
C	-3.19887300	0.93010500	0.34995400
C	-3.20126700	1.13465800	-2.43765400
H	-1.72948500	-0.45510500	-2.40659200
C	-4.03415800	1.88120700	-0.27133700
C	-4.01563700	1.99350700	-1.66745400
H	-3.22138300	1.18801100	-3.53224200
H	-4.71972500	2.47338700	0.34515300
H	-4.67094600	2.72022500	-2.16109700
P	1.19398000	1.16697600	0.06923000
C	2.41865800	0.72541400	1.55821300
C	2.26574500	1.46342900	-1.54040000
C	0.35098100	2.89394600	0.51681100
I	1.28509800	-2.91380400	-0.47114100
C	-2.64477600	-1.53289300	0.88060300
C	-1.53088100	-2.42390300	0.94156000
H	-0.96125100	-2.51657200	1.87671800
H	-1.56397500	-3.33985800	0.34146400
O	-3.41847500	0.66307800	1.68255500
C	-2.85595400	-0.61056900	2.07641500
H	-1.89624900	-0.44588700	2.60112500
H	-3.58767800	-1.04452600	2.78579700
C	-3.88737300	-2.02565000	0.14906800
H	-4.62491500	-1.22687200	-0.02891800
H	-3.62114200	-2.48063500	-0.81891400
H	-4.36150000	-2.81110100	0.77290100
C	-0.75349200	3.22502700	-0.52233400
H	-1.29680400	2.33973000	-0.87392500
H	-1.49058700	3.90294700	-0.05101900
H	-0.35034300	3.75022600	-1.40094600
C	-0.34141900	2.72077800	1.89081200
H	0.37423200	2.61188900	2.72129400
H	-0.94764200	3.62391700	2.09953700
H	-1.02718700	1.85691300	1.89859100
C	1.27585600	4.13497700	0.57640500
H	1.69775200	4.38261700	-0.41191000
H	0.65692900	5.00284500	0.88254200
H	2.10174100	4.05155200	1.29680900

C	1.58047600	-0.01490600	2.63319600
H	2.24789800	-0.30407100	3.46965300
H	0.76749200	0.59972500	3.05179800
H	1.14186600	-0.93936800	2.21512000
C	3.12953500	1.92681400	2.22513000
H	2.43919000	2.60334900	2.75436700
H	3.82787000	1.52712600	2.98737700
H	3.73148200	2.51890000	1.51557700
C	3.52153800	-0.26247100	1.10657800
H	3.11244600	-1.15806500	0.61265500
H	4.27210700	0.20337800	0.44814700
H	4.05851800	-0.60549900	2.01341200
C	2.65453400	0.09357800	-2.14377200
H	3.26501800	-0.52758100	-1.47391600
H	1.76641200	-0.49981200	-2.41588300
H	3.24298900	0.27736300	-3.06520500
C	3.55108700	2.29942200	-1.32524100
H	4.28747800	1.79302700	-0.68129400
H	4.03554400	2.45060900	-2.31104600
H	3.35305800	3.29691200	-0.90290000
C	1.39955400	2.17636000	-2.60878200
H	1.28048900	3.25304900	-2.40853500
H	1.91224700	2.08367400	-3.58623500
H	0.39869900	1.72245100	-2.71360100

7b-ts

Pd	-0.51104600	-0.91879400	-0.06625400
C	-2.17905400	0.39188600	-0.35972100
C	-2.27791800	0.63636300	-1.75501800
C	-2.92741300	1.22961900	0.49790900
C	-2.93727000	1.77560900	-2.24309600
H	-1.79483900	-0.05159300	-2.46030800
C	-3.57370500	2.39183400	0.02899800
C	-3.55780400	2.67051300	-1.34362900
H	-2.96532200	1.96872000	-3.32161000
H	-4.12211000	3.02160200	0.73835400
H	-4.06938000	3.56346000	-1.72062600
P	1.42961200	0.68559000	0.06933500
C	2.56942900	-0.08751900	1.48751900
C	2.51692500	0.86428700	-1.55094200
C	0.96992200	2.51378400	0.65597200
Br	0.79503800	-3.08481300	-0.61991300
C	-2.86033700	-1.33100900	0.67603000
C	-1.92315200	-2.40126300	0.56771100
H	-1.37211100	-2.73195800	1.45852100
H	-2.10299400	-3.18841800	-0.17342000
O	-3.17931800	0.83816300	1.79266400
C	-2.87363600	-0.56198600	1.99494200
H	-1.89260400	-0.65657500	2.49656200
H	-3.66745200	-0.93990100	2.66822700
C	-4.18619300	-1.47918400	-0.06000200
H	-4.75879700	-0.53881600	-0.10389700
H	-4.02936100	-1.84386100	-1.08814600
H	-4.79170700	-2.23655100	0.47908000
C	-0.08451600	3.12637200	-0.30073000
H	-0.88598900	2.42406700	-0.55437300
H	-0.54942700	3.99443500	0.20632600

H	0.35624900	3.50022000	-1.23595700
C	0.30071200	2.40325000	2.04929900
H	1.00448600	2.10989500	2.84450900
H	-0.10482200	3.39655400	2.32477000
H	-0.54478900	1.69391200	2.04657700
C	2.13043100	3.53718200	0.73316800
H	2.54657300	3.76403300	-0.26249800
H	1.71777100	4.48797200	1.12779000
H	2.95590500	3.23941900	1.39452600
C	1.62477200	-0.71681900	2.54493900
H	2.24198500	-1.14025500	3.36253100
H	0.92670400	0.00702800	2.99461600
H	1.03863700	-1.54149500	2.10381400
C	3.51447500	0.91120300	2.19818500
H	2.97958500	1.69204100	2.76111800
H	4.11823200	0.34234800	2.93304800
H	4.22146200	1.39654900	1.50469000
C	3.45281800	-1.24292700	0.95209100
H	2.86419600	-2.01523000	0.43306200
H	4.26378200	-0.89759300	0.29061800
H	3.93515800	-1.72649200	1.82518700
C	2.59941200	-0.51460400	-2.24656200
H	3.07889000	-1.29072000	-1.63455600
H	1.60136400	-0.89322800	-2.52086900
H	3.19346300	-0.39783000	-3.17514700
C	3.95089700	1.39846200	-1.31791700
H	4.57380100	0.70467400	-0.73246300
H	4.44196200	1.51865100	-2.30455500
H	3.97236700	2.38124000	-0.82096400
C	1.80963900	1.81437400	-2.54946800
H	1.91246700	2.87467900	-2.26785000
H	2.29105400	1.69398900	-3.53981300
H	0.73715700	1.58229700	-2.67164300

7c-ts

Pd	-0.54135700	-1.07324900	-0.24605100
C	-2.11652600	0.38209800	-0.32225500
C	-2.19396500	0.86807400	-1.65573500
C	-2.80544400	1.11741900	0.67025800
C	-2.76502400	2.11849500	-1.93785800
H	-1.76073100	0.27776500	-2.47311400
C	-3.36118900	2.38758000	0.41206200
C	-3.32076200	2.89168700	-0.89419500
H	-2.77506500	2.49354600	-2.96774100
H	-3.86418300	2.92674900	1.22248700
H	-3.76410800	3.87040100	-1.11073500
P	1.52331800	0.33909200	0.05626900
C	2.64261400	-0.68551300	1.33027100
C	2.55666800	0.61177500	-1.58282800
C	1.24361700	2.10937900	0.87190900
Cl	0.61632100	-3.08067000	-0.91799400
C	-2.93667600	-1.42293100	0.39207000
C	-2.07430400	-2.52093900	0.09733500
H	-1.57158700	-3.04975500	0.91831100
H	-2.28404300	-3.14120300	-0.78230700
O	-3.09665300	0.52863500	1.87899000
C	-2.90446500	-0.90488100	1.82898100

H	-1.93716700	-1.16601800	2.29682500
H	-3.73107700	-1.33293200	2.42867900
C	-4.26399300	-1.34370000	-0.35118800
H	-4.76976700	-0.37322100	-0.22157800
H	-4.12530500	-1.52747400	-1.42892900
H	-4.92415100	-2.14196300	0.04618800
C	0.19452600	2.91323400	0.06434900
H	-0.70564400	2.32820000	-0.15021000
H	-0.11196800	3.78689300	0.67274000
H	0.58897000	3.30382000	-0.88391800
C	0.62743300	1.87904400	2.27538300
H	1.33537900	1.43768900	2.99404200
H	0.31315600	2.85819300	2.68714500
H	-0.27059800	1.23846700	2.22738800
C	2.48509500	3.02816200	0.99882800
H	2.84313700	3.36764400	0.01223400
H	2.17931400	3.93810800	1.55420900
H	3.33141200	2.58297800	1.54016500
C	1.68413700	-1.36488700	2.34358000
H	2.28997500	-1.95016500	3.06443200
H	1.07826400	-0.65036800	2.92347400
H	1.00578200	-2.06569000	1.82632200
C	3.69037100	0.14925100	2.10487400
H	3.24754400	0.89460000	2.78451400
H	4.28018400	-0.54707600	2.73369100
H	4.40123500	0.66117300	1.43439900
C	3.41315700	-1.83146900	0.62763900
H	2.74491800	-2.49319600	0.05559900
H	4.22281500	-1.47031500	-0.02682400
H	3.89159800	-2.44262100	1.41900100
C	2.50839600	-0.68706300	-2.42301600
H	2.95623700	-1.55360300	-1.91813000
H	1.47465500	-0.96729000	-2.68372500
H	3.06938300	-0.50994700	-3.36262900
C	4.03463700	1.01736100	-1.36773700
H	4.62862800	0.22130300	-0.89184400
H	4.49070900	1.21163700	-2.35943500
H	4.14823100	1.93537100	-0.76977600
C	1.87444700	1.70889800	-2.43730800
H	2.06898300	2.72508900	-2.05705000
H	2.29379500	1.66071500	-3.46153000
H	0.78300900	1.56146500	-2.51661900

7d-ts

Pd	0.25417500	-0.29394100	-0.04379200
C	-1.87457400	-0.21456300	-0.31676100
C	-2.16309900	0.37777900	-1.57358100
C	-2.89281600	-0.18731800	0.66296500
C	-3.34008200	1.12033100	-1.76569600
H	-1.43843200	0.29196600	-2.39276100
C	-4.06430500	0.58061100	0.50209600
C	-4.27197200	1.24965700	-0.71210100
H	-3.53012500	1.60135400	-2.73224300
H	-4.81437200	0.59106600	1.30057000
H	-5.18670000	1.83608500	-0.85628700
P	0.47805300	2.01618000	0.30916800
C	1.51941900	2.44342500	1.78160600

C	1.30399500	2.94030800	-1.06859900
C	-1.05056400	3.02047800	0.61441500
I	2.93444400	-0.59182000	-0.18953300
C	-1.32011700	-2.15579600	0.11253900
C	0.08101600	-2.42148800	-0.08381300
H	0.70042600	-2.68210800	0.78489900
H	0.40227600	-2.88093700	-1.02747700
O	-2.82283300	-1.04741200	1.73046200
C	-1.75246100	-2.00964000	1.57503800
H	-0.88833200	-1.69049000	2.18734000
H	-2.15274100	-2.96203000	1.97189600
C	-2.30342400	-2.83638200	-0.83718400
H	-3.33176700	-2.45441600	-0.72845000
H	-1.99066500	-2.70862600	-1.88654400
H	-2.30094300	-3.92241500	-0.61255400
H	1.04274600	2.04842400	2.69521900
H	2.50842700	1.96803400	1.67303400
H	1.63619800	3.53867300	1.87741400
H	1.45531700	4.00203500	-0.80076500
H	2.27729800	2.46580200	-1.27878100
H	0.68350900	2.88179300	-1.97943700
H	-1.56164200	2.65210000	1.51989200
H	-1.74709700	2.91657500	-0.23387000
H	-0.79521300	4.08701800	0.75182800

8a

Pd	0.19726400	-0.50700100	0.00267900
C	-3.31587500	1.17324100	0.40327900
C	-3.96545100	0.76325100	1.57183700
C	-4.02560000	1.21022100	-0.81019900
C	-5.31982500	0.37559200	1.50284400
H	-3.43005600	0.72595300	2.52896900
C	-5.37212700	0.84276700	-0.90720000
C	-6.00923100	0.41879700	0.27581800
H	-5.83502500	0.03194900	2.40660600
H	-5.89672000	0.87191300	-1.86753600
H	-7.06020800	0.10943500	0.23406600
P	2.41046400	0.21911600	0.03004600
C	2.88793600	1.64655300	-1.21092400
C	3.11870200	0.65779900	1.80020800
C	3.23711600	-1.45172500	-0.58052600
I	-1.82448800	-2.19437500	-0.07814100
C	-1.92761800	1.76186000	0.16286900
C	-0.75841800	1.08562100	0.91187700
H	0.02470600	1.82532100	1.13513500
H	-1.10143900	0.62368200	1.85551400
O	-3.26640200	1.67048800	-1.86491400
C	-1.88306600	1.68296400	-1.39826700
H	-1.40113300	0.74073000	-1.72282800
H	-1.39267100	2.54871100	-1.87466400
C	-1.95603500	3.25902500	0.61290600
H	-2.78390100	3.79270100	0.11216100
H	-2.11113000	3.33882500	1.70401500
H	-1.00691200	3.76645800	0.35524700
C	2.34595800	-2.00430900	-1.72640600
H	2.31998200	-1.36002200	-2.61582700
H	2.73971800	-2.99279400	-2.03612900

H	1.29688400	-2.17263200	-1.40058400
C	3.17573700	-2.50982500	0.54959800
H	3.47384600	-3.48683800	0.12186400
H	3.86432500	-2.29880300	1.38357100
H	2.15203000	-2.62503600	0.94921600
C	4.69280000	-1.33325400	-1.08242900
H	5.05175200	-2.34358700	-1.36326800
H	4.78152400	-0.70070600	-1.98127600
H	5.38133600	-0.94237200	-0.31557400
C	2.64110100	1.17159000	-2.66414400
H	2.73234500	2.04798400	-3.33537400
H	3.37777000	0.42646100	-3.00508600
H	1.62587800	0.75702300	-2.79513400
C	1.90421700	2.82045400	-0.97663500
H	1.98766900	3.27335400	0.02199900
H	2.11628900	3.61488700	-1.71901500
H	0.86240300	2.49117200	-1.12148100
C	4.34176700	2.16281300	-1.09732600
H	4.54512400	2.65517900	-0.13206900
H	5.09007300	1.36662600	-1.24238800
H	4.51035500	2.92159800	-1.88720600
C	4.64079700	0.42552200	1.95783800
H	5.23938500	1.01181400	1.24094500
H	4.94111400	0.74501400	2.97561500
H	4.92587600	-0.63449800	1.86027900
C	2.35493100	-0.20382800	2.83940700
H	2.70293000	0.07785400	3.85315800
H	1.26658400	-0.02870600	2.78934200
H	2.52510500	-1.28338800	2.71894700
C	2.82622600	2.13588400	2.16361700
H	3.40324900	2.85476900	1.56019600
H	1.75462200	2.38571600	2.08709900
H	3.12003400	2.29142400	3.22012300

8b

Pd	0.12009200	-0.65102100	-0.00342900
C	-3.48021900	0.81810200	0.40736400
C	-4.04587500	0.42525400	1.62376400
C	-4.24541600	0.74986000	-0.77042800
C	-5.37357000	-0.05094000	1.63955000
H	-3.46644000	0.47102900	2.55459900
C	-5.56817900	0.29452900	-0.78384000
C	-6.12072000	-0.11084800	0.44748300
H	-5.82290200	-0.38138300	2.58260900
H	-6.13749400	0.24354400	-1.71744400
H	-7.15033800	-0.48678200	0.47205700
P	2.28091000	0.16962500	0.04521100
C	2.69479000	1.41579000	-1.39738700
C	2.92102100	0.91977300	1.73375000
C	3.21101300	-1.52613500	-0.28085100
Br	-1.77021400	-2.24041800	-0.15344500
C	-2.14844000	1.48569600	0.07017700
C	-0.90479200	0.94512300	0.80797600
H	-0.16950900	1.75158100	0.94506400
H	-1.17742300	0.53230200	1.79724500
O	-3.56613700	1.20361500	-1.88090900
C	-2.16531900	1.31691100	-1.48354900

H	-1.65071000	0.38350900	-1.77835000	C	2.73510700	0.82204300	1.76999900
H	-1.74660800	2.17851900	-2.03060300	C	3.13390900	-1.57406800	-0.28181300
C	-2.26619400	3.00259300	0.43181900	C	-2.35132000	1.23987100	0.08100000
H	-3.15061000	3.44498300	-0.06100100	C	-1.04994200	0.76688500	0.76043900
H	-2.38092700	3.13894600	1.52226600	H	-0.35335100	1.61220900	0.85976400
H	-1.36782500	3.55774900	0.10029800	H	-1.26059500	0.35073600	1.76378200
C	2.37379600	-2.30493300	-1.33281300	O	-3.79656600	0.93928900	-1.84565800
H	2.32209600	-1.81169400	-2.31316100	C	-2.39735600	1.14323800	-1.47734400
H	2.83264800	-3.30275000	-1.48142100	H	-1.82263200	0.26765900	-1.83016700
H	1.33321000	-2.49266900	-0.98863200	H	-2.06090500	2.06046200	-1.99006900
C	3.18320100	-2.39601600	1.00175200	C	-2.56745500	2.72637100	0.51836900
H	3.54787000	-3.40768700	0.73718900	H	-3.49602300	3.12428600	0.07072400
H	3.83832000	-2.01713000	1.80221700	H	-2.65938900	2.80508500	1.61672900
H	2.15856300	-2.50795700	1.39892000	H	-1.72207000	3.36095500	0.18968800
C	4.66866100	-1.40590900	-0.77773100	C	2.33737500	-2.35292700	-1.36532500
H	5.08788500	-2.42585100	-0.88904800	H	2.29255300	-1.84127000	-2.33646400
H	4.74157600	-0.91884700	-1.76430600	H	2.82419800	-3.33575400	-1.52454700
H	5.31740000	-0.85890100	-0.07397900	H	1.29522800	-2.57442200	-1.04631800
C	2.49592700	0.70120300	-2.75694400	C	3.10493000	-2.46989800	0.98266700
H	2.53842700	1.46300900	-3.55972800	H	3.49797200	-3.46743200	0.70531600
H	3.28219700	-0.04022700	-2.97292200	H	3.73739400	-2.09139500	1.80151200
H	1.51004200	0.20676600	-2.81964200	H	2.07671300	-2.61388800	1.35971300
C	1.64207000	2.55282400	-1.35664600	C	4.59694300	-1.40534900	-0.74656300
H	1.69017800	3.16620300	-0.44479700	H	5.04641300	-2.41085900	-0.87056300
H	1.81856100	3.22655400	-2.21806300	H	4.67629900	-0.89540500	-1.72096000
H	0.62076600	2.14691100	-1.44806300	H	5.21557700	-0.85589200	-0.01804600
C	4.11499500	2.02622300	-1.35860600	C	2.42093000	0.68267100	-2.73284700
H	4.28180100	2.66048100	-0.47257900	H	2.46592400	1.46180600	-3.51873300
H	4.90953800	1.26276300	-1.39038800	H	3.23082500	-0.03471000	-2.94267200
H	4.24619600	2.67396400	-2.24816200	H	1.44921000	0.16666500	-2.83253500
C	4.44864200	0.78946000	1.94462900	C	1.47526400	2.47659000	-1.31997200
H	5.03230800	1.29986100	1.16063000	H	1.47451000	3.06854500	-0.39278000
H	4.71253900	1.26071500	2.91228500	H	1.65664800	3.17717800	-2.15873100
H	4.78327300	-0.25821600	1.99522500	H	0.47117400	2.04023600	-1.45419300
C	2.17454700	0.18940200	2.87984300	C	3.96409500	2.02642300	-1.26913200
H	2.45449400	0.66185600	3.84203200	H	4.09194500	2.64438100	-0.36521900
H	1.08075000	0.26759600	2.76214500	H	4.78221900	1.28795800	-1.30065800
H	2.42607700	-0.87867200	2.95015500	H	4.09524100	2.69865000	-2.14035700
C	2.55531200	2.42109600	1.85645200	C	4.26119800	0.73379900	2.01220700
H	3.10337200	3.06011000	1.14589400	H	4.84713200	1.26181200	1.24189100
H	1.47471600	2.60646700	1.73976000	H	4.49139400	1.21007500	2.98598000
H	2.83320400	2.75731000	2.87454700	H	4.62437700	-0.30422400	2.07013600
8c				C	1.98904500	0.04836900	2.88747900
Pd	0.01869800	-0.77898900	-0.08567400	H	2.24283000	0.50557000	3.86421500
C	-3.61971500	0.46150400	0.41985700	H	0.89565900	0.10354400	2.75564100
C	-4.12064100	-0.02359000	1.63083200	H	2.26575900	-1.01462300	2.93772400
C	-4.40973900	0.38808500	-0.74087600	C	2.32219500	2.30979500	1.91264300
C	-5.40971500	-0.59625100	1.65867900	H	2.86659900	2.97728900	1.22574900
H	-3.51952300	0.02498400	2.54778300	H	1.23948600	2.46619300	1.77529300
C	-5.69601500	-0.16243300	-0.74158200	H	2.56815800	2.63487700	2.94258700
C	-6.18349100	-0.65915000	0.48392700	Cl	-1.74242100	-2.25286000	-0.37450800
H	-5.80765800	-0.99832400	2.59704500	8d			
H	-6.28663800	-0.21474500	-1.66180900	Pd	-1.16093100	0.46125000	0.04708200
H	-7.18256900	-1.10957600	0.51706200	C	2.21046100	-1.14212400	0.39667000
P	2.15210100	0.08873800	0.05473200	C	2.95781400	-0.40459400	1.32021400
C	2.56472500	1.37437100	-1.35457700	C	2.78128100	-1.48886600	-0.84075500

C	4.26990000	-0.01312200	0.98111300	H	3.51900500	4.59158300	-0.27648900
H	2.53207200	-0.12090300	2.29061600	H	5.82810800	4.14297700	-1.10827400
C	4.08272100	-1.12357300	-1.20062700	C	2.31417100	-0.09842300	2.05894300
C	4.82083700	-0.37386700	-0.26315500	H	1.36221900	0.45802700	1.96683600
H	4.85872000	0.58317500	1.68657400	H	2.05886800	-1.12578800	2.37467900
H	4.49872900	-1.40320500	-2.17376900	H	2.93642500	0.37249300	2.84032300
H	5.84002400	-0.05892300	-0.51572100	C	-2.33077000	-0.22620000	2.75044900
P	-3.10860200	-0.67721400	-0.09235200	H	-2.76448500	-0.75012100	3.62599800
C	-3.15019100	-2.37115400	-0.84819400	H	-1.41521000	-0.76322000	2.44053200
C	-4.01872200	-0.92617700	1.50368800	H	-2.03890000	0.78159000	3.08178600
C	-4.32845300	0.26441300	-1.12520100	C	-4.63814200	0.54180100	2.07290400
I	0.54648700	2.43723500	-0.08272400	H	-5.42638000	0.58329500	1.30292400
C	0.85022700	-1.82856500	0.49911600	H	-5.06662100	0.01905300	2.95208200
C	-0.27932800	-1.03217100	1.17388100	H	-4.41609600	1.57375100	2.39341500
H	-1.05646400	-1.71855200	1.55460800	C	-3.75048800	-1.70448900	1.37068200
H	0.09636500	-0.42793300	2.01989600	H	-2.88618600	-2.28352000	0.99914400
O	1.93910800	-2.24935500	-1.62862300	H	-4.06078700	-2.14577600	2.33861900
C	0.62294300	-2.16203100	-1.00973000	H	-4.59386400	-1.83267700	0.67272000
H	0.06535900	-1.33844700	-1.49886600	C	-3.28326600	-1.49383700	-1.92042600
H	0.11572700	-3.12577700	-1.18578700	H	-3.62527500	-2.20893000	-1.15815300
C	1.03253400	-3.14943300	1.31591700	H	-3.80271700	-1.74332100	-2.86776100
H	1.83522600	-3.76365900	0.86984600	H	-2.19837000	-1.64831800	-2.06468700
H	1.31325200	-2.92916200	2.36125100	C	-5.11589600	0.16130200	-1.39170100
H	0.09916100	-3.74482700	1.32189300	H	-5.61375900	-0.08283700	-2.35185400
H	-4.47665300	1.27056800	-0.69789800	H	-5.53593500	-0.51858900	-0.63170700
H	-3.93646200	0.37956100	-2.14987100	H	-5.40134900	1.19260800	-1.12572400
H	-5.30112500	-0.25991700	-1.16516700	C	-3.12384300	0.81448700	-2.78292300
H	-4.17994900	0.05200500	1.98701500	H	-2.02937500	0.75428000	-2.92001900
H	-4.99459100	-1.41731800	1.33613100	H	-3.59847600	0.39431500	-3.69182000
H	-3.41612000	-1.54958700	2.18626000	H	-3.41995900	1.87498500	-2.72738000
H	-4.18084200	-2.77027100	-0.87520000	C	-1.39339800	2.93734400	-0.90659200
H	-2.51816600	-3.05872300	-0.26091700	H	-1.69215500	2.78983200	-1.95498000
H	-2.75118900	-2.32841700	-1.87566200	H	-1.25019600	4.02583600	-0.75168400
9a-ts				H	-0.42266100	2.42987000	-0.75944400
Pd	-0.41507000	-0.44355300	-0.18393200	C	-1.90992900	2.82587200	1.50827800
C	2.14192200	-0.47887600	-0.46542700	H	-1.69840100	3.91375700	1.50490900
P	-2.48952100	0.46226500	-0.00729600	H	-2.63646900	2.64014900	2.31582900
C	-3.58946300	-0.01541900	-1.56124300	H	-0.96776800	2.30210500	1.75079500
C	-3.37711700	-0.21989300	1.60440500	C	-3.78338500	3.15064300	-0.13262800
C	-2.44262300	2.42233300	0.11243900	H	-3.63554100	4.23885300	0.02069400
I	1.24686200	-2.67878300	-0.24975400	H	-4.14922600	3.01977900	-1.16420800
H	1.35020200	0.31090400	-0.63290800	H	-4.57943400	2.82710800	0.55778700
H	2.67073900	-0.64338900	-1.41330800	9b-ts			
C	3.05671500	-0.11660600	0.71384500	Pd	-0.31221000	-0.41934100	-0.14909300
C	3.66415300	1.22858600	0.29690000	C	2.12512600	-0.59652600	-0.41932300
C	4.34980700	-0.98529500	0.75636600	P	-2.44240500	0.35696100	-0.01881100
C	4.97229800	0.99516000	-0.17120900	C	-3.52617600	-0.46768500	-1.43056100
H	4.74601200	-1.04344400	1.78827300	C	-3.21662100	-0.12829000	1.71700200
H	4.21260100	-2.00209300	0.35662000	C	-2.57674200	2.30455300	-0.21834500
O	5.35968900	-0.31849200	-0.06662000	Br	1.19333600	-2.63001300	-0.30372900
C	3.12558700	2.52144900	0.25506200	H	1.42305200	0.30559000	-0.40746100
C	5.77471600	2.02073600	-0.68779500	H	2.53680200	-0.71260000	-1.42963200
H	6.79036600	1.81699700	-1.04137400	C	3.17932900	-0.46967100	0.68668000
C	3.91903500	3.57225200	-0.24790100	C	3.90952600	0.83300500	0.33326600
C	5.22323000	3.31644500	-0.71758400	C	4.35302800	-1.48142700	0.51823600
H	2.10601200	2.71455200	0.60899500	C	5.13026000	0.49859800	-0.28595300

H	4.83128300	-1.68542600	1.49537400	C	-3.57960000	-1.27111100	0.24917400
H	4.05565000	-2.42966100	0.04619500	C	-2.55512800	1.45974400	1.49483800
O	5.35821400	-0.85409700	-0.34141200	Cl	1.10728500	-2.63496400	-0.42374200
C	3.53438000	2.17670500	0.46350800	H	1.50550700	0.26081100	-0.42635100
C	6.00463500	1.47226500	-0.78590300	H	2.47408100	-0.86243600	-1.49550800
H	6.95041400	1.18970500	-1.25888500	C	3.16065100	-0.76749400	0.61733400
C	4.40407400	3.17471900	-0.02038300	C	4.00891800	0.47963400	0.33647200
C	5.61845100	2.81898400	-0.64177600	C	4.23154400	-1.87395200	0.37237600
H	2.58220300	2.44856000	0.93454600	C	5.18984400	0.07176100	-0.31468200
H	4.13305000	4.23096300	0.08290700	H	4.69305500	-2.18577000	1.32886800
H	6.28363400	3.60564500	-1.01643800	H	3.84149700	-2.75529000	-0.15686700
C	2.56775700	-0.50278400	2.09630800	O	5.28973800	-1.28992800	-0.45543900
H	1.71366600	0.19532600	2.16711800	C	3.76288100	1.84206000	0.55166500
H	2.18783900	-1.51254200	2.33066200	C	6.14876700	0.98885200	-0.76500000
H	3.32254400	-0.21981100	2.85106600	H	7.06107900	0.64876300	-1.26512000
C	-2.13809600	0.14754900	2.79847000	C	4.71891700	2.78304300	0.11863500
H	-2.48168600	-0.27676000	3.76328500	C	5.89104200	2.35455900	-0.53685700
H	-1.18041900	-0.33356900	2.52448700	H	2.84398800	2.17350800	1.05008800
H	-1.94515200	1.21869400	2.95953100	H	4.54827300	3.85163000	0.28865500
C	-4.53054000	0.58366500	2.11482400	H	6.62459600	3.09728000	-0.87154000
H	-5.34706800	0.41604000	1.39232800	C	2.56042600	-0.83121800	2.03121200
H	-4.87152000	0.18458700	3.09175300	H	1.79818700	-0.04301500	2.16824600
H	-4.40366900	1.67177200	2.24307900	H	2.06273300	-1.80253100	2.19597400
C	-3.45854200	-1.65805900	1.74441800	H	3.34986500	-0.69541300	2.79157800
H	-2.55686500	-2.21817100	1.43932900	C	-2.91821800	-2.25647900	1.24856200
H	-3.70459400	-1.95614600	2.78298500	H	-3.53780000	-3.17411800	1.30251100
H	-4.30370500	-1.97156900	1.11027300	H	-1.90611200	-2.54256100	0.90982100
C	-3.09375000	-1.95260400	-1.55025700	H	-2.83507200	-1.85649100	2.27011300
H	-3.35399100	-2.55642400	-0.66873300	C	-4.99829800	-0.91137600	0.74721600
H	-3.60648900	-2.40187800	-2.42459800	H	-5.51523100	-0.19682800	0.08522700
H	-2.00237700	-2.03346200	-1.70429400	H	-5.61251900	-1.83391200	0.77955500
C	-5.05768300	-0.39822300	-1.23660900	H	-4.99792300	-0.49534000	1.76893100
H	-5.55235500	-0.84589800	-2.12226500	C	-3.70788500	-2.05140300	-1.08284700
H	-5.39789300	-0.97072600	-0.35743100	H	-2.71911900	-2.30600400	-1.50439800
H	-5.43184500	0.63422100	-1.14016500	H	-4.23843000	-3.00273800	-0.88076800
C	-3.16439400	0.18389900	-2.78779600	H	-4.29384200	-1.51114800	-1.84421100
H	-2.07212800	0.19622000	-2.95352300	C	-2.30630300	0.37371000	-2.85509200
H	-3.61868500	-0.42021500	-3.59799800	H	-2.81231600	-0.58872300	-3.02148000
H	-3.55374000	1.20982700	-2.89437800	H	-2.42920600	0.97718000	-3.77682600
C	-1.59580400	2.73551700	-1.33980300	H	-1.22865600	0.16891900	-2.71079500
H	-1.88641600	2.37574200	-2.33778700	C	-4.39377000	1.39706200	-1.85892700
H	-1.56585700	3.84323900	-1.38030200	H	-4.54893500	1.96168900	-2.80037700
H	-0.57546400	2.36556800	-1.13150700	H	-4.95126600	0.45057500	-1.95558600
C	-2.05815500	2.97925200	1.07425000	H	-4.85220500	1.98397700	-1.04516500
H	-1.95213800	4.06601100	0.88540800	C	-2.16514400	2.54695100	-1.68511400
H	-2.74627600	2.86366000	1.92740300	H	-1.07954700	2.44463100	-1.50680400
H	-1.06472400	2.59117300	1.36241400	H	-2.29904900	2.99106900	-2.69137200
C	-3.98499300	2.85863100	-0.53266600	H	-2.58066400	3.26369700	-0.95821200
H	-3.93925100	3.96640400	-0.55413800	C	-1.31695600	2.39379400	1.51839100
H	-4.35718500	2.53587800	-1.51935900	H	-1.27842100	3.08907600	0.66696300
H	-4.73381500	2.57608700	0.22548700	H	-1.34597600	3.00181100	2.44496200
				H	-0.38274300	1.80306400	1.51633000
				C	-2.49262900	0.64465200	2.80963000
				H	-2.40765000	1.35157500	3.65879400
				H	-3.39607700	0.03806700	2.98285500
				H	-1.60918300	-0.01824100	2.83507400
				C	-3.83754300	2.32313400	1.50309200
9c-ts							
Pd	-0.19541400	-0.53379000	-0.21313500				
C	2.08480900	-0.73618900	-0.47731800				
P	-2.35042700	0.23365700	-0.01782600				
C	-2.87804200	1.17313300	-1.65406600				

H	-3.86307900	2.92187700	2.43592100
H	-3.86831900	3.03759700	0.66324000
H	-4.75952900	1.71986900	1.47421800

9d-ts

Pd	-1.47526300	0.09067000	-0.11810800
C	1.01141500	-0.40979300	-0.42745600
P	-3.31847500	1.34195300	0.00632400
C	-4.61561500	0.99843100	-1.28621100
H	-5.50321300	1.64606300	-1.15207000
H	-4.18953000	1.16856500	-2.28957500
H	-4.92325000	-0.05919900	-1.22330900
C	-4.33451100	1.20990300	1.56353900
H	-3.72533700	1.51752400	2.43056300
H	-5.23861000	1.84618300	1.51012600
H	-4.63745700	0.16003900	1.71614300
C	-3.16366300	3.19519300	-0.14517700
H	-2.69102100	3.44714500	-1.10991800
H	-4.15121100	3.69153500	-0.08431600
H	-2.51648400	3.57856100	0.66224300
I	-0.28028200	-2.40914600	-0.22971800
H	0.38659900	0.52543500	-0.55987600
H	1.47829500	-0.64943900	-1.39165000
C	2.00304900	-0.25390100	0.73450700
C	2.84407200	0.95943900	0.31824600
C	3.10823900	-1.35264900	0.72876400
C	4.07083100	0.49099300	-0.19178200
H	3.51302400	-1.50438700	1.74771800
H	2.77063800	-2.31761800	0.31939200
O	4.20474800	-0.87387100	-0.11419600
C	2.55613900	2.33067500	0.30531600
C	5.03792600	1.35550000	-0.72085500
H	5.98646800	0.97024400	-1.10800500
C	3.51961000	3.22111800	-0.20967900
C	4.73925400	2.73191300	-0.72035200
H	1.59973100	2.70427400	0.69021400
H	3.31818500	4.29779100	-0.21688800
H	5.47785700	3.43619100	-1.12051800
C	1.30962700	-0.11608500	2.09885800
H	0.49100100	0.62611200	2.04382700
H	0.85915300	-1.07651000	2.40642000
H	2.03309600	0.20264800	2.86990900

10a

Pd	1.08559100	-0.26423900	-0.04480700
C	-2.88057100	0.10395200	-0.26100200
P	3.26739100	0.33220700	0.05769400
C	4.06725400	-0.23736100	1.75533500
C	4.28085400	-0.49059300	-1.40387400
C	3.45762800	2.27773900	-0.08940600
I	-1.26102200	-1.50133700	-0.12216100
H	-2.57385600	0.68203500	-1.14466000
H	-2.72537800	0.68654600	0.65856000
C	-4.29392700	-0.46719500	-0.37312600
C	-5.30556000	0.67749100	-0.23630400
C	-4.68581800	-1.31904100	0.88108100
C	-6.27198800	0.30400600	0.71663100

H	-4.70352700	-2.40354900	0.68674700
H	-4.00954600	-1.11145500	1.73280100
O	-6.03467400	-0.92702300	1.27876500
C	-5.43151300	1.89423400	-0.91797500
C	-7.37661200	1.11084000	1.01792800
H	-8.11625500	0.79665900	1.76128700
C	-6.53061100	2.72891500	-0.62624400
C	-7.48821800	2.33481600	0.32940400
H	-4.69212500	2.19830800	-1.66902800
H	-6.63901800	3.68746100	-1.14542400
H	-8.33801500	2.99241500	0.54635600
C	-4.52272700	-1.23889300	-1.69414300
H	-4.34920400	-0.58179400	-2.56560300
H	-3.83944800	-2.10455800	-1.77220100
H	-5.56208500	-1.60780400	-1.74795300
C	3.90671300	0.21676100	-2.72939000
H	4.32214000	-0.37271500	-3.57082800
H	2.81050500	0.26493400	-2.86230000
H	4.32339700	1.23464000	-2.81179600
C	3.78044400	-1.95139700	-1.55484800
H	2.67977300	-1.97596700	-1.65320400
H	4.22876400	-2.38797300	-2.47093300
H	4.05755100	-2.59818900	-0.71061300
C	5.81934400	-0.48814900	-1.25336500
H	6.16069800	-1.09672600	-0.39840800
H	6.26996600	-0.93234100	-2.16412100
H	6.23873300	0.52625500	-1.14142800
C	2.45572300	2.76290200	-1.17090700
H	2.42769300	3.87176700	-1.16121100
H	2.72779300	2.44770300	-2.19016300
H	1.43783100	2.38271600	-0.95851300
C	2.98743600	2.92551000	1.23531400
H	2.90883000	4.02029900	1.08162700
H	1.99015700	2.55451700	1.53353500
H	3.69132000	2.76561200	2.06845100
C	4.87108400	2.80389900	-0.42658600
H	5.21191100	2.48887100	-1.42702900
H	4.85269200	3.91273900	-0.42597800
H	5.62860700	2.48699900	0.30907300
C	3.03699800	0.05361000	2.88085100
H	3.39621500	-0.40974900	3.82185700
H	2.89553700	1.12727300	3.07671800
H	2.04982800	-0.37888100	2.62927000
C	5.42347900	0.40877300	2.12006100
H	5.34225500	1.49709500	2.27856700
H	5.78654200	-0.02943200	3.07211100
H	6.20212700	0.22994600	1.35936500
C	4.23813700	-1.77655400	1.72905500
H	5.05491600	-2.10975100	1.06763600
H	4.48808300	-2.12081700	2.75252400
H	3.30282500	-2.27973700	1.42413200

10b

Pd	0.63393100	-0.76201700	-0.18008500
C	-3.08777300	-1.31626700	-0.53573800
P	2.59111400	0.33231500	0.01381800
C	2.84888400	1.05229000	1.82075300

C	4.07258500	-0.89478000	-0.36565000	H	4.13646400	-0.55701700	2.65861900
C	2.70231400	1.82927600	-1.24981800	H	3.08049400	0.26196500	3.83030100
Br	-1.30869200	-2.40425500	-0.43349600	H	2.37759600	-0.91915600	2.68754000
H	-3.83788700	-2.11506700	-0.63150800				
H	-2.98305400	-0.76035700	-1.47780800	10c			
C	-3.35202400	-0.40434200	0.67204300	Pd	0.79645000	-0.64924700	-0.07322300
C	-4.67478500	0.28291200	0.31362200	C	-2.65736500	-0.25978200	-0.25819500
C	-2.40983700	0.83392600	0.69281200	P	2.87742800	0.18378300	0.05649400
C	-4.37769100	1.57042700	-0.17691800	C	3.43409400	0.43023600	1.92142700
H	-2.31853100	1.23329100	1.72112100	C	4.16005700	-1.02098900	-0.80686500
H	-1.39425100	0.63616700	0.28586000	C	2.97299200	1.92329700	-0.84534200
O	-3.03946900	1.87147900	-0.12843100	Cl	-1.40062900	-1.63720400	-0.22312700
C	-5.99860300	-0.17448800	0.32605600	H	-2.35127500	0.37931700	-1.09997100
C	-5.37140900	2.42965400	-0.66346800	H	-2.51600200	0.27792800	0.69106300
H	-5.11946700	3.42744500	-1.03629700	C	-4.08583600	-0.79323900	-0.41641300
C	-7.01788000	0.67830000	-0.14574500	C	-5.07880400	0.35955700	-0.24289800
C	-6.69920400	1.95935400	-0.63891100	C	-4.50708700	-1.69662800	0.79044700
H	-6.24455600	-1.17521500	0.70238400	C	-6.06894300	-0.04433700	0.67212500
H	-8.06049600	0.34283700	-0.13010000	H	-4.53616200	-2.76996200	0.54594400
H	-7.50095300	2.61140000	-1.00450500	H	-3.84578400	-1.53951300	1.66411000
C	-3.35915200	-1.16584200	2.00762600	O	-5.85835300	-1.30299500	1.18182700
H	-4.04062600	-2.03521000	1.96767500	C	-5.17399300	1.60959800	-0.86699900
H	-2.34969900	-1.54091100	2.25132900	C	-7.16756800	0.76387400	0.99080400
H	-3.69535400	-0.50348800	2.82419600	H	-7.92638100	0.42585200	1.70347400
C	4.09894000	-1.19493800	-1.88473600	C	-6.26480500	2.44752300	-0.55372200
H	4.79897000	-2.03531400	-2.06333300	C	-7.24690700	2.02175500	0.36171600
H	3.10314500	-1.50424500	-2.25018000	H	-4.41821700	1.93809000	-1.59114700
H	4.45484000	-0.34507600	-2.49009700	H	-6.34854100	3.43188100	-1.02675500
C	3.74964800	-2.24962500	0.31977600	H	-8.09093700	2.68118300	0.59454100
H	2.74487900	-2.60441700	0.02361600	C	-4.29706300	-1.50264200	-1.77518000
H	4.49955100	-2.99965600	-0.00415400	H	-4.10955200	-0.80756200	-2.61336000
H	3.78174900	-2.20509400	1.41858700	H	-3.61750300	-2.36698300	-1.88233600
C	5.47670500	-0.42232600	0.07425100	H	-5.33748800	-1.86221200	-1.85836600
H	5.55873300	-0.30954100	1.16804100	C	3.96476300	-0.94444300	-2.34069700
H	6.22302100	-1.18463900	-0.22828100	H	4.54529000	-1.76363000	-2.80990900
H	5.77315100	0.53111400	-0.39383900	H	2.90448900	-1.08111100	-2.61987400
C	2.07137900	1.35832200	-2.58682500	H	4.33005000	0.00030500	-2.77609500
H	2.00782300	2.22540300	-3.27529300	C	3.77908400	-2.47136300	-0.40694800
H	2.65496800	0.57507300	-3.09304400	H	2.70899300	-2.66236000	-0.61185700
H	1.05180000	0.96358300	-2.41960700	H	4.38742700	-3.17843400	-1.00675600
C	1.80172400	2.98483400	-0.74765200	H	3.96410300	-2.69414300	0.65424500
H	1.71254700	3.73631000	-1.55739600	C	5.65129900	-0.77593800	-0.48340800
H	0.78284200	2.63100800	-0.51015500	H	5.88360500	-0.93774600	0.58238600
H	2.21259200	3.50713100	0.13198200	H	6.26735200	-1.49521300	-1.06027600
C	4.11881700	2.38647600	-1.51917000	H	5.98929600	0.23772300	-0.75680200
H	4.77260800	1.65484100	-2.02334700	C	2.14283000	1.81892600	-2.15218200
H	4.03816600	3.26346600	-2.19297400	H	2.03075400	2.83306200	-2.58678500
H	4.62620800	2.72241800	-0.59956300	H	2.61071700	1.18080300	-2.91680700
C	1.49294200	1.65127900	2.27796200	H	1.13804800	1.40769600	-1.93873900
H	1.56510500	1.92254700	3.35079000	C	2.24973900	2.97513400	0.03029800
H	1.20449500	2.55883900	1.72670200	H	2.13162800	3.90528900	-0.56072900
H	0.68556000	0.90550100	2.15585700	H	1.24142200	2.63106800	0.32334300
C	3.95856100	2.11553200	1.98527500	H	2.81316000	3.23944700	0.93989600
H	3.74711900	3.03638700	1.41704600	C	4.38828100	2.44548700	-1.18160100
H	4.02487100	2.40401000	3.05394000	H	4.91318900	1.80198900	-1.90756200
H	4.95329300	1.74799900	1.68269800	H	4.30062800	3.44881300	-1.64601000
C	3.13331300	-0.11984200	2.79105800	H	5.03020400	2.55357300	-0.29120400

C	2.21878400	0.99782900	2.70213800
H	2.45902700	0.99668400	3.78479300
H	1.96207500	2.03083500	2.42311900
H	1.32384500	0.36902300	2.53788600
C	4.66302200	1.33608900	2.15904200
H	4.48272800	2.38114600	1.85662800
H	4.89474300	1.35058200	3.24354300
H	5.56517900	0.97746800	1.63617000
C	3.71502400	-0.95997500	2.54472400
H	4.64638300	-1.42123900	2.17636800
H	3.82688400	-0.83671600	3.64049800
H	2.87641400	-1.65768500	2.36911500

10d

Pd	1.86524400	-0.19531700	-0.09215800
C	-1.83905500	-1.11430600	-0.44667500
P	3.51052100	1.29923200	0.04110900
C	4.11644500	1.77693000	1.73905900
C	5.11840500	0.84296100	-0.78310400
C	3.20063800	2.98077400	-0.70225500
I	0.14362400	-2.22622300	-0.28238100
H	-2.56028100	-1.93772200	-0.55912600
H	-1.72851000	-0.56613400	-1.39290400
C	-2.18606300	-0.19466700	0.73794700
C	-3.51740900	0.43717800	0.31297300
C	-1.29518300	1.08065900	0.78809500
C	-3.25041600	1.73303200	-0.17307400
H	-1.25960600	1.48731200	1.81706000
H	-0.25537700	0.92330500	0.42157200
O	-1.93073400	2.09067700	-0.06159900
C	-4.82072700	-0.07411200	0.26564400
C	-4.25388600	2.54706200	-0.71475000
H	-4.02501200	3.55183900	-1.08373000
C	-5.85008500	0.73279300	-0.26135200
C	-5.56088200	2.02274400	-0.74992100
H	-5.04353300	-1.08207100	0.63704900
H	-6.87761800	0.35457500	-0.29284400
H	-6.37006100	2.63862000	-1.15927300
C	-2.22618600	-0.93738200	2.08346400
H	-2.85858400	-1.84191700	2.02141400
H	-1.21329600	-1.25637700	2.38744900
H	-2.63870800	-0.28340900	2.87131000
H	2.96440900	2.86911000	-1.77420800
H	2.33105100	3.44893000	-0.21014500
H	3.28349000	2.21067000	2.31848300
H	4.94325000	2.51139400	1.68582600
H	4.46566600	0.87500900	2.27021100
H	4.08161500	3.64134700	-0.58952300
H	5.87542400	1.64211700	-0.66572400
H	5.50426900	-0.09101500	-0.34031200
H	4.94259300	0.66293800	-1.85729500

11a

C	0.60447000	-0.75340900	-0.35096700
I	2.74284100	-0.10913500	-0.20153000
H	0.62862500	-1.80491800	-0.02904600
H	0.38814700	-0.69323700	-1.42721700

C	-0.36513400	0.09145700	0.48129400
C	-1.80258900	-0.30759100	0.12535800
C	-0.38223400	1.58843800	0.02492300
C	-2.53373900	0.86438000	-0.14510800
H	0.12378000	2.26653000	0.72956100
H	0.06546100	1.70810300	-0.98027000
O	-1.77896000	2.00863500	-0.05879900
C	-2.44720400	-1.55066500	0.10861700
C	-3.90342800	0.84108300	-0.43814100
H	-4.44980500	1.76705600	-0.64339000
C	-3.82431900	-1.60194100	-0.19277700
C	-4.53713300	-0.41654800	-0.45944300
H	-1.89721900	-2.47417900	0.32789900
H	-4.34115700	-2.56738700	-0.21730800
H	-5.60715500	-0.46945000	-0.69137600
C	-0.11956300	-0.04899800	2.00116000
H	-0.23270500	-1.10059600	2.32155300
H	0.89844600	0.28800600	2.26746900
H	-0.85004500	0.55788400	2.56410600

11b

C	1.08519400	-0.76043100	-0.42412100
Br	3.03145700	-0.16732500	-0.28805200
H	1.10576400	-1.81595400	-0.11527000
H	0.85340200	-0.68192200	-1.49605900
C	0.13900900	0.08171900	0.43472200
C	-1.30813700	-0.30778500	0.11285500
C	0.12092900	1.58070600	-0.01297800
C	-2.03937700	0.87034900	-0.12936100
H	0.64939700	2.25094000	0.68242600
H	0.54266700	1.70447300	-1.02862100
O	-1.27551800	2.00950700	-0.05738600
C	-1.96008300	-1.54707900	0.10499700
C	-3.41689400	0.85678200	-0.38386300
H	-3.96371800	1.78722400	-0.56629900
C	-3.34518200	-1.58857900	-0.15964200
C	-4.05813000	-0.39723700	-0.39724400
H	-1.41031300	-2.47534100	0.30390400
H	-3.86788200	-2.55100000	-0.17754800
H	-5.13449700	-0.44243800	-0.59952600
C	0.42461800	-0.06803600	1.94707900
H	0.31768700	-1.12122500	2.26437000
H	1.44942300	0.26637100	2.18728200
H	-0.29046100	0.53674900	2.53157200

11c

C	1.65788800	-0.81130900	-0.57315500
Cl	3.41763600	-0.30642000	-0.50140000
H	1.63792600	-1.87576700	-0.28902100
H	1.35571700	-0.71074100	-1.62755600
C	0.75585000	0.02987000	0.34437900
C	-0.71215300	-0.31617300	0.08531400
C	0.75773500	1.53828800	-0.06982000
C	-1.42392000	0.88372600	-0.10030300
H	1.33137800	2.18047700	0.61631800
H	1.13919500	1.67540700	-1.09975900
O	-0.62813800	2.00240600	-0.04556000

C	-1.39568400	-1.53825300	0.08421300
C	-2.81151400	0.90972500	-0.29086300
H	-3.34208300	1.85680100	-0.43076100
C	-2.79231700	-1.54047300	-0.11674700
C	-3.48485500	-0.32752100	-0.29798000
H	-0.86168100	-2.48381400	0.24072900
H	-3.33958500	-2.48927300	-0.12850100
H	-4.57025900	-0.34209900	-0.45045200
C	1.11250300	-0.16035700	1.83750600
H	0.98337700	-1.21549600	2.14010900
H	2.15964600	0.13250500	2.03213900
H	0.45046800	0.45675600	2.46977800

12

Pd	2.07250700	-0.00504700	0.01426800
P	-0.13538600	-0.00054300	-0.00126100
C	-0.84179100	-0.10508400	1.82720600
C	-0.82328400	-1.53398700	-1.01574300
C	-0.81379300	1.64482400	-0.82931700
C	-0.57234000	1.57089200	-2.35652100
H	-0.77324500	2.56980500	-2.79219900
H	0.47632800	1.30879700	-2.58577000
H	-1.23936000	0.85669700	-2.86653400
C	0.05827400	-1.69589800	-2.28128000
H	-0.21869800	-2.64198200	-2.78902000
H	-0.06613500	-0.88114900	-3.00968400
H	1.12829100	-1.74256100	-2.00503100
C	-2.30498600	1.96473600	-0.57556200
H	-2.52110700	2.15888300	0.48826600
H	-2.57200600	2.88652800	-1.13091000
H	-2.98096400	1.16617200	-0.92438300
C	0.05919400	2.82244900	-0.32245500
H	1.13207500	2.60611200	-0.48377600
H	-0.20892400	3.73531700	-0.89183300
H	-0.08306300	3.04453500	0.74539100
C	-2.30985300	-1.45434000	-1.43239400
H	-2.50722500	-0.62949900	-2.13756900
H	-2.58680700	-2.39440500	-1.95093400
H	-2.99024100	-1.34202700	-0.57203400
C	-0.60265100	-2.82088900	-0.18384700
H	-0.80547000	-3.69647000	-0.83205700
H	0.44219700	-2.89746700	0.16749400
H	-1.27805100	-2.89790300	0.68382600
C	-2.33305700	-0.49507900	1.95237400
H	-2.53452600	-1.51921700	1.59578100
H	-2.62215900	-0.46579200	3.02239900
H	-3.00332700	0.19447800	1.41286000
C	0.02314700	-1.12641400	2.61142200
H	-0.27328000	-1.09745800	3.67949600
H	-0.09906700	-2.16199600	2.26139300
H	1.09569600	-0.86676900	2.53486700
C	-0.62339800	1.25702800	2.53000500
H	-1.29211100	2.04945000	2.15565100
H	-0.83990600	1.13270600	3.60957900
H	0.42377200	1.59610200	2.43398000

12d

Pd	1.31328800	-0.00003600	0.00000000
P	-0.86133500	0.00026700	-0.00014400
C	-1.70513100	-0.55408000	1.56579100
C	-1.70519000	1.63326100	-0.30312900
C	-1.70528400	-1.07934100	-1.26248400
H	-1.39529000	-0.77151200	-2.27534000
H	-1.39712900	-2.12807700	-1.11430100
H	-2.80718900	-1.00740200	-1.17989500
H	-1.39401900	-1.58474300	1.80590300
H	-2.80707000	-0.52008300	1.46174900
H	-1.39796200	0.09904500	2.39997400
H	-2.80704600	1.52610100	-0.28002000
H	-1.39832200	2.02867400	-1.28611600
H	-1.39356900	2.35661300	0.46912500

13-ts

Pd	1.37675000	-0.57592800	-0.19300600
P	3.46387500	-1.35837900	0.12953300
C	4.78005600	0.09640400	0.13378100
C	3.56315500	-2.27154500	1.86472000
C	3.99044100	-2.63977600	-1.26209300
C	2.77143300	-3.54668500	-1.57246900
C	4.27767300	-1.86943000	-2.57485400
C	5.21108900	-3.52949500	-0.93077100
C	4.98641800	-2.51372200	2.41794200
C	2.75244300	-1.43254900	2.88699500
C	2.83086900	-3.63170000	1.76308300
C	6.26563200	-0.30933800	0.00259400
C	4.60167400	0.91745600	1.43327100
C	4.40945400	1.05468500	-1.02710000
H	2.47623300	-4.19095300	-0.73122200
H	3.03242700	-4.20878800	-2.42269600
H	1.89478700	-2.93948600	-1.85891600
H	3.44884500	-1.18513700	-2.83059700
H	5.21992900	-1.29755400	-2.54701200
H	4.37086800	-2.60475000	-3.39872400
H	5.01848400	-4.21409600	-0.08768900
H	6.11782900	-2.94636500	-0.70037100
H	5.44154100	-4.16193000	-1.81197100
H	5.50895600	-1.57447000	2.66623100
H	5.62360900	-3.08712700	1.72494500
H	4.91189600	-3.09678200	3.35809900
H	2.69433300	-1.99491400	3.84104900
H	3.20652200	-0.45483700	3.10629500
H	1.72439700	-1.25536900	2.52004900
H	2.72288900	-4.04845300	2.78410400
H	1.81652700	-3.51324200	1.34172500
H	3.38150100	-4.37704500	1.16609400
H	6.89287600	0.60310100	0.06528600
H	6.59594400	-0.98933100	0.80522000
H	6.48859700	-0.78596100	-0.96645700
H	5.18520000	1.85517000	1.34215800
H	4.97104200	0.39257600	2.32923900
H	3.54403200	1.19375200	1.59384600
H	3.34744900	1.35475700	-0.96257700
H	5.03726500	1.96573500	-0.95360800
H	4.57483600	0.61899400	-2.02327300

P	-0.10505100	3.29429000	0.08679100	C	-7.69471000	-0.80412600	-1.05871800
C	1.11928600	4.68897400	0.72366300	H	-5.94527400	-1.20383800	-2.29596500
C	-0.31912600	3.53945300	-1.84644400	H	-7.89639700	-1.30835600	2.35423800
C	-1.84734800	3.63252700	0.92120300	C	-8.23941000	-0.83708600	0.23996000
C	0.57621600	6.13261300	0.82558800	H	-8.30501900	-0.45407900	-1.89845100
C	1.61560100	4.22493700	2.12032400	H	-9.27330600	-0.51051300	0.40174200
C	2.37819900	4.70657800	-0.17740800				
C	0.90212800	2.84819900	-2.51115400	15d-ts			
C	-1.55348100	2.73847600	-2.32783100	Pd	1.13182400	0.20998100	0.15309100
C	-0.44330100	4.98790900	-2.36927000	P	3.46899500	0.07415800	-0.12467400
C	-1.65316100	3.82170700	2.44635700	C	4.35206900	1.32510200	-1.19024100
C	-2.67868100	4.81834300	0.38320700	H	5.43917800	1.12404000	-1.24159500
C	-2.66238900	2.32012400	0.77145600	H	3.93375600	1.29672600	-2.21137600
H	1.38877900	6.80545500	1.17046600	H	4.19304700	2.33827300	-0.78332800
H	-0.24658300	6.22643700	1.55397700	C	4.50745700	0.16422200	1.42212100
H	0.21859600	6.51885200	-0.14396700	H	4.20023800	-0.63314200	2.12036300
H	2.01225800	3.19483700	2.07883500	H	5.58557300	0.05401000	1.19826500
H	0.83284000	4.25405500	2.89309100	H	4.33906600	1.13367000	1.92216600
H	2.43445300	4.89351900	2.45559700	C	4.10983900	-1.50353800	-0.88468700
H	2.18804800	5.12708300	-1.17807800	H	3.65625500	-1.63838600	-1.88168700
H	3.14711200	5.34548500	0.30203800	H	5.21223500	-1.49637600	-0.98261500
H	2.81333000	3.69871400	-0.29604000	H	3.80751700	-2.36256000	-0.26128300
H	1.85619600	3.35693200	-2.30707300	I	-0.34946100	-1.86481000	-1.33149200
H	0.99837500	1.79740600	-2.17611500	P	0.15909900	2.32789400	-0.14935500
H	0.75994400	2.84271600	-3.61106900	C	-0.74933300	3.08837400	1.29048700
H	-1.52278300	1.69138900	-1.97668100	H	-0.04996700	3.23143900	2.13261300
H	-1.54810400	2.71409300	-3.43613500	H	-1.19914300	4.06357500	1.02260800
H	-2.50976100	3.19146400	-2.01928800	H	-1.54344300	2.40025700	1.62569100
H	0.45724500	5.59013500	-2.16406300	C	1.31127200	3.73568300	-0.57251100
H	-0.57690300	4.97168800	-3.47089100	H	0.76254700	4.69082200	-0.68346600
H	-1.31125600	5.51582000	-1.93958000	H	2.07029200	3.84924100	0.22101100
H	-1.18968600	4.78740200	2.70570400	H	1.83270800	3.51392900	-1.51965600
H	-1.04950800	3.00874900	2.88909200	C	-1.09807200	2.52671300	-1.50896400
H	-2.64755700	3.79890500	2.93574400	H	-0.64665800	2.22891000	-2.47124800
H	-2.14356900	5.77856300	0.47024200	H	-1.94957900	1.85646600	-1.30918200
H	-2.97132300	4.68512700	-0.67181000	H	-1.45733200	3.57127700	-1.58310300
H	-3.61665900	4.90569800	0.96977200	C	-0.47398100	-0.97875400	0.86997200
H	-2.94155300	2.10356100	-0.27038900	C	0.38938100	-1.64639100	1.78160400
H	-3.60304300	2.40612400	1.35207800	C	-1.75144700	-0.52334000	1.32449000
H	-2.09500300	1.45599300	1.16239400	C	0.07947800	-1.67903900	3.16413800
I	-0.96808500	-1.89457500	-0.46943400	H	1.24081300	-2.21779700	1.40052300
C	-3.19499000	-1.31270100	-0.82910000	C	-2.05061300	-0.58311200	2.69402400
H	-3.27835000	-1.34989600	-1.92530500	C	-1.12963300	-1.14413500	3.61271200
H	-3.23823600	-0.27645300	-0.46558300	H	0.76456700	-2.17669900	3.86023100
C	-4.17971600	-2.23783500	-0.11605200	H	-2.99492400	-0.17368600	3.06731500
C	-5.59881400	-1.65838000	-0.19612100	H	-1.39544600	-1.18400400	4.67524700
C	-3.97940400	-2.22609700	1.43638500	O	-2.59671500	-0.00865600	0.37132300
C	-4.15581500	-3.67547800	-0.68872300	C	-3.96806500	0.24138100	0.75116100
C	-6.16223000	-1.68132000	1.09369500	H	-4.02268400	1.10226800	1.44746600
C	-6.36589500	-1.22181900	-1.28287100	H	-4.35819200	-0.65808400	1.27407600
H	-3.48333500	-3.13041700	1.82217500	C	-4.76896500	0.50984100	-0.50419500
H	-3.41351900	-1.33228300	1.76060900	C	-5.48624600	1.64718000	-0.62086000
O	-5.30347400	-2.15989900	2.05328600	H	-5.47414600	2.42018100	0.15750700
H	-4.41962000	-3.67154800	-1.76190900	H	-6.11504500	1.84089100	-1.49817300
H	-3.15291400	-4.12737500	-0.58018800	C	-4.74456500	-0.57362900	-1.55620400
H	-4.88708400	-4.31334400	-0.16155100	H	-3.70998800	-0.76542300	-1.89564200
C	-7.48098800	-1.27928100	1.34179300	H	-5.12031200	-1.53145900	-1.14497400

H	-5.36254500	-0.30342000	-2.42928000	C	1.91674300	-0.41539800	-1.54874600
16d				C	2.74387500	-0.34645100	0.75793200
Pd	-0.48173100	0.21380200	-0.38948100	C	2.22386600	-1.79112700	-1.57795300
C	1.33986100	0.80335000	-1.08747400	H	1.54022900	0.09062500	-2.44561200
C	1.46915900	1.56311700	-2.26593700	C	3.05699600	-1.70783100	0.73992400
C	2.52955300	0.46663700	-0.39051300	C	2.77739100	-2.41688700	-0.44629600
C	2.72706600	1.99266900	-2.74493300	H	2.01077300	-2.37728800	-2.47708900
H	0.56665300	1.83287000	-2.83009800	H	3.50291300	-2.19704700	1.61109000
C	3.79292900	0.89637200	-0.84953200	H	2.99876400	-3.48944100	-0.48285800
C	3.88563400	1.66137500	-2.02943900	P	-2.29981800	1.30564000	0.00988000
H	2.79169500	2.58275200	-3.66711400	I	-1.18082600	-2.09864000	0.18771900
H	4.70826900	0.64475000	-0.30381300	C	2.13793300	1.82712600	-0.07603200
H	4.87098300	1.99033800	-2.38005000	C	0.71299300	2.30045300	-0.38968200
P	-0.24315900	-1.82562800	-1.50212200	H	0.33905100	3.07564200	0.30189200
C	1.30785300	-2.13278000	-2.46658200	H	0.60320100	2.65509500	-1.43206000
C	-0.31399900	-3.29398000	-0.37781500	O	3.03200100	0.50791300	1.78496900
C	-1.56287600	-2.16640400	-2.75543600	C	2.40565500	1.79290900	1.46248400
I	-2.99762300	-0.54659000	0.49064100	H	1.45447200	1.83886800	2.02693800
O	2.35803800	-0.31198300	0.74627900	H	3.09255400	2.58051600	1.81293800
C	3.53277400	-0.70291300	1.48320100	C	3.24852300	2.57875400	-0.84341400
H	4.24518200	-1.23410300	0.82071100	H	4.24835500	2.17330200	-0.59780500
H	4.03731500	0.20995000	1.87253100	H	3.10120900	2.48460600	-1.93423500
C	3.10438300	-1.59519500	2.62809300	H	3.23393900	3.65542900	-0.58823700
C	3.68535100	-2.80106600	2.80097000	C	-3.47910500	0.68356600	-1.27198900
H	4.44111200	-3.18305200	2.10349000	H	-3.11546400	0.96395900	-2.27498600
H	3.43023500	-3.44444100	3.65155800	H	-3.51487200	-0.41653900	-1.20802700
C	2.04778700	-1.04268200	3.55529700	H	-4.48757900	1.10878800	-1.11411600
H	2.37093200	-0.07669000	3.99223000	C	-3.13744900	0.93012200	1.61482400
H	1.11125500	-0.84681000	3.00125300	H	-2.54904200	1.35369100	2.44622800
H	1.82841600	-1.74075000	4.38087000	H	-4.15728700	1.35690000	1.63090700
H	1.27221300	-3.12768000	-2.94673600	H	-3.17870500	-0.16450700	1.74032400
H	1.43125200	-1.35442700	-3.23762300	C	-2.49739500	3.14519000	-0.12296600
H	2.18009100	-2.08128600	-1.79450600	H	-3.56719700	3.41802800	-0.07241000
H	-1.42970700	-3.16780600	-3.20461100	H	-1.96442900	3.64724500	0.70190900
H	-1.52097400	-1.40286900	-3.55102900	H	-2.07819800	3.50572700	-1.07734300
H	-2.54745800	-2.10230400	-2.26324600	18d			
H	-0.24277900	-4.23450300	-0.95467300	Pd	0.70031500	0.07041400	0.23177600
H	-1.26326000	-3.26816500	0.18281700	C	-1.35707000	0.42698400	0.52400600
H	0.52072600	-3.24029500	0.34133000	P	1.25513300	2.33713100	0.45070200
P	-0.69783800	2.25137400	0.73910000	C	0.02024200	3.55761500	1.12119700
C	-2.10971700	3.29083300	0.14233100	H	0.50593000	4.54022100	1.26228300
H	-3.03894000	2.70129200	0.21130600	H	-0.83324900	3.68122700	0.43495800
H	-2.20342100	4.21324900	0.74460600	H	-0.36494300	3.20952300	2.09512200
H	-1.94643300	3.56251800	-0.91464900	C	2.62145400	2.53980400	1.68935900
C	0.72264300	3.43998600	0.69146400	H	3.49946400	1.96294900	1.35555900
H	0.96603600	3.69455100	-0.35327300	H	2.88902900	3.60685400	1.80213300
H	0.47598100	4.36139500	1.24972900	H	2.29288900	2.14217200	2.66490200
H	1.61604000	2.97078900	1.13614100	C	1.90652900	3.22507200	-1.04012900
C	-1.01693200	2.09312600	2.55612900	H	1.11369200	3.30939000	-1.80279400
H	-1.16013600	3.08738400	3.01805400	H	2.26236000	4.23688700	-0.77301400
H	-1.91601600	1.47332700	2.70883900	H	2.73805800	2.63574900	-1.46167000
H	-0.15979200	1.58934800	3.03428000	I	3.32264600	-0.40883800	-0.63303600
17d				H	-1.49195600	1.37607900	1.07293200
Pd	-0.22372300	0.45598700	-0.18691000	H	-1.76150900	-0.36606400	1.17556700
C	2.15724400	0.30974600	-0.35585800	C	-2.20909300	0.49697100	-0.78249800
				C	-3.68054900	0.55456200	-0.35586600

C	-2.24014300	-0.84589200	-1.56773500
C	-4.23324100	-0.73391300	-0.49039400
H	-2.44508700	-0.67427300	-2.64318200
H	-1.31852900	-1.43605000	-1.46188000
O	-3.34890400	-1.64254800	-1.03642000
C	-4.45899500	1.58325900	0.18806100
C	-5.53987000	-1.04109900	-0.09484900
H	-5.94407400	-2.05140300	-0.21643100
C	-5.78486900	1.30592700	0.58473300
C	-6.31079300	0.00659300	0.44940100
H	-4.04861800	2.59419700	0.30511500
H	-6.40813800	2.10548300	1.00062400
H	-7.34183000	-0.19617700	0.76186600
C	-1.79026400	1.65355000	-1.70784200
H	-1.85541300	2.62393100	-1.18372900
H	-0.74712500	1.51964200	-2.04795700
H	-2.44709100	1.71159400	-2.59502500
P	0.47462600	-2.22835900	0.65367500
C	0.84372100	-3.42682200	-0.71246300
H	1.83546800	-3.19084000	-1.13238700
H	0.83549200	-4.46375700	-0.32981100
H	0.09138800	-3.33592100	-1.51445800
C	-1.11836300	-2.89809100	1.33508900
H	-1.95262000	-2.74012900	0.62984400
H	-1.01243200	-3.98076300	1.53050100
H	-1.36512400	-2.39196300	2.28457100
C	1.67392500	-2.73756800	1.97357300
H	1.56783300	-3.81514700	2.19777900
H	2.69941500	-2.52221700	1.63129800
H	1.48114600	-2.15472600	2.89036300

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C	4.64932100	-1.17438000	-0.44178900
H	5.22365100	-2.09570200	-0.29480800
H	4.98260300	-0.50879900	-1.24857200
C	3.59174100	-0.87405600	0.33259200
C	0.81005800	2.43108300	0.03606700
C	2.80430600	0.40000100	0.21146700
C	0.48718500	1.05586700	0.04086000
H	2.93595700	1.02886800	1.11775500
H	3.12706600	0.98506000	-0.67287900
O	1.40830100	0.04561900	0.09211500
C	-0.20591300	3.40093000	-0.02351400
C	-0.87778600	0.68435500	-0.01667400
C	-1.55378000	3.01940200	-0.08009000
C	-1.88754000	1.65131200	-0.07707400
H	0.06950800	4.46165000	-0.02641500
H	-2.34797300	3.77215700	-0.12685400
H	-2.93535900	1.33747400	-0.12062300
H	3.26794800	-1.56002600	1.12718600
H	1.85567400	2.75020000	0.07440800
I	-1.40285000	-1.39816800	-0.00862600

19d-ts

Pd	-1.29010200	0.24692400	0.21601100
C	1.13270200	0.04409300	-0.29695300
P	-1.58764300	2.52709000	-0.28093700

C	-3.05907900	2.86959600	-1.37323100
H	-3.15066200	3.94720200	-1.60904800
H	-2.95515100	2.29952300	-2.31237300
H	-3.98002000	2.52965100	-0.86931000
C	-1.89150400	3.76191900	1.08752700
H	-1.02688400	3.77443700	1.77400200
H	-2.05459200	4.78454700	0.69544500
H	-2.77828400	3.45117700	1.66677200
C	-0.25820100	3.42972000	-1.23585500
H	-0.04189500	2.87740400	-2.16750200
H	-0.55983300	4.46325200	-1.49221000
H	0.67003100	3.47034500	-0.63848900
I	-0.45276300	-1.08448300	-2.08154000
H	0.73236500	0.48384100	0.64804700
H	1.44521400	0.81818100	-1.00763100
C	2.19932100	-1.01859800	-0.00120000
C	3.24419500	-0.21619300	0.78948000
C	3.05441700	-1.40426500	-1.24695700
C	4.31988200	0.07999600	-0.07155800
H	3.47252700	-2.42302800	-1.13721300
H	2.50397500	-1.32932300	-2.19588300
O	4.18557200	-0.47401500	-1.31737000
C	3.24146600	0.27906700	2.10113400
C	5.40733600	0.86529700	0.33527700
H	6.23365000	1.07930800	-0.34997900
C	4.33092900	1.05878600	2.53726900
C	5.39359000	1.35036400	1.65704200
H	2.40730700	0.06246400	2.77957300
H	4.35152600	1.44199000	3.56332100
H	6.23336500	1.96104700	2.00860800
C	1.65146000	-2.24282400	0.74636600
H	1.08559700	-1.93089300	1.64232600
H	0.96375300	-2.81197100	0.09666900
H	2.47713900	-2.90230600	1.06753800
P	-2.42497400	-1.23403100	1.61757500
C	-1.93407200	-1.32420600	3.41776300
H	-2.01451300	-0.32078600	3.87015200
H	-2.57358300	-2.02927800	3.98255700
H	-0.88308700	-1.65202500	3.50062100
C	-4.25883800	-0.93069700	1.79979200
H	-4.73627400	-1.67853500	2.46221200
H	-4.42487000	0.07866100	2.21386100
H	-4.73663300	-0.97415800	0.80578700
C	-2.45235300	-3.05123000	1.18975100
H	-2.82466200	-3.17351900	0.15798800
H	-1.42546900	-3.45438100	1.22343200
H	-3.09173000	-3.63245900	1.88133300

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Pd	-0.41630000	0.88010100	-0.08254800
C	3.72794700	-0.51844300	-0.34750000
C	4.38443000	-0.84082200	-1.54193900
C	4.02273200	-1.23523000	0.83102000
C	5.34278400	-1.87667300	-1.53731200
H	4.16380100	-0.29149100	-2.46542500
C	4.96094000	-2.27520300	0.85846200
C	5.61716900	-2.58432400	-0.35029500

H	5.87719600	-2.13000800	-2.45958200	C	-3.65211400	-0.39884300	1.52408000
H	5.18023700	-2.81228000	1.78697900	C	-4.45725000	0.49899000	-0.58866500
H	6.36488400	-3.38614300	-0.35962800	C	-4.76799900	0.18509200	2.15809000
P	-1.84251000	-0.94780200	-0.02676000	H	-2.91077400	-0.96331200	2.10190800
C	-1.90037700	-2.11307000	-1.59765300	C	-5.56814600	1.09535200	0.01933200
C	-1.65109200	-2.04366700	1.57439800	C	-5.70711400	0.92442600	1.41096900
C	-3.52350500	0.05585000	0.07635300	H	-4.90400600	0.06486800	3.23830900
I	0.44750800	3.39639900	-0.07977200	H	-6.29512600	1.66409200	-0.56891900
C	2.60544700	0.46611900	-0.03309300	H	-6.56855100	1.37320400	1.91885900
C	1.30735000	-0.07372600	-0.66636400	P	1.42898100	1.14591100	0.01282700
H	1.30903700	0.08948800	-1.76027100	C	2.04856200	1.09465100	1.87050500
H	1.19233500	-1.14758800	-0.45373400	C	2.98879800	1.20923700	-1.16984200
O	3.30099000	-0.80746800	1.91860600	C	0.43298800	2.82272700	-0.23843000
C	2.65413600	0.45185600	1.51744000	I	1.29850000	-2.97725400	0.15222400
H	1.66246300	0.48347700	1.99407900	C	-2.43476000	-0.68386100	-0.82992600
H	3.27441400	1.28067700	1.90581100	C	-1.70973200	-1.96999600	-0.65598300
C	-3.86611300	0.64179200	-1.31600500	H	-1.95448100	-2.56733800	0.23239800
H	-4.19039200	-0.12104400	-2.04134900	H	-1.55256100	-2.58308000	-1.55539000
H	-4.70837200	1.35054400	-1.19373100	O	-4.16572300	0.58472400	-1.93506200
H	-3.01832800	1.20706200	-1.74272600	C	-3.11959100	-0.39622500	-2.19724500
C	-3.26567300	1.28208500	0.99535700	H	-3.60128500	-1.31857300	-2.57441000
H	-4.18100600	1.90704900	1.01709700	H	-2.45203500	0.01838400	-2.96723000
H	-3.01709200	1.01953800	2.03278800	C	-0.61168100	2.97515700	0.89677700
H	-2.45822900	1.94146200	0.60611500	H	-0.15694400	3.20010600	1.87452700
C	-4.74533300	-0.72676800	0.60609400	H	-1.27939000	3.82234600	0.64549600
H	-5.62978100	-0.05965100	0.57445100	H	-1.24830500	2.07855700	1.00356100
H	-4.98333600	-1.61483200	-0.00247300	C	-0.38406500	2.75698800	-1.55604400
H	-4.62306500	-1.04837000	1.65376200	H	-0.97344800	3.69038800	-1.64849800
C	-1.59303600	-1.25098500	-2.84945600	H	0.23487900	2.66671400	-2.45980700
H	-1.53020900	-1.92093800	-3.72960400	H	-1.10277700	1.92057100	-1.55130500
H	-2.36680700	-0.49940200	-3.06163100	C	1.29927100	4.10533300	-0.28646300
H	-0.62941800	-0.72343100	-2.75382700	H	0.62724200	4.98559600	-0.33163900
C	-3.25179000	-2.84105700	-1.79320200	H	1.94159900	4.22666100	0.59946900
H	-4.08537900	-2.14842500	-1.99264200	H	1.93879700	4.14505700	-1.18395800
H	-3.16804200	-3.50674200	-2.67524500	C	0.86723400	0.57435800	2.73223300
H	-3.52321400	-3.47147200	-0.93048900	H	1.21598800	0.46421300	3.77846500
C	-0.78657000	-3.18557700	-1.51514400	H	0.00162100	1.25374700	2.74216200
H	-0.77179600	-3.73833900	-2.47488800	H	0.52662300	-0.41667900	2.38149400
H	0.21610200	-2.74814600	-1.37847200	C	2.55524100	2.43408700	2.45339800
H	-0.96219800	-3.92636700	-0.71944500	H	1.76458000	3.19879700	2.52799100
C	-2.57244600	-3.28557200	1.63436400	H	2.92291100	2.24976800	3.48251900
H	-2.32510700	-4.03574000	0.86492100	H	3.39503100	2.85794800	1.87830800
H	-2.43539500	-3.77814900	2.61742200	C	3.17938200	0.04578200	2.01381500
H	-3.64101200	-3.03201300	1.53994800	H	3.37946200	-0.09453100	3.09448800
C	-0.17360500	-2.50038300	1.69592200	H	2.89034900	-0.93586800	1.60112700
H	-0.06836900	-3.08039400	2.63374800	H	4.12608500	0.36859800	1.55124500
H	0.16055600	-3.15135200	0.87462400	C	4.12256300	2.15652900	-0.71144600
H	0.51830000	-1.64466900	1.76149000	H	4.59493900	1.82536800	0.22790700
C	-1.92566300	-1.16209100	2.81842000	H	4.91531300	2.15550100	-1.48628700
H	-1.32666800	-0.23392200	2.80466100	H	3.79043400	3.19917600	-0.58257500
H	-2.98967000	-0.89917000	2.93457400	C	3.55052700	-0.22705400	-1.30636400
H	-1.63149300	-1.73397300	3.71993600	H	4.40642700	-0.20039800	-2.01029200
H	2.80027400	1.48305000	-0.40874700	H	3.90985700	-0.65239500	-0.35884800
				H	2.79436500	-0.92040300	-1.70944500
21				C	2.54163700	1.62469400	-2.59293700
Pd	-0.06635300	-0.73282000	-0.33792500	H	1.70187900	1.00546900	-2.95653100
C	-3.50952400	-0.24319300	0.14111100	H	2.26321400	2.68855800	-2.66686900

H	3.39261400	1.46236100	-3.28310300
H	-1.59710000	0.19882200	-0.74212900
22-ts			
Pd	-0.35989300	-0.48032200	-0.18067000
C	2.19286600	-0.55911800	-0.51704300
P	-2.40777000	0.47471500	0.02104600
C	-3.78805500	-0.81537800	-0.50827400
C	-2.74014900	0.99955800	1.88058900
C	-2.60685400	2.07029600	-1.10733600
I	1.30144100	-2.71639200	-0.14092200
H	1.40471500	0.21283900	-0.75812000
H	2.75421200	-0.77802500	-1.43577200
C	3.05775400	-0.13810800	0.67090600
C	3.66274600	1.22248200	0.33717600
C	4.34776600	-0.98158100	0.86945500
C	5.02605100	1.03027000	0.03887400
H	4.61341400	-1.06111800	1.93958600
H	4.29277800	-1.98959200	0.42975600
O	5.43941200	-0.26934900	0.19792400
C	3.09193300	2.49709400	0.22511300
C	5.85335600	2.08128300	-0.37860700
H	6.91070000	1.91056900	-0.60402500
C	3.90825400	3.57274000	-0.17888300
C	5.26834100	3.35835500	-0.48150600
H	2.03000700	2.65356400	0.44844900
H	3.48333100	4.57900900	-0.26048300
H	5.89063700	4.20376100	-0.79740300
C	-3.81190700	2.98591500	-0.78958100
H	-3.73345300	3.46077900	0.20305000
H	-3.84473400	3.80697100	-1.53444000
H	-4.77903800	2.45874100	-0.84271500
C	-1.29988700	2.89815400	-1.00394400
H	-0.42044700	2.26818800	-1.22958100
H	-1.34013300	3.72085200	-1.74581100
H	-1.14883200	3.35304200	-0.01372800
C	-2.69991900	1.61948100	-2.58560200
H	-2.60842400	2.51352100	-3.23387500
H	-1.87920300	0.92818300	-2.84917200
H	-3.66136300	1.13949500	-2.82920200
C	-5.19760100	-0.23803400	-0.77163000
H	-5.22252200	0.43497400	-1.64519500
H	-5.89193200	-1.07415900	-0.99132200
H	-5.60657300	0.30800200	0.09492100
C	-3.28714500	-1.54519500	-1.78260000
H	-3.98272800	-2.37761600	-2.01160900
H	-3.24572500	-0.89680500	-2.67034500
H	-2.27754500	-1.96632300	-1.62247800
C	-3.89428900	-1.90467500	0.58766800
H	-4.51256300	-2.73675700	0.19686500
H	-2.90246600	-2.31637700	0.84635600
H	-4.38274000	-1.54374800	1.50778100
C	-2.16707900	-0.11593600	2.79411900
H	-2.21171900	0.22765400	3.84748600
H	-2.72633500	-1.06078500	2.72994100
H	-1.11323100	-0.33023000	2.53673300
C	-4.21497100	1.26120800	2.26138200

H	-4.83429500	0.35116700	2.19453400
H	-4.25876000	1.60429200	3.31487900
H	-4.68464400	2.04273500	1.64185000
C	-1.91239900	2.26914700	2.19543500
H	-2.31065200	3.17533800	1.71060100
H	-1.94094100	2.44605500	3.28885100
H	-0.85415600	2.14354300	1.90317100
H	2.44245100	-0.12184800	1.58678700
23			
Pd	-0.73748000	-0.66761200	-0.10346700
C	3.10983500	-1.09008300	-0.66640400
P	-2.67694500	0.49747200	0.03276400
C	-4.09908200	-0.43323800	-0.94597000
C	-3.25263800	0.70609300	1.89686600
C	-2.46794600	2.28351500	-0.74699200
I	1.29718100	-2.37906200	-0.23177400
H	3.02489200	-0.88751900	-1.74308700
H	3.96489000	-1.75287000	-0.46266800
C	3.11879900	0.18613200	0.17786100
C	4.34442300	1.00380400	-0.21323300
C	3.40167200	-0.04582400	1.68597300
C	5.29652000	0.87528200	0.81790500
H	2.87917800	0.70227200	2.30957400
H	3.14695700	-1.05745300	2.03910900
O	4.84281200	0.14025700	1.88608100
C	4.65860200	1.72792800	-1.37054700
C	6.57294000	1.44581500	0.73048300
H	7.29678800	1.33463000	1.54390200
C	5.93252900	2.32329200	-1.47547800
C	6.87396700	2.17391400	-0.43736900
H	3.92627100	1.83691500	-2.17988300
H	6.19116100	2.90416000	-2.36740500
H	7.86135200	2.64036400	-0.53308100
C	-3.56468000	3.31591500	-0.40186300
H	-3.59641800	3.55682500	0.67374500
H	-3.34995200	4.26272100	-0.93789600
H	-4.57079400	2.98584000	-0.70967800
C	-1.08652600	2.82751300	-0.29552500
H	-0.28804700	2.10043600	-0.53752900
H	-0.87838700	3.77300600	-0.83666400
H	-1.03048500	3.04419200	0.78155600
C	-2.38030700	2.14969700	-2.28684200
H	-2.06783000	3.12651000	-2.70719900
H	-1.62674800	1.39840500	-2.58414900
H	-3.34490400	1.89198300	-2.75403800
C	-5.35834400	0.40012800	-1.27662900
H	-5.14294200	1.23957000	-1.95901200
H	-6.09490400	-0.25042400	-1.79019000
H	-5.85158500	0.80742200	-0.37803000
C	-3.48387500	-0.98257000	-2.25988000
H	-4.22320900	-1.64997300	-2.74717100
H	-3.22220100	-0.19613500	-2.98344400
H	-2.56772100	-1.56445400	-2.04629400
C	-4.52466700	-1.67777200	-0.13042600
H	-5.18315500	-2.30575000	-0.76285200
H	-3.65052100	-2.28945300	0.15645100

H	-5.09477500	-1.42319200	0.77740900
C	-2.99119400	-0.64148900	2.62108600
H	-3.14647900	-0.49685300	3.70947400
H	-3.66401000	-1.44994200	2.29769500
H	-1.95090800	-0.97838900	2.45376400
C	-4.72289400	1.12909900	2.11423600
H	-5.43746900	0.36596200	1.76278000
H	-4.90286200	1.26224800	3.20032600
H	-4.97038600	2.08417500	1.62116200
C	-2.32947100	1.73895600	2.58849000
H	-2.51067300	2.77346700	2.25354400
H	-2.52635400	1.71179400	3.67876200
H	-1.26287400	1.49398700	2.43470500
H	2.16432400	0.72516900	0.03525400

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C	0.52585500	-0.55840600	-0.39099800
I	2.69857000	-0.14505000	-0.09983200
H	0.46120000	-1.65582600	-0.40445000
H	0.29212700	-0.15699900	-1.38837800
C	-0.35080000	0.05695500	0.70738300
C	-1.80193200	-0.30857200	0.41423100
C	-0.43682500	1.60719100	0.66797600
C	-2.44255100	0.83970600	-0.09174400
H	-0.56447200	2.02551800	1.68343600
H	0.42224400	2.09116200	0.17724600
O	-1.63511000	1.95081900	-0.10294000
C	-2.49568700	-1.52331700	0.48527000
C	-3.76971200	0.81824600	-0.53968500
H	-4.24809400	1.72315000	-0.92721800
C	-3.83706500	-1.56710900	0.05244200
C	-4.45664500	-0.40862800	-0.45771800
H	-2.00882300	-2.42590500	0.87471500
H	-4.39909800	-2.50531600	0.11209900
H	-5.49935200	-0.45704800	-0.79237000
H	-0.00689200	-0.29405800	1.69661700

25-ts

Pd	-0.08798600	-0.74067500	-0.27941900
C	-3.41999400	-0.50716200	0.14748500
C	-3.62517400	-0.69198200	1.52298400
C	-4.27529200	0.34258600	-0.58547800
C	-4.70058800	-0.02647000	2.13921400
H	-2.95837400	-1.33816900	2.10519900
C	-5.34574600	1.02145400	0.00933600
C	-5.54358100	0.82135200	1.38876300
H	-4.88397300	-0.16588800	3.21001400
H	-5.99791500	1.67287500	-0.58064700
H	-6.37531800	1.33272400	1.88676900
P	1.25474000	1.21413700	0.01858400
C	2.35265900	1.09650000	1.64125900
C	2.42984300	1.46183700	-1.52262100
C	0.13541000	2.82100500	0.19284200
I	1.52591900	-2.89365200	0.20059200
C	-2.39910800	-1.02993000	-0.80248300
C	-1.61224700	-2.21143700	-0.62558800
H	-1.72437400	-2.79494800	0.29510400

H	-1.31156200	-2.79034200	-1.50730800
O	-3.93760900	0.43829500	-1.91768200
C	-2.96300000	-0.61479300	-2.17629100
H	-3.50591900	-1.47255800	-2.62025100
H	-2.22432600	-0.23169600	-2.89382800
C	-0.57698600	2.79127400	1.56818200
H	0.10104400	2.97847700	2.41539400
H	-1.34485500	3.58959700	1.58099100
H	-1.09722200	1.83106600	1.73488500
C	-1.00295800	2.82694700	-0.85920400
H	-1.54151500	3.79146300	-0.77672600
H	-0.65579100	2.72837700	-1.89687000
H	-1.74128200	2.03084700	-0.66640800
C	0.90668300	4.15757400	0.04348900
H	0.22052400	4.98976900	0.29731400
H	1.78106300	4.23985600	0.70621600
H	1.24340900	4.32634600	-0.99341500
C	1.48875000	0.41855500	2.73725700
H	2.12068700	0.26712600	3.63488400
H	0.61891400	1.01970900	3.04351900
H	1.13152500	-0.57198800	2.40648900
C	2.89870900	2.44109700	2.17857800
H	2.11004200	3.12916600	2.52334000
H	3.53687600	2.22274100	3.05777900
H	3.52940200	2.96999400	1.44428700
C	3.56485500	0.16295200	1.40044900
H	4.07316500	0.01183500	2.37347300
H	3.25721600	-0.83033000	1.03443800
H	4.31025700	0.59212200	0.71148300
C	3.59464700	2.45915900	-1.30970900
H	4.30210100	2.12849500	-0.53252000
H	4.16749500	2.53581600	-2.25546700
H	3.24998100	3.47372500	-1.05271600
C	3.00763100	0.07742900	-1.91240300
H	3.66579500	0.21173500	-2.79418700
H	3.60172100	-0.39599000	-1.11818400
H	2.20846000	-0.63277000	-2.18523900
C	1.60174500	1.93697100	-2.74207000
H	0.72442100	1.28936700	-2.91842800
H	1.26550900	2.98372100	-2.65815400
H	2.24465200	1.87328400	-3.64173800
H	-1.34598300	0.19112500	-0.68886000

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Pd	-0.21728200	-0.25106500	-0.84353700
C	-3.20540600	0.48433300	-0.21129100
C	-3.61307400	-0.49018700	0.72233200
C	-3.52983500	1.84573900	0.00997800
C	-4.33872000	-0.07755600	1.84970400
H	-3.33833900	-1.54076900	0.57906700
C	-4.24648400	2.27611800	1.13343500
C	-4.64582300	1.28811300	2.05124100
H	-4.66496100	-0.82046500	2.58527700
H	-4.48551700	3.33422500	1.27870600
H	-5.21240100	1.58714800	2.94086500
P	1.77137000	0.57488700	0.16566300
C	2.26066600	-0.26491900	1.87435400

C	3.18818100	0.24981300	-1.13859300	H	-2.92021300	1.98714800	0.00007400
C	1.64022200	2.51208300	0.48560900	H	-1.96466200	-2.26413300	-0.00001200
I	-0.51594900	-2.88207500	0.08166400	H	-3.65448500	-0.39743600	0.00005300
C	-2.44101800	0.41870200	-1.46148000	C	1.61251400	0.45681300	-0.00004700
C	-1.96492300	-0.68676900	-2.17438200	C	2.48531200	1.49076100	-0.00005700
H	-2.26379600	-1.70077900	-1.89500100	H	2.13984900	2.53012600	-0.00002800
H	-1.62021600	-0.54851800	-3.20680000	H	3.56929600	1.33130700	-0.00003300
O	-3.06761900	2.68355900	-0.97507400	O	0.73165100	-1.77829900	-0.00010300
C	-2.58845800	1.82441700	-2.05049700	C	1.98562200	-1.02564800	0.00013600
H	-3.37977300	1.80649800	-2.82759800	H	2.55193100	-1.32790500	0.89928700
H	-1.67680700	2.27001400	-2.46985900	H	2.55238600	-1.32817300	-0.89862200
C	0.76067100	2.76091100	1.73644700				
H	1.25940300	2.49403600	2.68108800	28			
H	0.52700300	3.84246800	1.78610200	Pd	0.91810500	0.03444700	0.04575800
H	-0.19898200	2.21816200	1.67237200	P	-1.37070800	0.00966800	0.01908300
C	0.90405300	3.22589900	-0.67661200	C	-1.79625600	-1.35558500	-1.31076600
H	0.94808900	4.31689400	-0.48689100	C	-2.16274000	-0.47191700	1.73131200
H	1.34870100	3.04496600	-1.66660900	C	-2.06287000	1.73663300	-0.56524300
H	-0.15941400	2.93894700	-0.70962900	I	3.52657200	0.02205700	0.04331600
C	3.01179500	3.20717700	0.67453800	C	-1.68540200	1.95680700	-2.05139800
H	2.83409300	4.25604300	0.98397200	H	-2.23589900	1.29888800	-2.74298700
H	3.63818500	2.73955100	1.44797400	H	-1.94205900	2.99937300	-2.32231700
H	3.59108300	3.24388200	-0.26289300	H	-0.60081100	1.83092300	-2.21888000
C	0.97622100	-0.39830400	2.73344300	C	-1.32198700	2.84874500	0.22454100
H	1.23157100	-0.97208100	3.64616800	H	-1.64965000	3.83095100	-0.16929400
H	0.56519800	0.56874800	3.05867800	H	-1.53427600	2.84043000	1.30341000
H	0.18988800	-0.95692500	2.19993800	H	-0.22900000	2.77184300	0.08950800
C	3.33508300	0.49493000	2.69128100	C	-3.58993900	1.91276100	-0.40094500
H	2.99183800	1.47802000	3.05150400	H	-3.87987200	2.89992800	-0.81209600
H	3.56443800	-0.11129900	3.58992600	H	-4.17038400	1.14743000	-0.94295400
H	4.28195700	0.63112600	2.14248800	H	-3.90392700	1.89978200	0.65577400
C	2.78388400	-1.70130700	1.62715900	C	-0.74231500	-1.21580400	-2.44282600
H	2.90643900	-2.18643100	2.61549600	H	-0.88863400	-2.03718800	-3.17216400
H	2.06696300	-2.31185000	1.05441800	H	-0.80441000	-0.26655000	-2.99322900
H	3.76934600	-1.72525700	1.13404900	H	0.29267600	-1.31999600	-2.05315600
C	4.62826200	0.38216600	-0.58737900	C	-3.21973300	-1.28660000	-1.90551700
H	4.85448600	-0.35897900	0.19506400	H	-3.40441800	-0.35289500	-2.46128500
H	5.33795300	0.20106700	-1.41870100	H	-3.34851000	-2.12191700	-2.62250100
H	4.84210100	1.38667000	-0.18649100	H	-4.00383300	-1.39143000	-1.13666400
C	2.97474600	-1.18024000	-1.69941000	C	-1.57971200	-2.76202800	-0.69978500
H	3.74843900	-1.37648100	-2.46824400	H	-1.64168800	-3.50682000	-1.51720800
H	3.04882600	-1.96836800	-0.93645100	H	-0.58280500	-2.86195800	-0.23537600
H	1.98165300	-1.27645000	-2.17545600	H	-2.34773900	-3.03234600	0.04243700
C	3.04422300	1.21688600	-2.33943700	C	-3.62958400	-0.95734600	1.64189600
H	2.03068300	1.18398700	-2.77599000	H	-3.73079300	-1.89654600	1.07327300
H	3.29306300	2.26059500	-2.08640400	H	-3.99867500	-1.15941000	2.66682600
H	3.75454700	0.89424100	-3.12575700	H	-4.30284900	-0.20888000	1.19247300
H	0.09937900	1.03647100	-1.65688900	C	-1.28986900	-1.57877600	2.37973500
				H	-1.65212100	-1.74779700	3.41288300
27				H	-1.34485500	-2.54184300	1.85211900
C	0.14522200	0.47526500	-0.00001000	H	-0.22871700	-1.27809200	2.43141300
C	-0.80274100	1.51424200	0.00000700	C	-2.09943200	0.74374500	2.68844200
C	-0.29462500	-0.86789700	-0.00004000	H	-1.07634400	1.15053100	2.77428200
C	-2.17007500	1.18887200	0.00004100	H	-2.78426000	1.55761800	2.40054500
H	-0.48014700	2.56205600	-0.00001100	H	-2.40494300	0.40377500	3.69689200
C	-1.65172200	-1.21539200	-0.00001500	H	0.89732600	0.76983800	1.38472500
C	-2.58403300	-0.16144900	0.00000500				

P(*t*-Bu)₃

P	-0.00143600	-0.00150600	-0.71420200
C	-1.82512200	-0.01397900	0.00017800
C	0.90028500	1.58641800	-0.00137500
C	0.92566600	-1.57319000	0.00028100
C	0.64922700	1.95096800	1.47982700
H	1.24195600	2.85156600	1.74318800
H	-0.40751600	2.19228500	1.68404900
H	0.95252400	1.14388100	2.16787200
C	2.42851500	1.44452900	-0.21198500
H	2.67958000	1.17176400	-1.25296300
H	2.90671300	2.42252900	-0.00243800
H	2.89043200	0.70855200	0.46631000
C	0.46864200	2.77306900	-0.90649500
H	1.04954200	3.67452100	-0.62423900
H	0.67360900	2.55693300	-1.97054100
H	-0.59733000	3.02851100	-0.81303900
C	2.17317000	-1.78708000	-0.90031400
H	2.93156100	-0.99772400	-0.79127600
H	2.65637600	-2.74743500	-0.62812900
H	1.89002300	-1.84033000	-1.96711400
C	1.36041200	-1.53743500	1.48248700
H	1.85062600	-2.49746500	1.74671200
H	2.09070000	-0.73709400	1.68859900
H	0.50678200	-1.40439200	2.16847400
C	0.04239700	-2.82602200	-0.21997100
H	-0.30963500	-2.90387000	-1.26461600
H	0.64958300	-3.72916100	-0.00889100
H	-0.83229300	-2.86210000	0.44975400
C	-2.01489100	-0.40721700	1.48334100
H	-3.09260200	-0.35393500	1.74356800
H	-1.68485800	-1.43865400	1.69347800
H	-1.47719900	0.26901700	2.16958300
C	-2.46765200	1.37840100	-0.22003600
H	-2.36142900	1.72043500	-1.26550100
H	-3.55265800	1.30448000	-0.00553000
H	-2.05899600	2.15427700	0.44782100
C	-2.63781100	-0.98643600	-0.89929500
H	-2.54950500	-0.71090300	-1.96577400
H	-2.33195300	-2.03820400	-0.79566900
H	-3.70952800	-0.92704400	-0.62052200

PMe₃

P	0.00065400	-0.00098700	-0.61166600
C	-1.23410800	-1.09146500	0.28338000
H	-1.15537300	-1.01204200	1.38502500
H	-2.25976700	-0.81303100	-0.01838800
H	-1.07721800	-2.14557000	-0.00773100
C	-0.33013700	1.61358000	0.28255200
H	-0.30832400	1.50384000	1.38420500
H	0.42603200	2.36282500	-0.01300900
H	-1.31956300	2.00572300	-0.01377900
C	1.56335300	-0.52083400	0.28390500
H	2.39691800	0.14036500	-0.01361400
H	1.45837200	-0.48494000	1.38564600
H	1.83446300	-1.55005000	-0.01238700

PH₃-8

Pd	1.69175500	0.20120100	-0.05355500
C	-2.06063300	0.57574300	0.40044200
C	-2.53754800	-0.45433100	1.21738500
C	-2.72991600	0.87995400	-0.79843200
C	-3.67805500	-1.17678600	0.80940900
H	-2.03076000	-0.71050200	2.15573000
C	-3.86876600	0.18789500	-1.22353200
C	-4.33272400	-0.85282200	-0.39431000
H	-4.05110000	-1.99935200	1.42906300
H	-4.36672400	0.44392100	-2.16408100
H	-5.21624000	-1.42466800	-0.70094800
P	2.96281800	2.06522900	-0.27506100
I	0.72757900	-2.20878300	-0.06176800
C	-0.96680700	1.62032100	0.60700200
C	0.34690300	1.13157600	1.22874000
H	0.90246300	1.95898600	1.70224100
H	0.18233300	0.33982800	1.97886700
O	-2.16469000	1.94418700	-1.47462300
C	-0.86712900	2.16818900	-0.85334100
H	-0.10929100	1.59492500	-1.42453900
H	-0.65549700	3.24922300	-0.91554100
C	-1.52427700	2.73513700	1.55413600
H	-2.47364700	3.13047400	1.15059200
H	-1.72391600	2.33089100	2.56219600
H	-0.80693800	3.57259900	1.64635200
H	3.04822100	3.02759500	0.77801700
H	2.74376500	2.98905900	-1.34286900
H	4.36386100	1.88604800	-0.47995700

PH₃-9-ts

Pd	-1.77084600	0.85126000	-0.11672900
C	0.42818000	-0.30029500	-0.43535800
P	-3.12693100	2.59877600	0.05860700
I	-1.41237900	-1.86354900	-0.23104400
H	0.12841600	0.77889500	-0.60524000
H	0.79932400	-0.70259900	-1.38643600
C	1.40743800	-0.43010700	0.73914900
C	2.57064700	0.47442700	0.31381500
C	2.13713500	-1.80672200	0.75815800
C	3.60738200	-0.34418600	-0.17641900
H	2.47010900	-2.05753100	1.78331600
H	1.53195600	-2.63379400	0.35522400
O	3.33254500	-1.68596300	-0.07702100
C	2.69988400	1.86967800	0.27808100
C	4.78994900	0.18769900	-0.70635300
H	5.58528800	-0.46645600	-1.07697300
C	3.88641500	2.42690700	-0.23841000
C	4.91043700	1.59066400	-0.72862200
H	1.89457300	2.51610700	0.64716500
H	4.01215300	3.51463400	-0.26306700
H	5.82638900	2.03883300	-1.13064800
C	0.77459100	-0.07484000	2.09342900
H	0.20993800	0.87404800	2.02229100
H	0.05988900	-0.85638300	2.40669600
H	1.55370200	0.02877400	2.86900300
H	-3.83754800	2.85981500	1.27349900

H	-4.26633500	2.71412700	-0.79924700
H	-2.68163700	3.94833900	-0.12846500

PH₃-17

Pd	0.24657300	0.15842600	-0.19141600
C	-1.95785800	-0.36276000	-0.33056000
C	-1.90589900	0.51684400	-1.44605900
C	-2.68049300	0.01563000	0.83749600
C	-2.56627900	1.76878900	-1.34889900
H	-1.46912700	0.19072700	-2.39715900
C	-3.33320200	1.24729000	0.93941600
C	-3.26046900	2.11315300	-0.17721200
H	-2.54584400	2.46013500	-2.19798800
H	-3.89977300	1.51431600	1.83671000
H	-3.77510800	3.07990500	-0.12534100
P	0.57735300	2.45752800	0.35106800
I	2.85747100	-0.28367600	0.09225800
C	-1.56423800	-1.85141800	-0.20900800
C	-0.07244100	-1.86741300	-0.55385200
H	0.56423500	-2.49702100	0.08597700
H	0.13820100	-2.06110600	-1.62007900
O	-2.72898700	-0.97731800	1.76674500
C	-1.81263400	-2.04050500	1.32117300
H	-0.87625200	-1.91760100	1.89634600
H	-2.29318500	-2.99745300	1.57977600
C	-2.44986900	-2.77810100	-1.06821100
H	-3.51870000	-2.67013400	-0.80215300
H	-2.33806800	-2.54141500	-2.14133900
H	-2.15651300	-3.83431200	-0.92113500
H	-0.48878400	3.39477600	0.53859400
H	1.30580600	2.75965400	1.53680400
H	1.35668500	3.25331100	-0.53921700

PH₃-18

Pd	-0.91620000	0.11530800	-0.29893700
C	1.15938300	0.37439900	-0.60616000
P	-1.32375700	2.37554000	-0.21257100
I	-3.63226500	-0.23927700	0.13565300
H	1.29424600	1.29585800	-1.20380500
H	1.49981300	-0.46473600	-1.23938600
C	2.05323600	0.46159400	0.66400300
C	3.50725900	0.41225800	0.17809500
C	2.04245400	-0.84594600	1.50875800
C	3.98203900	-0.90398100	0.34247100
H	2.31796000	-0.63667600	2.56196700
H	1.08256800	-1.38429000	1.48627300
O	3.06536800	-1.73237000	0.95627000
C	4.32348000	1.36974600	-0.43590900
C	5.25121400	-1.30647900	-0.08812900
H	5.59695800	-2.33493700	0.05788800
C	5.61332000	0.99449600	-0.86840800
C	6.06281500	-0.32969200	-0.70020300
H	3.97126700	2.39899500	-0.57889300
H	6.26789700	1.73669500	-1.33858200
H	7.06660100	-0.60815000	-1.04149600
C	1.73189100	1.68775500	1.53603400
H	1.78349900	2.61973200	0.94352800

H	0.71486100	1.60942400	1.96383200
H	2.45085600	1.78259700	2.36975500
P	-0.77606800	-2.16638800	-0.56674800
H	-0.30385700	3.34894000	-0.45224000
H	-1.85556000	2.91518800	0.99042000
H	-2.30137500	2.86295200	-1.12073500
H	-1.55133900	-2.70950700	-1.62627200
H	-1.23378100	-3.00111400	0.48864000
H	0.46650700	-2.81672400	-0.84308600

PH₃

P	-0.00014200	-0.00001500	-0.13152900
H	0.56526400	1.05910300	0.65711400
H	0.63593500	-1.01816400	0.65723400
H	-1.19906400	-0.04071000	0.65858200

P(*i*-Pr)₃-8

Pd	0.38693500	-0.41708400	0.09595100
C	-2.91148100	1.26240100	0.39073800
C	-3.46039000	0.89634900	1.62343800
C	-3.68641500	1.15200500	-0.77719200
C	-4.78196700	0.40519900	1.66564000
H	-2.87330900	0.97713400	2.54710800
C	-5.00357100	0.68015600	-0.76455700
C	-5.53901100	0.30280700	0.48283700
H	-5.21766500	0.09422900	2.62149500
H	-5.58109700	0.59556900	-1.69056600
H	-6.56306700	-0.08603200	0.52763400
P	2.57845400	0.22128500	0.09298500
C	3.15468200	1.86183000	-0.67876900
C	3.31641600	0.19018000	1.83986300
C	3.49947200	-1.15137000	-0.82966800
I	-1.46790400	-2.26368000	-0.08564100
C	-1.58995500	1.93143000	0.02254600
C	-0.32939200	1.40957300	0.73957500
H	0.46469300	2.17414600	0.71366400
H	-0.55064500	1.16987600	1.79811300
O	-3.02387900	1.58222000	-1.90720500
C	-1.62264800	1.73504600	-1.52779100
H	-1.08724500	0.80966100	-1.81478700
H	-1.22816000	2.59479100	-2.09542800
C	-1.70392600	3.45366600	0.36618200
H	-2.59618600	3.88617200	-0.12129100
H	-1.80493800	3.60418400	1.45592100
H	-0.81149500	4.00660500	0.01579400
C	2.98098200	-1.27916900	-2.27771400
H	3.12036600	-0.35147600	-2.85894700
H	3.52984000	-2.08587500	-2.79925600
H	1.90491400	-1.53157500	-2.29446700
C	3.38330600	-2.49952300	-0.08706200
H	3.89472500	-3.28576700	-0.67369000
H	3.85056600	-2.47783100	0.91291300
H	2.32747400	-2.80559300	0.03345200
C	2.19882500	2.35189800	-1.78603600
H	2.49594100	3.36650200	-2.11309100
H	2.22883200	1.69404500	-2.67228400
H	1.15419500	2.39182800	-1.44126100

C	4.61125800	1.86237600	-1.19387400
H	5.34024300	1.51960200	-0.44215000
H	4.72068400	1.22645400	-2.09088900
H	4.89361100	2.89084400	-1.48916300
C	4.85254900	0.28423000	1.94476200
H	5.21326300	1.30520300	1.72559800
H	5.16086600	0.04931100	2.98139100
H	5.37889100	-0.42096200	1.27781900
C	2.64164900	1.22992300	2.75669200
H	2.84992900	2.26713100	2.43254900
H	1.54940800	1.08966600	2.79446400
H	3.03288500	1.12634000	3.78628200
H	3.08661900	2.57708500	0.16639700
H	3.00248100	-0.81093100	2.19536700
H	4.56521800	-0.85051400	-0.85824700

P(*i*-Pr)₃-9-ts

Pd	-0.70871500	-0.29453600	-0.12856000
C	1.86968700	-0.42305900	-0.41870100
P	-2.77796400	0.56965900	0.04469400
C	-4.09359900	-0.55140500	-0.73341300
C	-3.33980300	0.73541200	1.85420500
C	-3.11866400	2.30756100	-0.68208800
I	0.89452900	-2.57415700	-0.19494000
H	1.09991700	0.39338500	-0.55422400
H	2.36981700	-0.59058700	-1.38147300
C	2.82528300	-0.10373400	0.74095200
C	3.49749500	1.20200700	0.29946800
C	4.06876600	-1.04269600	0.76768300
C	4.78127300	0.89217700	-0.19101000
H	4.48081200	-1.11407500	1.79250400
H	3.86769200	-2.05382400	0.38083900
O	5.09760700	-0.43996400	-0.08040200
C	3.02810300	2.52133200	0.25229800
C	5.62836500	1.86689700	-0.73356600
H	6.62431700	1.60433500	-1.10398200
C	3.86788100	3.52184000	-0.27733200
C	5.14728500	3.19029300	-0.76757800
H	2.02674200	2.77214300	0.62197900
H	3.52354100	4.56111400	-0.31087800
H	5.78875100	3.97840000	-1.17875100
C	2.10981200	-0.03170400	2.09881300
H	1.21081900	0.60836900	2.02829400
H	1.77164400	-1.03444400	2.41564400
H	2.78384100	0.37977000	2.87069000
C	-4.55355300	2.56779500	-1.18719800
H	-5.32510900	2.35357500	-0.42871300
H	-4.65758900	3.63177100	-1.47645100
H	-4.78401200	1.96519200	-2.08411000
C	-2.08630100	2.66635700	-1.77045900
H	-2.20533500	3.72399300	-2.07787600
H	-1.05402100	2.51597500	-1.40966400
H	-2.21375700	2.03824400	-2.67146300
C	-3.72955500	-0.83505900	-2.20533900
H	-4.49543700	-1.48756700	-2.66800900
H	-3.66264200	0.08528800	-2.81211800
H	-2.75093200	-1.34638600	-2.26692100

C	-4.22255200	-1.87403100	0.04791600
H	-4.91391800	-2.55729400	-0.48195200
H	-3.24118300	-2.37764900	0.12891500
H	-4.61984700	-1.72836500	1.06822300
C	-4.78154100	1.22609100	2.08656400
H	-5.52916200	0.63273200	1.53032300
H	-5.03544500	1.15368500	3.16215400
H	-4.89987800	2.28645800	1.79709700
C	-2.33115800	1.58209000	2.65572100
H	-2.33457100	2.64108400	2.33370600
H	-2.58930500	1.56629500	3.73227300
H	-1.30446000	1.19305100	2.53538100
H	-2.93508700	2.97638600	0.18391700
H	-3.25554900	-0.30637800	2.22087700
H	-5.06453300	-0.01986600	-0.69946200

P(*i*-Pr)₃-17

Pd	0.24272000	0.28831200	-0.22198800
C	2.57865200	0.92603300	-0.34077700
C	2.62741000	0.21864700	-1.56603400
C	3.33059400	0.46089200	0.76901100
C	3.38397900	-0.96764900	-1.63199500
H	2.11399600	0.60364300	-2.45489400
C	4.08864500	-0.71111700	0.71610100
C	4.09194600	-1.41941800	-0.50259900
H	3.40542700	-1.55039900	-2.55816400
H	4.65272000	-1.06071500	1.58595300
H	4.66398100	-2.35180600	-0.56840400
P	-2.04184800	0.37403900	-0.01550400
I	0.36364800	-2.42750400	0.21025900
C	2.05063600	2.33708500	-0.01369200
C	0.56077600	2.33808100	-0.37300800
H	-0.05765200	2.94121900	0.31465100
H	0.39170400	2.67714800	-1.41120300
O	3.28709300	1.31492800	1.83593700
C	2.27600000	2.33084200	1.53055500
H	1.34943400	2.03701100	2.05953900
H	2.65232000	3.28682400	1.93028400
C	2.87547200	3.44164300	-0.71336900
H	3.94617700	3.37197100	-0.44274800
H	2.79478200	3.35302600	-1.81162000
H	2.50442100	4.44301400	-0.42303600
C	-3.00638800	-0.66343900	-1.28712100
C	-2.48712900	-0.28194600	1.70390500
C	-2.78047000	2.11189700	-0.23576600
C	-1.62033000	0.40216800	2.78033700
H	-1.80911600	-0.06862200	3.76380900
H	-0.54571600	0.29476400	2.54977300
H	-1.85702300	1.47933000	2.87622100
C	-3.97242100	-0.31256000	2.13314600
H	-4.10642300	-1.10644400	2.89209000
H	-4.27836800	0.63691500	2.60472300
H	-4.67569700	-0.52043600	1.30941500
C	-3.36887000	-2.09104500	-0.83070000
H	-2.45978600	-2.68994900	-0.64554000
H	-3.99266600	-2.11514900	0.07778000
H	-3.94241100	-2.58359800	-1.63931700

C	-2.23471200	-0.72878000	-2.62368600	H	2.51513400	-1.42767600	2.20690000
H	-2.85888700	-1.23506100	-3.38508000	H	0.96005300	-1.55879600	3.07427500
H	-1.96308200	0.26619300	-3.01278200	C	2.60621000	-3.91022000	1.06903900
H	-1.30494700	-1.31011600	-2.49348300	H	3.27538400	-3.21760100	0.53093100
C	-4.24370000	2.31288000	0.21214300	H	3.17073500	-4.32359600	1.92754400
H	-4.56901500	3.33267500	-0.07117100	H	2.36239200	-4.75369500	0.40291100
H	-4.93489800	1.60476600	-0.28086700	C	-1.83005300	-4.46414200	1.03648500
H	-4.37376200	2.21769300	1.30029300	H	-2.76915300	-4.63171400	1.59840200
C	-2.62499000	2.59459500	-1.69531900	H	-1.98698600	-4.84770800	0.01683900
H	-3.35574600	2.09531600	-2.35745700	H	-1.04909200	-5.07987300	1.52035900
H	-2.82479900	3.68156400	-1.74751500	C	0.31009600	-4.85594100	-1.37684000
H	-1.61684000	2.41407100	-2.10049000	H	-0.73808300	-5.05601900	-1.66014400
H	-2.12178800	-1.32359300	1.60455000	H	0.94690800	-5.29186100	-2.17083000
H	-2.13817300	2.74580200	0.40431000	H	0.51808300	-5.40618800	-0.44456300
H	-3.94622400	-0.09457500	-1.44362500	C	0.07896500	-2.63553000	-2.55991700
P(<i>i</i>-Pr)₃-18				H	-0.99507300	-2.82654800	-2.73492900
Pd	0.42922300	-0.01890100	0.01624300	H	0.25112700	-1.54579900	-2.51478500
C	-1.64501300	0.37008700	0.22037000	H	0.62634600	-3.02706500	-3.43855000
P	1.02299700	2.33140000	0.26880100	C	-1.63119900	-2.43365400	2.51346200
C	-0.41501900	3.55908200	0.57117100	H	-2.68450000	-2.53040900	2.83687700
H	-1.19800900	3.19471600	-0.11851800	H	-1.01638500	-3.02587300	3.21541800
C	2.15241200	2.64800700	1.77756300	H	-1.34240600	-1.37416000	2.62093200
H	1.99271200	3.71883400	2.02332100	C	1.72865400	1.78778200	2.98760100
C	2.03820500	2.98371000	-1.19761300	H	1.87549600	0.71900300	2.75993000
H	2.86025300	2.24202300	-1.18416300	H	2.36027700	2.04260900	3.86061700
I	3.07439300	-0.56011000	-0.82530600	H	0.67730400	1.92678700	3.28202500
H	-1.73650400	1.34285500	0.72380000	C	3.65841000	2.42691600	1.52190200
H	-2.06972100	-0.36706900	0.92066400	H	4.21312600	2.67671700	2.44713800
C	-2.57518000	0.42514600	-1.04024200	H	3.86942800	1.37375700	1.26934200
C	-3.95318300	0.86540100	-0.52664200	H	4.06711500	3.05307000	0.71301000
C	-2.96973800	-0.97723800	-1.58030000	C	1.30068100	2.78477500	-2.53443100
C	-4.76514900	-0.27711200	-0.39107000	H	1.01902300	1.72796200	-2.67780100
H	-3.25829600	-0.92319700	-2.64928000	H	0.38983800	3.40798000	-2.60791100
H	-2.18942400	-1.73791000	-1.45602800	H	1.96806100	3.07185900	-3.36942000
O	-4.14637400	-1.42724100	-0.83428600	C	2.66961900	4.39505900	-1.12051500
C	-4.44852500	2.11094400	-0.12197100	H	2.95873700	4.70432700	-0.10218100
C	-6.05620700	-0.22807100	0.14701100	H	3.58723800	4.40542300	-1.73970400
H	-6.66499700	-1.13365800	0.23770700	H	2.00004700	5.17122200	-1.52653100
C	-5.75217700	2.19408500	0.41188400	C	-0.14852200	5.03695200	0.22227200
C	-6.53836100	1.03370800	0.55037200	H	0.02618800	5.19074500	-0.85414900
H	-3.83474700	3.01544100	-0.21973000	H	-1.03579700	5.63885800	0.50030300
H	-6.15459500	3.16542600	0.72065000	H	0.71344200	5.45081900	0.77567400
H	-7.54903000	1.11037400	0.96814500	C	-0.99009200	3.48008000	2.00352900
C	-2.03708100	1.29900500	-2.18432300	H	-0.30203900	3.93789300	2.73686400
H	-1.83527300	2.33115000	-1.84849000	H	-1.93752500	4.05010600	2.04373600
H	-1.09066900	0.88467100	-2.57373100	H	-1.21042300	2.45121800	2.33269500
H	-2.76737400	1.35710300	-3.01281000	P(<i>i</i>-Pr)₃			
P	0.17459200	-2.40526900	0.31884500	P	0.01459200	-0.05083300	-0.74191600
C	0.59137700	-3.34090200	-1.28955900	C	1.73526600	-0.60837200	-0.13799900
H	1.68835900	-3.18825300	-1.28048200	C	-1.15788100	-1.20826600	0.20681800
C	-1.49889900	-2.95768800	1.06267600	C	-0.19515000	1.64422600	0.13069500
H	-2.26683100	-2.44330600	0.46011600	C	-2.60951900	-0.92367600	-0.23632000
C	1.36208600	-3.17997300	1.61442400	H	-2.73326800	-1.11214200	-1.31926600
H	0.72630800	-3.93396300	2.11904300	H	-3.31538900	-1.58294100	0.30592800
C	1.80283700	-2.13735300	2.66193300	H	-2.91632200	0.11995700	-0.04452200
H	2.31296300	-2.64725800	3.50254600	C	-0.80524100	-2.68455000	-0.06737100

H	-1.57266900	-3.34806200	0.37668500
H	-0.77301400	-2.89452100	-1.15378300
H	0.16902200	-2.97413900	0.36446500
C	-0.99513700	2.59593200	-0.78641600
H	-2.03838700	2.25066900	-0.91411900
H	-1.03252800	3.61585300	-0.35531600
H	-0.54562600	2.66334600	-1.79286900
C	-0.77205900	1.64768300	1.56054800
H	-0.75546000	2.67618900	1.97232000
H	-1.82462300	1.31069700	1.57735200
H	-0.20219900	1.00322100	2.25127500
C	2.00570800	-0.58604100	1.37809900
H	2.98735900	-1.04919900	1.60182400
H	2.04118600	0.44917700	1.76510500
H	1.24014400	-1.13857200	1.95241000
C	2.82229500	0.17284800	-0.90690500
H	2.67073900	0.11243600	-1.99954400
H	2.83167400	1.24365900	-0.62636000
H	3.82706000	-0.23142100	-0.67613500
H	0.84251500	2.03385600	0.18437000
H	1.78733200	-1.66043200	-0.48446500
H	-1.07612000	-1.02382600	1.29649800

P(OMe)₃-8

Pd	-0.68588400	-0.63610800	-0.07245500
C	2.47082200	1.25348900	-0.42975300
C	3.36322400	0.40332300	-1.09043900
C	2.87964100	1.91729100	0.74127000
C	4.65519100	0.21869900	-0.55473900
H	3.06576000	-0.12574200	-2.00401900
C	4.15788200	1.76271700	1.28872300
C	5.04285500	0.89549700	0.61728300
H	5.35654300	-0.46184700	-1.04949800
H	4.44766500	2.28996600	2.20330600
H	6.04900700	0.74068100	1.02408100
P	-2.62256100	0.45562800	0.05160400
I	1.05510200	-2.57004000	0.09678300
C	1.08332800	1.77152700	-0.80179100
C	0.09834600	0.76304100	-1.39865800
H	-0.74288100	1.27115200	-1.89592400
H	0.59008700	0.07947000	-2.11293200
O	1.90473000	2.74762700	1.25731900
C	0.66926200	2.39588100	0.56741400
H	0.13573300	1.64466600	1.18230500
H	0.06217900	3.31039900	0.48182400
C	1.25168200	2.90536400	-1.86992900
H	1.95063300	3.67216900	-1.49021900
H	1.66572200	2.50193600	-2.81090600
H	0.28106000	3.38854800	-2.08733700
O	-2.59616800	2.09294700	0.05389100
O	-3.73754300	0.20494000	-1.13156400
O	-3.55345400	0.00691100	1.34889300
C	-3.82926300	2.87007500	0.04781800
H	-3.52286900	3.91208700	0.22372000
H	-4.32817800	2.77596700	-0.92991700
H	-4.50541100	2.53219500	0.85114100
C	-2.94865800	-0.08348300	2.66699000

H	-3.65840500	-0.65348400	3.28511500
H	-1.97914300	-0.61233000	2.62681600
H	-2.80526600	0.92482300	3.09332200
C	-4.03881600	-1.15856000	-1.52889100
H	-4.64011200	-1.07699200	-2.44672300
H	-3.10796600	-1.71783600	-1.73559900
H	-4.61896100	-1.66575900	-0.73927100

P(OMe)₃-9-ts

Pd	-0.99984800	-0.16630800	-0.16189900
C	1.44598200	-0.41277600	-0.45560600
P	-2.91574300	0.92227300	-0.06076300
I	0.35735700	-2.56986900	-0.21207200
H	0.75911300	0.46315100	-0.68543700
H	1.97055600	-0.67400400	-1.38373700
C	2.36792300	-0.10783800	0.73241200
C	3.08991500	1.16663400	0.27698600
C	3.57994500	-1.08289200	0.81505300
C	4.37705700	0.80671000	-0.16863800
H	3.96059300	-1.14337700	1.85253200
H	3.35802300	-2.09597600	0.44488600
O	4.64999000	-0.53099400	-0.01618300
C	2.65773300	2.49696900	0.18401300
C	5.26768300	1.74385700	-0.70755400
H	6.26590400	1.44507800	-1.04249300
C	3.54211700	3.45895500	-0.34241400
C	4.82559500	3.07882600	-0.78596100
H	1.65256900	2.78379500	0.51521600
H	3.22894600	4.50611600	-0.41221700
H	5.50095000	3.83844700	-1.19638800
C	1.61362800	0.01883000	2.06484000
H	0.73027300	0.67573100	1.95016800
H	1.24768800	-0.96791100	2.40057800
H	2.27343400	0.43994300	2.84378400
O	-3.92986000	0.96596700	-1.37350000
O	-4.06274800	0.41818900	1.05500700
O	-2.79605100	2.54597600	0.20362400
C	-3.97677300	3.39081900	0.23667600
H	-4.73379800	2.97886100	0.92624100
H	-3.63219500	4.37283200	0.59697600
H	-4.40539200	3.48628800	-0.77475800
C	-4.29147900	-0.28827500	-1.99041900
H	-4.99920100	-0.84459100	-1.35007200
H	-4.77462200	-0.03130400	-2.94624400
H	-3.39361500	-0.90712500	-2.18004400
C	-3.60185000	-0.08003100	2.32829200
H	-3.41095800	0.75582300	3.02662500
H	-4.40813800	-0.71683600	2.72669000
H	-2.67641700	-0.67765600	2.20863000

P(OMe)₃-17

Pd	-0.02322100	0.31738400	-0.18841700
C	2.33008900	0.76467200	-0.34528700
C	2.25179500	0.19818900	-1.64218200
C	3.07017800	0.10062900	0.66786900
C	2.87052400	-1.04529100	-1.87452700
H	1.75026600	0.73255700	-2.45779400

C	3.69540800	-1.12932800	0.44732000
C	3.56997200	-1.69259900	-0.83821800
H	2.78910400	-1.51958800	-2.85733900
H	4.25351500	-1.63103000	1.24335100
H	4.03332500	-2.66604400	-1.03389200
P	-2.18936100	0.68331500	0.09576600
I	-0.24011400	-2.39642300	0.01988800
C	1.95867400	2.17266200	0.16572100
C	0.46485400	2.35042300	-0.12272700
H	-0.09458800	2.89867400	0.65405100
H	0.28500300	2.81995700	-1.10682400
O	3.15710500	0.82592500	1.82207600
C	2.23540800	1.95803900	1.68715700
H	1.30471700	1.68260300	2.21934100
H	2.71217900	2.82016900	2.18091400
C	2.86062200	3.27174100	-0.43951500
H	3.92758300	3.07846500	-0.21946600
H	2.74118800	3.31441800	-1.53689200
H	2.59104300	4.26244800	-0.02712900
O	-3.12850300	-0.32955100	-0.78875500
O	-2.77567400	0.67061500	1.62642100
O	-2.81393400	2.18042100	-0.23807000
C	-4.56854200	-0.35215300	-0.59664100
H	-4.96813800	-0.94451000	-1.43351800
H	-4.81426800	-0.84140200	0.36047400
H	-4.99258200	0.66711800	-0.61115400
C	-2.78692000	2.62059400	-1.61479900
H	-3.53467900	2.07372900	-2.21699600
H	-3.03671100	3.69244800	-1.59272000
H	-1.78653700	2.47983700	-2.06335700
C	-2.23603600	-0.24360300	2.61934700
H	-1.13321300	-0.25831200	2.58378900
H	-2.58773400	0.14167000	3.58872100
H	-2.61295100	-1.26534000	2.44859500

P(OMe)₃-18

Pd	0.58182200	0.03755700	0.11413400
C	-1.48125600	0.43879800	0.44792600
P	1.12746200	2.26133700	0.45880900
I	3.18775800	-0.50162700	-0.73310300
H	-1.54657800	1.38153900	1.01277700
H	-1.87533200	-0.37080800	1.08278900
C	-2.33086000	0.56707600	-0.84810100
C	-3.77289600	0.81552100	-0.39005500
C	-2.54189100	-0.78373600	-1.59616700
C	-4.49689000	-0.38576900	-0.51020300
H	-2.71441200	-0.61060200	-2.67726600
H	-1.72099800	-1.50576500	-1.47224300
O	-3.75389200	-1.40890800	-1.06014900
C	-4.39333800	1.94288900	0.16141900
C	-5.82959000	-0.50719000	-0.09959300
H	-6.37113700	-1.45236900	-0.21083000
C	-5.73959200	1.85257500	0.57461000
C	-6.44183400	0.63824200	0.44875700
H	-3.84114000	2.88404700	0.27273900
H	-6.24023500	2.73043700	0.99819000
H	-7.48692300	0.58005300	0.77485000

C	-1.79931600	1.64657700	-1.80925300
H	-1.66693700	2.60661200	-1.28214200
H	-0.81364300	1.34758600	-2.21357900
H	-2.49406500	1.80117300	-2.65519900
P	0.20860500	-2.20329800	0.52846100
O	-1.13330700	-2.58313900	1.39548500
O	0.01948000	-3.31920500	-0.68469800
O	1.43218000	-2.76461000	1.46683100
O	-0.15428900	3.26123300	0.70988600
O	2.10803300	3.11090400	-0.56760600
O	1.93096500	2.55451200	1.85890300
C	0.04636200	4.63528100	1.13788300
H	-0.93386900	5.12593200	1.03514900
H	0.37514200	4.65860500	2.18937300
H	0.79161600	5.13829800	0.49855100
C	1.99418800	2.94916100	-2.00338700
H	2.84650500	3.49919900	-2.43114500
H	2.06915400	1.88281300	-2.27926000
H	1.04759100	3.38494100	-2.37049200
C	3.27968100	2.07615600	2.10214800
H	3.54123600	2.44892800	3.10467600
H	3.31114700	0.97465800	2.07888000
H	3.97226300	2.48343900	1.34732600
C	-2.09839000	-3.62163900	1.07998200
H	-1.60054600	-4.58049700	0.86209200
H	-2.72298800	-3.71480000	1.98226400
H	-2.72162500	-3.31218600	0.22539000
C	1.36067800	-4.07788200	2.07444500
H	2.33146300	-4.22922600	2.57015300
H	0.54777000	-4.11143100	2.82027700
H	1.20737600	-4.85929000	1.30934000
C	0.91070100	-3.34087500	-1.83118900
H	0.87198800	-2.38199700	-2.37528500
H	1.95007200	-3.52998600	-1.51582300
H	0.54322800	-4.15865600	-2.47087100

P(OMe)₃

P	-0.00127900	-0.00350700	0.44490500
O	-1.44300800	-0.16170500	-0.38761600
O	0.86215300	-1.17419800	-0.38113600
O	0.58753000	1.32720300	-0.38089700
C	-2.35673900	-1.18477000	0.06041900
H	-3.34430800	-0.92823700	-0.35480600
H	-2.04303700	-2.17419000	-0.31851000
H	-2.42380900	-1.21834900	1.16598000
C	0.14141300	2.62697100	0.05882800
H	0.14119700	2.70809000	1.16403700
H	0.85055000	3.35983600	-0.35770200
H	-0.87331900	2.83640300	-0.32507200
C	2.21230500	-1.43049600	0.05878900
H	2.49753400	-2.41004700	-0.35660900
H	2.89679300	-0.65312900	-0.32595600
H	2.28231400	-1.46839300	1.16404200

Q-Phos^{*}-8

Pd	-0.41495500	0.04885800	0.09520300
C	-4.28572400	0.34560500	0.31204900

C	-4.77440300	-0.25972800	1.47391500	H	-0.02377800	3.25677800	2.21624000
C	-4.91859400	0.10035400	-0.91940100	H	1.36450600	4.29459200	1.75784900
C	-5.88469200	-1.12449800	1.38089800	H	3.54471100	2.85344300	3.06718600
H	-4.29734000	-0.07846200	2.44539200	H	3.75943700	3.16566400	1.32649200
C	-6.02882600	-0.74252700	-1.04067700	H	3.97323700	1.51017900	1.98508800
C	-6.50100500	-1.35683200	0.13630200	H	5.69420800	-0.47949600	-1.75866400
H	-6.26476800	-1.62204500	2.27997900	H	3.60594900	-1.62122800	-3.09161200
H	-6.49703500	-0.92199400	-2.01375800	H	1.55223400	-1.91897500	1.77666000
H	-7.36118900	-2.03394400	0.07622800	H	4.16119900	-1.39536700	2.46408200
I	-1.65723500	-2.27386800	-0.03448700	H	5.75621800	-2.63851700	0.64289700
C	-3.21677400	1.41363900	0.09389800	H	4.15190200	-3.92564400	-1.14089800
C	-1.90648800	1.24104800	0.88931400	H	1.55221100	-3.45128900	-0.42578000
H	-1.45377000	2.22233800	1.09581300	Q-Phos* -9-ts			
H	-2.08772400	0.72090300	1.84833400	Pd	-0.44603300	-0.06192900	-0.45666500
O	-4.35314700	0.79971400	-1.96437800	C	-2.82980800	-0.72969500	0.27884100
C	-3.09056600	1.33413200	-1.46177200	I	-1.77663600	-2.44366000	-0.99266000
H	-2.28324400	0.63272900	-1.74539400	H	-2.13142900	0.11950800	0.54477200
H	-2.93878400	2.31154000	-1.94997100	H	-3.02123400	-1.32233200	1.18270800
C	-3.82547600	2.79335800	0.50676500	C	-4.09681600	-0.20518500	-0.41354200
H	-4.77393200	2.96996000	-0.03193400	C	-4.71732700	0.71806600	0.64244200
H	-4.04074000	2.81834000	1.59020300	C	-5.21832800	-1.28285000	-0.51015700
H	-3.12958300	3.62001900	0.26827400	C	-5.77766200	0.02768400	1.26212800
P	1.32282900	1.57683700	0.11917200	H	-5.89898500	-1.06027600	-1.35400700
C	2.64846300	0.54958400	-0.64524000	H	-4.83730800	-2.31170200	-0.60509900
C	1.26294000	3.09172200	-1.09523500	O	-6.00600700	-1.21410700	0.72129600
C	1.86603600	2.13892700	1.89527100	C	-4.36058800	1.99879400	1.08459400
Fe	3.42722100	-1.33789000	-0.29249900	C	-6.50693300	0.57810800	2.32394000
C	2.31600000	-0.39074700	-1.71077200	H	-7.33009600	0.02562700	2.78787000
C	4.10082500	0.58981300	-0.57578000	C	-5.08849400	2.57867800	2.14295500
C	1.16070300	2.51101500	-2.52702700	C	-6.14203200	1.86872500	2.75412200
C	2.52393800	3.97796300	-1.00778800	H	-3.53154600	2.54160000	0.61525900
C	-0.00796700	3.93597200	-0.84632600	H	-4.83222700	3.58394100	2.49447700
C	1.49434600	0.98412100	2.85423100	H	-6.69765700	2.33093900	3.57831100
C	1.06642100	3.39342100	2.31880400	C	-3.80400200	0.46686600	-1.76382000
C	3.37524700	2.43322900	2.05581400	H	-2.96072900	1.17565600	-1.66908300
C	4.63363500	-0.28433800	-1.58418700	H	-3.51463200	-0.28541300	-2.51915800
C	3.53374500	-0.88447000	-2.28905200	H	-4.69308300	1.01243400	-2.12605700
C	2.44948800	-2.28269600	1.27272500	P	1.39547100	1.24000100	-0.63221000
C	3.81885900	-2.00241300	1.62330200	C	2.96238000	0.26086300	-0.48622400
C	4.66475200	-2.66827200	0.66676700	C	1.59794500	1.93430100	-2.44092000
C	3.81520800	-3.35366400	-0.27369400	C	1.46158200	2.69324900	0.65279400
C	2.44666000	-3.11099500	0.09974300	Fe	3.97796500	-0.85277300	0.94953100
H	1.30245700	-0.66705100	-2.01618100	C	2.95204600	-1.16036400	-0.78913900
H	4.70327200	1.18135200	0.11098900	C	4.36076000	0.64945000	-0.41278200
H	0.96755600	3.34343900	-3.23143800	C	1.94770800	0.71937200	-3.33434900
H	0.32838800	1.78964500	-2.61944200	C	2.69295800	3.00749400	-2.60941000
H	2.09016000	2.00899700	-2.84196500	C	0.23365100	2.48623700	-2.91859500
H	2.48147600	4.74520500	-1.80616000	C	0.97703200	2.09996000	1.99675100
H	3.44778100	3.39203100	-1.16165000	C	0.44829600	3.77914700	0.22704100
H	2.60085900	4.51252300	-0.04546400	C	2.84928100	3.33357000	0.87429200
H	-0.05041500	4.74472500	-1.60217200	C	5.17819000	-0.50264700	-0.68201400
H	-0.03337200	4.41423700	0.14544300	C	4.30559400	-1.62094400	-0.92269600
H	-0.92001900	3.32648200	-0.96234000	C	2.87543200	-1.07371700	2.68003600
H	1.76612200	1.27357200	3.88885200	C	3.97557600	-0.16796100	2.89709900
H	2.04255900	0.06166500	2.60538200	C	5.19603700	-0.87374000	2.60804900
H	0.41415700	0.75800100	2.82818000	C	4.85007500	-2.21489200	2.21405300
H	1.27098900	3.59168400	3.38905600				

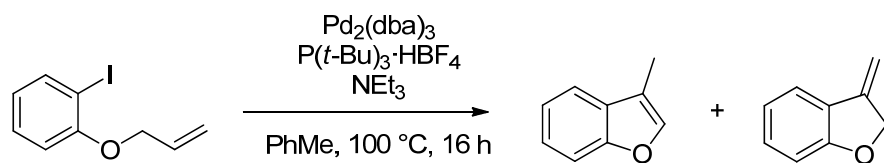
C	3.41577600	-2.33706600	2.25877900
H	2.04176700	-1.75600200	-0.88976100
H	4.74362300	1.64420300	-0.18593900
H	1.90546500	1.03252000	-4.39647400
H	1.22544600	-0.10522000	-3.19133300
H	2.96073300	0.33176500	-3.13417600
H	2.80226800	3.24909000	-3.68593600
H	3.67688900	2.65558400	-2.25146800
H	2.44525700	3.95005300	-2.09092100
H	0.30400500	2.74896300	-3.99325800
H	-0.07964000	3.39290000	-2.37549700
H	-0.55709200	1.72267100	-2.79789100
H	0.93499700	2.90507400	2.75806200
H	1.65940400	1.31837200	2.36674000
H	-0.02930400	1.65412400	1.89643900
H	0.31982800	4.49834400	1.06023500
H	-0.54217900	3.34234500	0.00245100
H	0.78771400	4.35225300	-0.65239000
H	2.74725400	4.17798100	1.58558400
H	3.29256900	3.73541100	-0.05200500
H	3.55559400	2.61294200	1.31931500
H	6.27049300	-0.52889700	-0.66499900
H	4.61723300	-2.64888000	-1.12077900
H	1.81312700	-0.84252600	2.77489400
H	3.90003600	0.87426300	3.21345100
H	6.20466500	-0.45729800	2.65152300
H	5.55052000	-2.99090400	1.89803800
H	2.83638000	-3.22046500	1.98306600

Q-Phos* -17

Pd	1.12699100	0.05220100	-0.28846000
C	2.53042800	2.16646000	-0.58861900
C	3.11748400	1.60604400	-1.74451700
C	3.33606100	2.46174800	0.53800200
C	4.48933500	1.29680500	-1.72211200
H	2.51909800	1.42822400	-2.64585200
C	4.70268300	2.17490400	0.57133400
C	5.25912100	1.57420500	-0.57510700
H	4.95746900	0.82233000	-2.59047300
H	5.30738700	2.39873700	1.45525900
H	6.32353900	1.31359300	-0.56983500
I	3.21891100	-1.53518300	0.54155300
C	1.15128300	2.81334400	-0.37485300
C	0.08798300	1.77958100	-0.74894100
H	-0.86334500	1.88492700	-0.20532800
H	-0.10105400	1.80115500	-1.83853100
O	2.64833800	3.10641400	1.53098400
C	1.23178900	3.06241500	1.16237100
H	0.77555100	2.22098900	1.71912000
H	0.78637700	4.01768100	1.48564100
C	1.02116200	4.14071000	-1.16172100
H	1.81980900	4.85096700	-0.87518800
H	1.09953300	3.95990600	-2.24872000
H	0.04189200	4.61657700	-0.96202900
P	-0.73265700	-1.31783400	-0.10792200
C	-2.41255700	-0.65416500	-0.59687900
C	-0.65512100	-2.81134800	-1.37230900

C	-0.85010500	-1.93271700	1.74614400
Fe	-3.80773400	0.79380400	-0.06117600
C	-2.61264800	0.31946400	-1.66011500
C	-3.73041500	-1.23186900	-0.34879900
C	-0.82261200	-2.20517600	-2.78757800
C	-1.78343100	-3.83799200	-1.12232600
C	0.70973700	-3.52788700	-1.33171400
C	-0.32801400	-0.76193000	2.61395400
C	0.05426000	-3.16129700	1.98835500
C	-2.27542400	-2.28737800	2.22095900
C	-4.68494700	-0.63700900	-1.24147000
C	-3.99283000	0.32437100	-2.05270300
C	-3.14678300	1.91194800	1.54594800
C	-4.32360900	1.16306400	1.90169500
C	-5.38420500	1.55800100	1.01191100
C	-4.86069900	2.54803700	0.10607800
C	-3.47693400	2.76674000	0.43687300
H	-1.83772700	0.94026500	-2.10249600
H	-3.97698100	-1.99138300	0.38875000
H	-0.66640200	-3.01043100	-3.53163400
H	-0.06929500	-1.41986400	-2.98209900
H	-1.82685500	-1.78256700	-2.95530800
H	-1.71182800	-4.62768400	-1.89601200
H	-2.78801500	-3.39006900	-1.20254400
H	-1.69182000	-4.33613500	-0.14167700
H	0.69866800	-4.32599000	-2.10040300
H	0.92603600	-3.99918800	-0.36174200
H	1.54211300	-2.84279000	-1.55767300
H	-0.40079200	-1.04833000	3.68196400
H	-0.92639500	0.15469700	2.46880400
H	0.72876000	-0.53586100	2.38766300
H	0.07392900	-3.35838600	3.07847300
H	1.09472200	-2.98876600	1.66564400
H	-0.33596000	-4.07054200	1.49975400
H	-2.20999900	-2.59910900	3.28176100
H	-2.70939600	-3.13496200	1.66294200
H	-2.96032000	-1.42589000	2.16794900
H	-5.75525900	-0.85379800	-1.26398100
H	-4.43826300	0.97514600	-2.80818900
H	-2.16775200	1.83104400	2.02045200
H	-4.39932900	0.42352700	2.70121300
H	-6.39925300	1.15545500	1.00535900
H	-5.40936400	3.02691100	-0.70750500
H	-2.79507000	3.44593500	-0.07832900

4. Experimental. A typical procedure

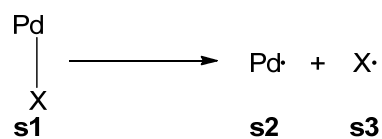


To a 0.5-2 mL biotage microwave vial equipped with a magnetic stir bar was added the aryl iodide (0.1 mmol). The vial was purged with argon for 5 minutes, after which $\text{Pd}_2(\text{dba})_3$ (2.5 mol%), $\text{P}(t\text{-Bu})_3 \cdot \text{HBF}_4$ (10 mol%), toluene (0.5 mL), and NEt_3 (0.2 mmol) were added. The vial was capped and added to an oil bath pre-heated to $100\text{ }^\circ\text{C}$. After stirring for 16 hours, the vial was cooled and 1,3,5-trimethoxybenzene (0.0333 mmol) was added as an internal standard. The contents were filtered over a pad of SiO_2 and washed with Et_2O . ^1H analysis of the crude reaction mixture revealed 34% recovery of starting material and a 15% of the known Heck-type products. The remainder of the mass balance was unidentifiable decomposition products.

5. The computation of bond dissociation energy.

The bond dissociation energy can be computed by the energy increase from the optimized complex to the sum of the single point energies of two bond-broken radicals.

For this type bond dissociation energy:



$$E_{\text{(BDE)}} = E_{\text{(s1)}} - (E_{\text{(s2)}} + E_{\text{(s3)}})$$