

Supporting Information

Mechanism, Reactivity, and Selectivity in Palladium-Catalyzed Organosilicon-Based Cross Coupling Reaction

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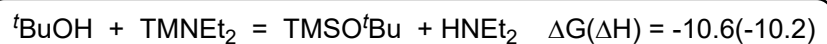
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1. Reaction energies for formation of TMSO^tBu



The reaction free energy is -10.6 kcal/mol, indicating that the formation of the TMSO^tBu is favorable. In addition, TMSO^tBu is a good nucleophile because it contains the ^tBuO group.

2. 3D geometries for the key intermediate and TSs in the transmetalation and C-O reductive elimination steps

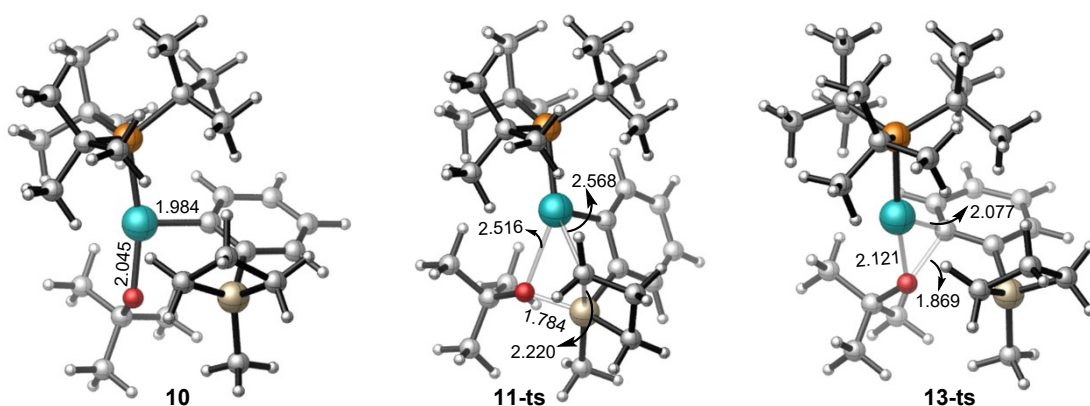


Figure S1. 3D geometries for **10**, **11-ts**, and **13-ts** (bond distances are in Å).

3. 3D geometries for the key intermediate and TS in the final C-C reductive elimination step

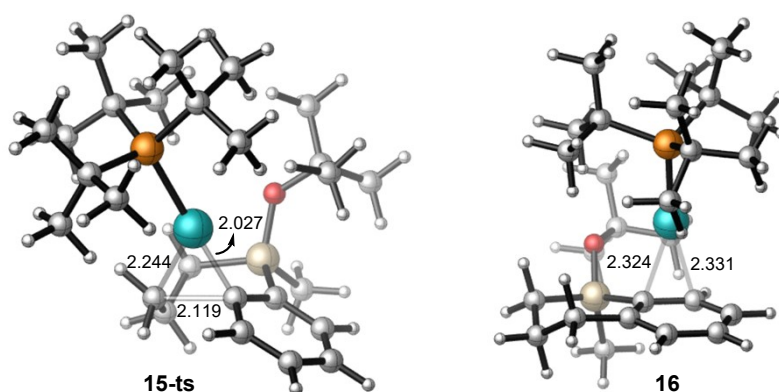


Figure S2. 3D geometries for **15-ts** and **16** (bond distances are in Å).

4. 3D geometries for the key intermediates and TSs in the transmetalation and C-O RE steps with coordination of different bases

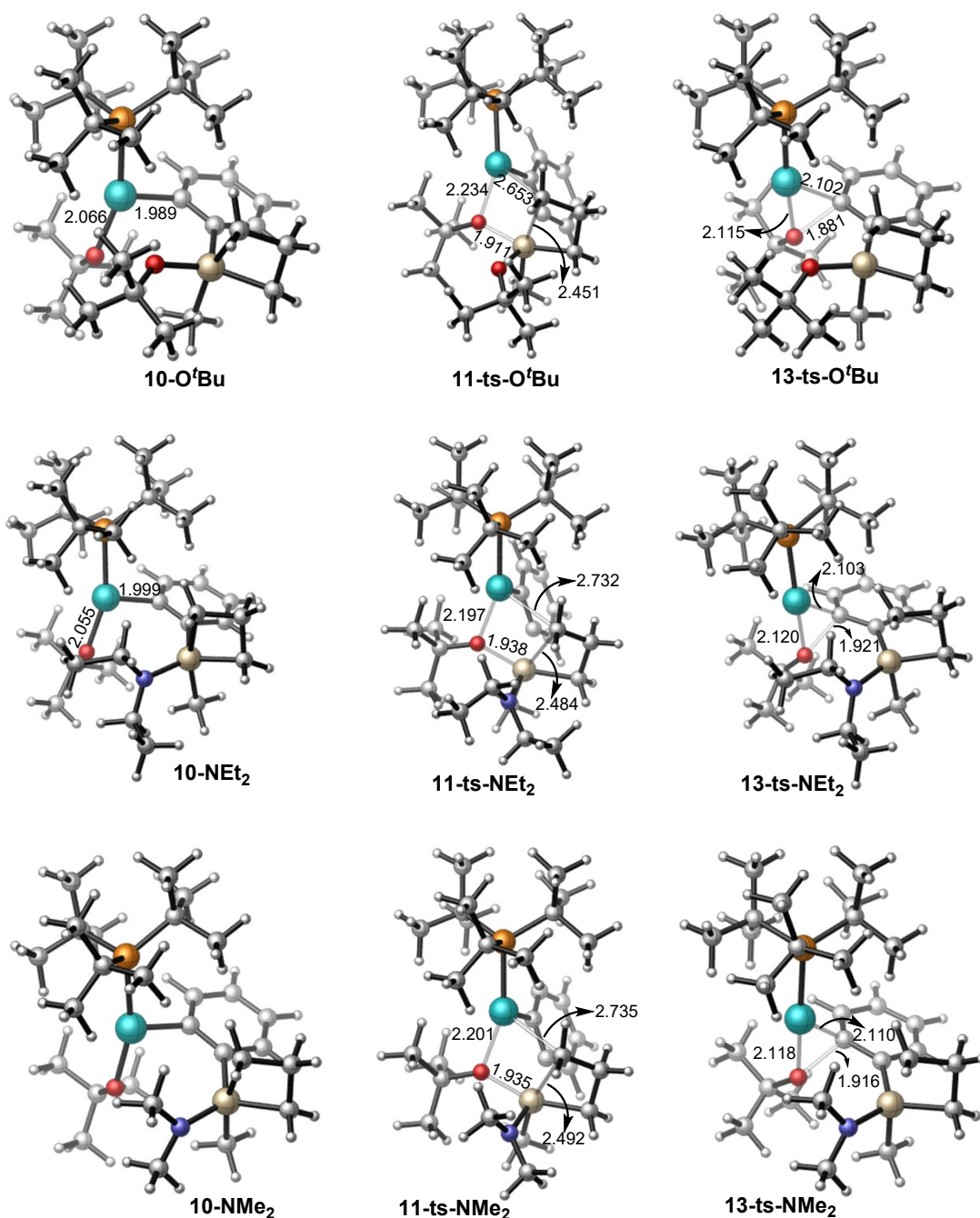


Figure S3. 3D geometries for the key intermediates and TSs in the transmetalation and C-O reductive elimination pathways with the coordination of O^tBu , NEt_2 , and NMe_2 bases.

5. Ring tension of silacyclobutane, silacyclopentane, and silacyclohexane

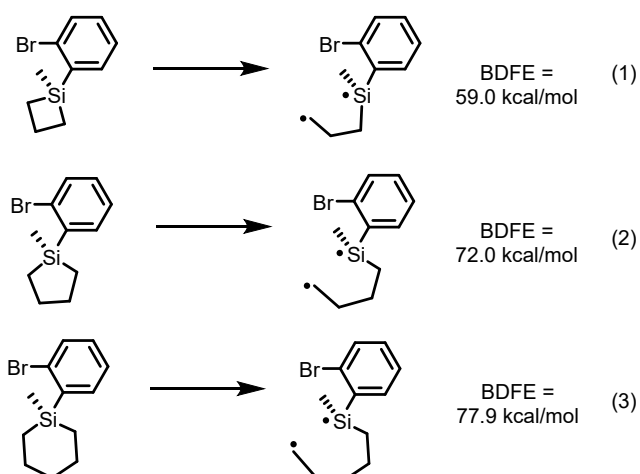


Figure S4. Bond dissociation free energy of the silacyclobutane, silacyclopentane, and silacyclohexane. Note that the lower the BDFE, the higher the ring tension.

6. Results for the high-level single point calculations

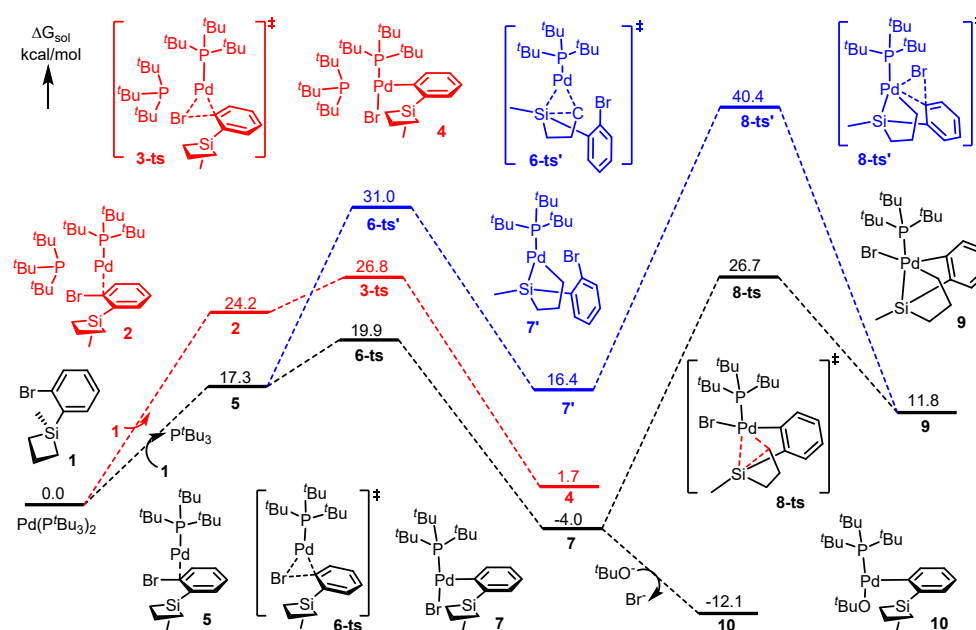


Figure S5. High-level free energy for the oxidative addition and ligand exchange steps. Calculated at B3LYP-D3(BJ)/[6-311++G(d,p) + SDD (Pd)]// B3LYP-D3(BJ)/[6-31+G(d,p) + Lanl2dz (Pd)] level.

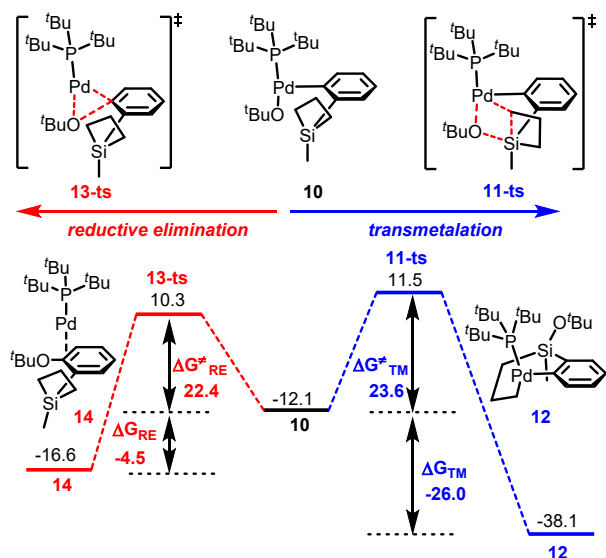


Figure S6. High-level energy profiles for the competing transmetalation and the C-O reductive elimination. Calculated at B3LYP-D3(BJ)/[6-311++G(d,p) + SDD (Pd)]// B3LYP-D3(BJ)/[6-31+G(d,p) + Lanl2dz (Pd)] level.

7. Energetic for all calculated species

Table S1. Energetics (in Hartree) and Imaginary Frequencies (for TSs) for All Calculated Species.

Species	Electronic Energy (EE)	EE + ZPE	Enthalpy	Free Energy	Imaginary Frequency (cm ⁻¹ *i)
1	-691.628875	-691.428197	-691.414118	-691.468945	
2	-2448.468604	-2447.524127	-2447.468980	-2447.609922	
3-ts	-2448.463690	-2447.519669	-2447.465068	-2447.605323	-111.22
4	-2448.505355	-2447.558518	-2447.503832	-2447.642716	
5	-1633.459716	-1632.887072	-1632.851493	-1632.951762	
6-ts	-1633.455319	-1632.883331	-1632.848272	-1632.947217	-109.47
6-ts-prime	-1633.438555	-1632.865473	-1632.830796	-1632.929581	-72.92
7	-1633.496938	-1632.921508	-1632.886644	-1632.983352	
7-prime	-1633.457789	-1632.883802	-1632.848598	-1632.948449	
8-ts	-1633.445851	-1632.871725	-1632.837274	-1632.933176	-200.79
8-ts-prime	-1633.421941	-1632.848873	-1632.814250	-1632.910204	-245.14
9	-1633.468474	-1632.892787	-1632.858098	-1632.954436	
10	-1853.380639	-1852.681764	-1852.641346	-1852.749454	
10-bp86d3	-1853.425925	-1852.748176	-1852.706895	-1852.815662	
10-m06	-1852.259822	-1851.566504	-1851.526613	-1851.632191	
10-m06I	-1853.064036	-1852.365488	-1852.325556	-1852.431763	
10-NEt2	-2066.665160	-2065.827792	-2065.780817	-2065.901497	

10-NMe2	-1988.021509	-1987.241166	-1987.196859	-1987.311003	
10-OtBu	-2086.570389	-2085.746115	-2085.699380	-2085.818191	
10-pbe0d3	-1851.651693	-1850.950397	-1850.910155	-1851.017784	
10-wb97xd	-1852.853475	-1852.148430	-1852.108810	-1852.214877	
11-ts	-1853.345877	-1852.647503	-1852.608137	-1852.712864	-204.05
11-ts-bp86d3	-1853.395554	-1852.718548	-1852.678213	-1852.784516	-193.97
11-ts-m06	-1852.230286	-1851.535446	-1851.497378	-1851.597479	-151.02
11-ts-m061	-1853.035519	-1852.336941	-1852.298316	-1852.400025	-168.62
11-ts-NEt2	-2066.632196	-2065.796393	-2065.750217	-2065.867407	-181.72
11-ts-NMe2	-1987.989212	-1987.210759	-1987.167183	-1987.210759	-181.06
11-ts-OtBu	-2086.535964	-2085.712043	-2085.666329	-2085.781527	-217.46
11-ts-pbe0d3	-1851.620359	-1850.918909	-1850.879977	-1850.983122	-175.46
11-ts-wb97xd	-1852.816762	-1852.110910	-1852.072737	-1852.174863	-169.63
12	-1853.427854	-1852.726887	-1852.687417	-1852.792800	
13-ts	-1853.348577	-1852.650906	-1852.610985	-1852.717718	-358.88
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13-ts-m061	-1853.034809	-1852.338096	-1852.298256	-1852.404642	-316.54
13-ts-NEt2	-2066.634418	-2065.799120	-2065.752364	-2065.872224	-305.72
13-ts-NMe2	-1987.989915	-1987.212124	-1987.167838	-1987.281950	-312.13
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16	-1853.483148	-1852.780836	-1852.740973	-1852.848795	
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NEt2_b3_n	-213.251115	-213.118612	-213.110967	-213.148734	
NMe2_b3_n	-134.608690	-134.533630	-134.528602	-134.558661	
Pd_2PtBu3_b3_n	-1756.852325	-1756.108621	-1756.068770	-1756.175285	
Prod	-911.652393	-911.322437	-911.304026	-911.367221	
PtBu3_b3_n	-814.995620	-814.625144	-814.606603	-814.666170	
tBuO_b3_n	-233.167350	-233.046201	-233.038894	-233.074886	
tBuOH_b3_n	-233.711908	-233.576133	-233.568531	-233.605038	
TMSNEt2_b3_n	-622.555476	-622.304698	-622.289364	-622.345166	
TMSOtBu_b3_n	-642.456211	-642.218523	-642.203500	-642.257723	

8. Reference

Full citation of Gaussian 09 software:

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J., *Gaussian 09*, Revision D.01, Gaussian, Inc., Wallingford CT, **2009**.

9. Cartesian coordinates

1	C	-4.101873	0.614813	-0.291628	C	1.372152	1.958260	-2.789067
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H	-5.240911	4.056628	1.904728	C	0.217355	-2.057601	-4.445889
H	-3.871337	5.167871	1.849702	H	0.724670	-3.026527	-4.536093
H	-4.366942	4.317560	0.390170	H	-0.682646	-2.214076	-3.843626
C	-3.009794	3.158538	3.367176	H	-0.085687	-1.759656	-5.450886
H	-2.525443	4.115177	3.598740	C	2.387687	-0.856226	-4.725014
H	-3.927377	3.112136	3.955240	H	3.169763	-0.241756	-4.275319
H	-2.339932	2.357868	3.694556	H	2.835909	-1.834018	-4.950029

H	2.104170	-0.401040	-5.675906	C	-1.215587	0.485434	4.807552
C	-0.133860	1.018955	-6.185374	C	-0.573855	0.417153	6.048723
H	0.112697	-0.006284	-6.467115	C	0.263491	-0.658526	6.344059
H	-0.812699	1.409461	-6.956146	H	1.163766	-2.455517	5.603520
H	0.782141	1.611555	-6.225576	H	-1.859287	1.329352	4.592497
C	-1.304580	2.548674	-4.599951	H	-0.737882	1.205731	6.778428
H	-0.503248	3.283414	-4.686647	H	0.756274	-0.724169	7.309913
H	-2.046444	2.787827	-5.372659	C	-0.227559	-4.715545	3.229334
H	-1.789623	2.678951	-3.630175	C	-0.457271	-3.330730	1.256489
C	-2.104493	0.236139	-4.836472	C	-0.463218	-4.836088	1.687105
H	-2.784355	0.618874	-5.608964	H	-1.172537	-4.735265	3.781756
H	-1.911194	-0.811248	-5.064240	H	0.436106	-5.469868	3.662673
H	-2.628190	0.280610	-3.876947	H	-1.463375	-2.914373	1.175872
C	-4.565186	0.023802	-1.061530	H	0.073303	-3.099218	0.329586
H	-5.232773	-0.595031	-0.465318	H	-1.379537	-5.374353	1.415981
H	-4.932860	0.001562	-2.094960	H	0.373939	-5.363894	1.217849
H	-3.573789	-0.430565	-1.049687	Si	0.396743	-2.941118	2.899239
C	-3.548767	2.194808	-1.580066	C	2.270128	-2.846427	2.733154
H	-3.514906	3.276570	-1.445323	H	2.641977	-3.647612	2.083942
H	-2.532617	1.796924	-1.512689	H	2.555022	-1.887210	2.288059
H	-3.911137	2.007271	-2.597118	H	2.774287	-2.935799	3.701873
C	-5.896852	2.124534	-0.715078	Br	0.272875	0.345345	0.994226
H	-6.203867	2.102358	-1.768634	C	-2.232094	3.157017	-4.272606
H	-6.651153	1.574715	-0.149587	H	-1.508290	3.141044	-5.097288
H	-5.917676	3.165800	-0.390330	H	-2.599029	2.134307	-4.140022
C	-5.818665	-0.210074	1.955468	H	-3.064434	3.787269	-4.589027
H	-6.445350	-0.580841	2.775665	C	-0.281409	2.788494	-2.823939
H	-6.477346	-0.024544	1.106306	H	-0.564854	1.747251	-2.641061
H	-5.117702	-1.007995	1.691350	H	0.319804	2.817335	-3.742075
C	-4.392563	0.644509	3.758892	H	0.361061	3.104351	-2.003770
H	-5.162990	0.318106	4.468983	C	-1.078406	5.130979	-3.272698
H	-3.705758	-0.192831	3.597509	H	-0.454152	5.157791	-4.176421
H	-3.833361	1.451238	4.229585	H	-1.922782	5.802417	-3.440505
C	-6.125838	2.147485	2.736052	H	-0.478643	5.537655	-2.456685
H	-6.645557	2.484958	1.837942	C	-5.123794	2.967926	-2.738092
H	-6.881404	1.742190	3.421263	H	-6.172364	3.255516	-2.889925
H	-5.685459	3.019442	3.222785	H	-4.681443	2.824875	-3.723009
C	-4.084719	4.445598	1.116163	H	-5.114519	2.003669	-2.220055
H	-5.065830	4.352162	1.584519	C	-5.245631	4.174230	-0.604861
H	-3.659940	5.407706	1.430372	H	-6.291495	4.366841	-0.875551
H	-4.224927	4.495174	0.035006	H	-5.224437	3.247533	-0.024163
C	-2.832182	3.450925	3.038859	H	-4.924191	4.993680	0.038854
H	-2.314625	4.402903	3.208232	C	-4.494420	5.397759	-2.650068
H	-3.735216	3.460428	3.650588	H	-4.038703	5.346291	-3.640988
H	-2.175078	2.649912	3.391229	H	-5.548417	5.672320	-2.795427
C	-1.766149	3.516653	0.825802	H	-4.018322	6.211276	-2.099451
H	-1.054692	2.741924	1.128137	C	-2.249460	5.961094	-0.069186
H	-1.836119	3.502510	-0.259757	H	-3.314932	6.191309	-0.013753
H	-1.356732	4.491628	1.118389	H	-1.771271	6.444210	0.793890
				H	-1.848215	6.431984	-0.969175
				C	-0.441030	4.250034	0.093966
				H	0.116109	4.732118	-0.710653
				H	-0.105509	4.707322	1.034174
				H	-0.171435	3.191147	0.134950
				C	-2.552626	3.851988	1.273848
				H	-2.123244	4.374648	2.139155
				H	-3.635263	3.945541	1.341891
				H	-2.291503	2.793579	1.363686
				C	-3.941913	-1.831758	0.066164
				H	-3.715958	-2.847195	0.382928
				H	-4.407343	-1.887424	-0.925074
				H	-2.994414	-1.295203	-0.064417
				C	-5.022274	0.345945	0.430846
4							
Pd	-1.933109	-0.399696	2.117559				
P	-2.658042	3.383043	-1.475111				
P	-4.128357	-1.000038	2.769652				
C	-4.418004	4.058138	-1.899959				
C	-1.964158	4.451593	-0.022740				
C	-1.526423	3.684607	-3.008708				
C	-4.376159	-2.686489	3.650092				
C	-4.909539	-1.078615	1.008397				
C	-5.010421	0.374384	3.782705				
C	0.482467	-1.637398	5.376230				
C	-0.140563	-1.591949	4.109756				
C	-1.024041	-0.530927	3.869737				

H	-5.807958	0.937087	0.901043	C	1.051598	2.315524	-2.398524
H	-4.078513	0.894505	0.495380	H	1.649688	3.235218	-2.423368
H	-5.275192	0.259244	-0.631797	H	1.254910	1.799179	-1.454464
C	-6.288464	-1.754022	0.944949	H	1.396251	1.678249	-3.210895
H	-6.671341	-1.657607	-0.078583	C	-0.676211	3.441256	-3.829656
H	-6.239662	-2.819886	1.171489	H	-1.717765	3.736215	-3.966015
H	-7.016270	-1.292602	1.612590	H	-0.072248	4.357876	-3.832291
C	-3.997294	-3.830911	2.692449	H	-0.370887	2.854443	-4.698091
H	-3.983924	-4.763560	3.267944	C	-0.707684	3.662844	-1.337195
H	-4.712829	-3.963459	1.880396	H	-0.583660	3.167290	-0.369627
H	-3.003325	-3.692811	2.267939	H	0.024006	4.478188	-1.390915
C	-3.401528	-2.782941	4.840221	H	-1.698589	4.116560	-1.375427
H	-3.551231	-3.756539	5.322178	C	-3.360125	1.985523	-0.344778
H	-2.366019	-2.727325	4.509661	H	-2.758226	2.855963	-0.090663
H	-3.554671	-2.016220	5.597474	H	-4.401840	2.216276	-0.087757
C	-5.811446	-2.925796	4.151240	H	-3.028039	1.153312	0.283102
H	-6.556036	-2.841019	3.359143	C	-4.219138	0.380203	-1.989372
H	-5.866740	-3.946639	4.548421	H	-4.370061	0.081086	-3.027078
H	-6.089523	-2.250501	4.961214	H	-3.845130	-0.479095	-1.425542
C	-6.541794	0.390449	3.629348	H	-5.203422	0.639413	-1.580898
H	-7.005072	-0.551802	3.923588	C	-3.861944	2.753589	-2.687584
H	-6.941624	1.172769	4.286249	H	-4.916106	2.905005	-2.421743
H	-6.859478	0.630037	2.614164	H	-3.347638	3.699062	-2.506112
C	-4.681027	0.222415	5.280674	H	-3.821763	2.543946	-3.757765
H	-5.053647	1.114320	5.797648	C	-0.034640	-0.020135	-4.410339
H	-5.171321	-0.639831	5.733385	H	-0.015579	-0.757634	-5.221909
H	-3.609674	0.156149	5.469749	H	0.343402	0.917921	-4.818478
C	-4.452915	1.738466	3.328750	H	0.651013	-0.368486	-3.631661
H	-3.362588	1.761442	3.354190	C	-1.911666	-1.353322	-3.557907
H	-4.767298	2.004896	2.322714	H	-1.257783	-1.790004	-2.798799
H	-4.827867	2.512950	4.008272	H	-2.937761	-1.427705	-3.203648
5				H	-1.830976	-1.961859	-4.467530
Pd	-0.563943	-0.021607	-0.407922	C	-2.369872	0.646335	-5.010155
P	-1.480412	1.091442	-2.243942	H	-2.238798	0.027826	-5.907463
C	-1.478970	0.089957	-3.888133	H	-3.430423	0.617087	-4.753292
C	-3.295001	1.603406	-1.839702	H	-2.112209	1.671802	-5.279589
C	-0.441811	2.694666	-2.506169	6-ts			
C	-1.908487	-0.735414	2.564924	Pd	-1.369668	0.367704	0.021038
C	-0.917452	-1.393243	1.801504	P	-2.872380	1.558088	-1.393451
C	0.234225	-0.626873	1.482552	C	-3.265613	0.678115	-3.056787
C	0.392286	0.719914	1.895209	C	-4.509715	1.789862	-0.412433
C	-0.617245	1.308471	2.664639	C	-2.126819	3.291042	-1.770664
C	-1.755966	0.577713	3.013367	C	-1.559934	-1.387977	3.394922
H	-2.812980	-1.281177	2.820805	C	-1.044713	-1.502036	2.087022
H	1.308776	1.255597	1.677368	C	-0.353328	-0.374682	1.605783
H	-0.499007	2.336715	2.993589	C	-0.066285	0.758292	2.388565
H	-2.529758	1.034943	3.622425	C	-0.592526	0.813887	3.681668
C	-2.948203	-3.577345	0.920849	C	-1.340375	-0.255682	4.182159
C	-0.961139	-3.640962	-0.447738	H	-2.136216	-2.213821	3.805272
C	-2.501565	-3.403655	-0.568268	H	0.546867	1.562127	1.997764
H	-3.768077	-2.930873	1.244867	H	-0.407503	1.691228	4.295276
H	-3.224670	-4.616635	1.134804	H	-1.739768	-0.213402	5.191089
H	-0.331240	-3.028036	-1.095695	C	-2.985948	-3.851322	1.405982
H	-0.705746	-4.696294	-0.602548	C	-1.924809	-3.015728	-0.596344
H	-2.681792	-2.372008	-0.883798	C	-3.346338	-3.213691	0.022893
H	-3.011746	-4.064032	-1.279761	H	-3.622454	-3.550723	2.242500
Si	-1.141719	-3.224107	1.391521	H	-2.986690	-4.946537	1.351757
C	-0.298950	-4.273935	2.704877	H	-1.782050	-2.103023	-1.178734
H	-0.450525	-5.340867	2.505706	H	-1.629330	-3.874652	-1.210943
H	0.778762	-4.082284	2.733539	H	-3.814244	-2.237903	0.180901
H	-0.706749	-4.052814	3.698305	H	-4.030491	-3.812732	-0.589753
Br	1.935258	-1.590881	0.917670	Si	-1.238339	-3.139260	1.164559

C	0.249744	-4.228647	1.531577	H	-1.782050	-2.103023	-1.178734
H	0.144811	-5.206817	1.048641	H	-1.629330	-3.874652	-1.210943
H	1.171306	-3.762892	1.168153	H	-3.814244	-2.237903	0.180901
H	0.355618	-4.391969	2.610603	H	-4.030491	-3.812732	-0.589753
Br	1.218653	-0.756768	-0.023446	Si	-1.238339	-3.139260	1.164559
C	-1.026116	3.143769	-2.837874	C	0.249744	-4.228647	1.531577
H	-0.479044	4.092039	-2.903401	H	0.144811	-5.206817	1.048641
H	-0.306454	2.364932	-2.568526	H	1.171306	-3.762892	1.168153
H	-1.419324	2.930196	-3.832281	H	0.355618	-4.391969	2.610603
C	-1.403183	3.782560	-0.497849	Br	1.218653	-0.756768	-0.023446
H	-0.666267	3.045120	-0.162704	C	-1.026116	3.143769	-2.837874
H	-0.872397	4.713429	-0.733848	H	-0.479044	4.092039	-2.903401
H	-2.074975	3.989718	0.333552	H	-0.306454	2.364932	-2.568526
C	-3.128753	4.361337	-2.232284	H	-1.419324	2.930196	-3.832281
H	-3.863207	4.602617	-1.461520	C	-1.403183	3.782560	-0.497849
H	-2.582544	5.285917	-2.459261	H	-0.666267	3.045120	-0.162704
H	-3.665573	4.069031	-3.136533	H	-0.872397	4.713429	-0.733848
C	-1.945770	0.097034	-3.607892	H	-2.074975	3.989718	0.333552
H	-2.174359	-0.518175	-4.486956	C	-3.128753	4.361337	-2.232284
H	-1.232609	0.858646	-3.919251	H	-3.863207	4.602617	-1.461520
H	-1.456946	-0.541470	-2.865989	H	-2.582544	5.285917	-2.459261
C	-4.173139	-0.535597	-2.781359	H	-3.665573	4.069031	-3.136533
H	-4.231643	-1.137988	-3.695976	C	-1.945770	0.097034	-3.607892
H	-3.767675	-1.174892	-1.993760	H	-2.174359	-0.518175	-4.486956
H	-5.192600	-0.253071	-2.516356	H	-1.232609	0.858646	-3.919251
C	-3.929470	1.554146	-4.130722	H	-1.456946	-0.541470	-2.865989
H	-3.279138	2.360126	-4.474863	C	-4.173139	-0.535597	-2.781359
H	-4.161102	0.931613	-5.004564	H	-4.231643	-1.137988	-3.695976
H	-4.865941	1.995859	-3.785437	H	-3.767675	-1.174892	-1.993760
C	-4.851280	0.444481	0.264809	H	-5.192600	-0.253071	-2.516356
H	-5.710152	0.594615	0.930865	C	-3.929470	1.554146	-4.130722
H	-5.118760	-0.341541	-0.438999	H	-3.279138	2.360126	-4.474863
H	-4.010604	0.090339	0.871240	H	-4.161102	0.931613	-5.004564
C	-4.264977	2.777535	0.744458	H	-4.865941	1.995859	-3.785437
H	-4.133354	3.806574	0.408489	C	-4.851280	0.444481	0.264809
H	-5.140846	2.761977	1.404231	H	-5.710152	0.594615	0.930865
H	-3.396132	2.486728	1.343429	H	-5.118760	-0.341541	-0.438999
C	-5.719953	2.271476	-1.227902	H	-4.010604	0.090339	0.871240
H	-6.033101	1.542271	-1.977225	C	-4.264977	2.777535	0.744458
H	-6.569372	2.420979	-0.549100	H	-4.133354	3.806574	0.408489
H	-5.534084	3.220836	-1.733051	H	-5.140846	2.761977	1.404231
6-ts-prime				H	-3.396132	2.486728	1.343429
Pd	-1.369668	0.367704	0.021038	C	-5.719953	2.271476	-1.227902
P	-2.872380	1.558088	-1.393451	H	-6.033101	1.542271	-1.977225
C	-3.265613	0.678115	-3.056787	H	-6.569372	2.420979	-0.549100
C	-4.509715	1.789862	-0.412433	H	-5.534084	3.220836	-1.733051
C	-2.126819	3.291042	-1.770664	7			
C	-1.559934	-1.387977	3.394922	Pd	-0.962644	0.856749	-0.130726
C	-1.044713	-1.502036	2.087022	P	-2.326479	2.770322	-0.345988
C	-0.353328	-0.374682	1.605783	C	-3.462655	3.396196	1.066090
C	-0.066285	0.758292	2.388565	C	-3.403634	2.280909	-1.867355
C	-0.592526	0.813887	3.681668	C	-1.110422	4.162173	-0.871535
C	-1.340375	-0.255682	4.182159	C	-1.465147	-0.437978	3.880243
H	-2.136216	-2.213821	3.805272	C	-1.513769	-0.388715	2.468801
H	0.546867	1.562127	1.997764	C	-0.904690	0.711175	1.846906
H	-0.407503	1.691228	4.295276	C	-0.202963	1.666884	2.585333
H	-1.739768	-0.213402	5.191089	C	-0.154758	1.575087	3.980163
C	-2.985948	-3.851322	1.405982	C	-0.806751	0.530824	4.634836
C	-1.924809	-3.015728	-0.596344	H	-1.948414	-1.266204	4.396033
C	-3.346338	-3.213691	0.022893	H	0.297335	2.489216	2.093583
H	-3.622454	-3.550723	2.242500	H	0.384110	2.330821	4.545586
H	-2.986690	-4.946537	1.351757	H	-0.790498	0.462901	5.718860

C	-4.044705	-2.258871	2.234909	C	-1.352452	-0.808087	4.421744
C	-3.181424	-1.803855	0.025911	H	-3.019915	-1.275744	3.162974
C	-4.506679	-1.704508	0.847308	H	1.901494	-1.495343	3.703755
H	-4.469402	-1.749515	3.104436	H	0.500792	-0.465415	5.480256
H	-4.257134	-3.330441	2.330138	H	-1.974369	-0.358644	5.190548
H	-2.985223	-0.993514	-0.676814	C	-3.803156	-1.965574	0.640249
H	-3.117591	-2.750183	-0.525163	C	-2.794136	-0.681712	-1.250638
H	-4.800113	-0.655574	0.952830	C	-3.637729	-0.573842	0.020104
H	-5.355716	-2.237816	0.402761	H	-4.331113	-1.954512	1.600971
Si	-2.250379	-1.936280	1.669814	H	-4.388799	-2.603173	-0.037320
C	-1.025179	-3.344096	1.903624	H	-2.510220	0.300417	-1.639859
H	-1.424733	-4.281566	1.499684	H	-3.347613	-1.221766	-2.026884
H	-0.087612	-3.114505	1.388361	H	-3.141439	0.091135	0.739415
H	-0.806582	-3.498218	2.966978	H	-4.607784	-0.106053	-0.217284
C	-4.619756	1.455135	-1.409476	Si	-2.016317	-2.610781	0.655041
H	-5.094177	1.030491	-2.301770	C	-1.956262	-4.504890	0.801970
H	-4.334521	0.624712	-0.764180	H	-2.487456	-4.967595	-0.038220
H	-5.372496	2.055242	-0.898325	H	-0.928636	-4.881160	0.796052
C	-3.907671	3.462305	-2.712575	H	-2.435072	-4.841275	1.730869
H	-3.098257	3.999613	-3.208143	Br	1.388398	-2.715767	1.057903
H	-4.562474	3.066409	-3.498644	C	0.837251	1.419170	-1.766953
H	-4.490029	4.175491	-2.127672	H	0.861693	2.514297	-1.705516
C	-2.561634	1.341705	-2.760633	H	0.032201	1.059185	-1.118142
H	-2.268837	0.428274	-2.227832	H	1.780162	1.048512	-1.367698
H	-3.178978	1.021804	-3.608559	C	1.745942	1.526505	-4.112406
H	-1.666540	1.807681	-3.166594	H	1.621351	1.259182	-5.163354
C	-4.094140	2.176103	1.765081	H	1.772187	2.622188	-4.052449
H	-4.697905	2.539103	2.605240	H	2.719783	1.163469	-3.780814
H	-4.752360	1.606202	1.112838	C	-0.698560	1.730168	-3.666790
H	-3.333720	1.503146	2.162280	H	-1.565766	1.408523	-3.085226
C	-4.578744	4.337528	0.577375	H	-0.564918	2.803819	-3.487185
H	-5.293622	3.837942	-0.076467	H	-0.923887	1.606936	-4.726578
H	-5.134262	4.688939	1.455270	C	-2.049879	-1.077643	-4.756539
H	-4.192616	5.216587	0.059784	H	-2.275003	-0.028314	-4.573612
C	-2.640576	4.142016	2.133688	H	-2.558598	-1.367690	-5.684296
H	-1.819270	3.537934	2.519539	H	-2.477180	-1.665373	-3.940977
H	-2.248380	5.095055	1.777610	C	-0.451197	-2.902263	-5.107305
H	-3.309585	4.361008	2.974176	H	0.549747	-3.237488	-5.381349
C	-1.758644	5.547844	-1.028380	H	-0.777105	-3.449162	-4.217245
H	-2.113673	5.948716	-0.077661	H	-1.121860	-3.181412	-5.928916
H	-1.000075	6.242304	-1.409621	C	-0.003648	-0.682426	-6.167598
H	-2.589607	5.549805	-1.734006	H	-0.532150	-1.079448	-7.043972
C	0.026088	4.248948	0.166726	H	-0.170670	0.395793	-6.154120
H	-0.314677	4.486234	1.172602	H	1.062136	-0.860240	-6.320976
H	0.589909	3.313028	0.198722	C	2.886647	-1.125302	-2.087280
H	0.713545	5.044069	-0.144945	H	3.768542	-1.755360	-1.919444
C	-0.424906	3.771407	-2.196103	H	3.247221	-0.130964	-2.352342
H	-1.090858	3.818446	-3.057535	H	2.345589	-1.060854	-1.141084
H	0.389804	4.482132	-2.376534	C	1.794537	-3.231885	-2.772500
H	0.018086	2.771368	-2.141902	H	1.183043	-3.297093	-1.866531
Br	0.785272	-0.989870	-0.550035	H	1.309138	-3.828332	-3.542641
7-prime				H	2.761596	-3.700391	-2.552142
Pd	-0.960369	-1.679017	-1.209716	C	2.845612	-1.750222	-4.504405
P	0.318766	-0.895038	-3.257769	H	3.812202	-2.239535	-4.327108
C	2.034852	-1.766272	-3.199339	H	2.351708	-2.296098	-5.309709
C	-0.543445	-1.377531	-4.906944	H	3.051139	-0.736720	-4.853063
C	0.593783	1.008729	-3.235949	8-ts			
C	-1.940660	-1.327970	3.267684	Pd	-1.571169	0.294915	0.472027
C	-1.183331	-1.919547	2.235508	P	-2.371706	2.685716	-0.354735
C	0.193333	-1.940936	2.458948	C	-3.698678	3.586649	0.712920
C	0.824252	-1.444003	3.592367	C	-3.194956	2.142227	-2.015042
C	0.030978	-0.866791	4.587329	C	-0.979310	3.946264	-0.778132
				C	-0.641222	-1.000704	4.274554

C	-1.009324	-0.858993	2.929331	P	-2.530507	2.707842	-0.388412
C	-1.043350	0.417617	2.375155	C	-3.693574	3.731733	0.763504
C	-0.701835	1.563867	3.078530	C	-3.499296	2.307730	-2.018289
C	-0.332217	1.399903	4.422010	C	-1.061027	3.868006	-0.883151
C	-0.302957	0.134569	5.016658	C	-1.046151	-0.920363	4.244625
H	-0.621851	-1.984364	4.737334	C	-0.797594	-0.836667	2.867140
H	-0.692860	2.542537	2.621169	C	-0.447262	0.425143	2.386037
H	-0.057729	2.277150	5.001948	C	-0.279600	1.567955	3.151335
H	-0.013561	0.035872	6.058986	C	-0.523450	1.430876	4.526781
C	-3.149705	-2.936147	2.180294	C	-0.892545	0.200119	5.071713
C	-3.504734	-0.990096	0.792158	H	-1.393691	-1.860739	4.665461
C	-4.068569	-1.712843	2.020139	H	0.019862	2.516240	2.726191
H	-3.105418	-3.370029	3.183920	H	-0.407667	2.301127	5.166933
H	-3.426013	-3.725140	1.470596	H	-1.070932	0.114392	6.139534
H	-3.965713	-0.018300	0.645969	C	-3.090947	-2.660217	1.922118
H	-3.642169	-1.584593	-0.117564	C	-3.816794	-0.558346	0.792966
H	-3.985385	-1.062100	2.898171	C	-4.025568	-1.450533	2.016382
H	-5.133528	-1.953532	1.896645	H	-3.038723	-3.252844	2.843156
Si	-1.622322	-2.005522	1.577948	H	-3.424876	-3.332727	1.120364
C	-0.366610	-3.057679	0.665280	H	-4.463912	0.312905	0.828891
H	-0.811545	-3.469335	-0.248245	H	-4.034405	-1.117182	-0.125242
H	0.514229	-2.472448	0.393898	H	-3.795728	-0.884280	2.928628
H	-0.072047	-3.901667	1.302650	H	-5.081707	-1.754767	2.098063
C	-4.581930	1.514825	-1.782369	Si	-1.457890	-1.860918	1.411181
H	-4.919400	1.079157	-2.730889	C	-0.220789	-3.076203	0.670305
H	-4.559741	0.709529	-1.048854	H	-0.634391	-3.530793	-0.237484
H	-5.334181	2.242684	-1.478380	H	0.722419	-2.589567	0.412611
C	-3.367938	3.247283	-3.070467	H	-0.013766	-3.883307	1.384914
H	-2.422531	3.666003	-3.413533	C	-4.916545	1.797740	-1.693699
H	-3.869542	2.819727	-3.948073	H	-5.370752	1.443286	-2.627362
H	-3.991499	4.065661	-2.704845	H	-4.906103	0.958735	-0.999438
C	-2.306914	1.007862	-2.572901	H	-5.569893	2.574941	-1.296443
H	-2.329874	0.126321	-1.914439	C	-3.644588	3.465548	-3.019245
H	-2.706448	0.676842	-3.539990	H	-2.690203	3.790219	-3.434563
H	-1.266385	1.290895	-2.718622	H	-4.259466	3.122312	-3.861188
C	-4.559026	2.501453	1.393067	H	-4.143816	4.331620	-2.582044
H	-5.277811	2.991656	2.061166	C	-2.774158	1.131025	-2.708254
H	-5.130598	1.899470	0.687748	H	-2.717026	0.260315	-2.046223
H	-3.942446	1.831324	1.999112	H	-3.342513	0.841294	-3.601066
C	-4.613379	4.559276	-0.051990	H	-1.761390	1.374129	-3.027732
H	-5.223879	4.061347	-0.806124	C	-4.650007	2.762847	1.486129
H	-5.303097	5.028493	0.661698	H	-5.278904	3.343279	2.172669
H	-4.054109	5.358489	-0.539808	H	-5.317174	2.229033	0.811138
C	-3.029510	4.365995	1.861346	H	-4.095705	2.031244	2.079652
H	-2.373518	3.731197	2.459803	C	-4.524852	4.824560	0.069089
H	-2.465104	5.234397	1.521018	H	-5.252769	4.414504	-0.632007
H	-3.819605	4.733649	2.527208	H	-5.088744	5.374475	0.833782
C	-1.454894	5.361056	-1.149089	H	-3.908215	5.547967	-0.464568
H	-1.958854	5.865799	-0.323349	C	-2.862242	4.390285	1.881130
H	-0.577037	5.966874	-1.408378	H	-2.193397	3.675937	2.369335
H	-2.123477	5.367555	-2.011332	H	-2.279126	5.241859	1.529744
C	-0.049156	4.023440	0.451211	H	-3.552131	4.768451	2.645399
H	-0.542101	4.412702	1.341302	C	-1.429105	5.305729	-1.290328
H	0.374958	3.042104	0.676721	H	-1.819154	5.881441	-0.448708
H	0.781579	4.701789	0.218376	H	-0.515286	5.812443	-1.627172
C	-0.100623	3.403844	-1.923102	H	-2.149396	5.358184	-2.105848
H	-0.604105	3.394895	-2.889830	C	-0.069698	3.959067	0.294587
H	0.768719	4.066201	-2.021113	H	-0.473606	4.476444	1.161562
H	0.274658	2.403150	-1.699283	H	0.275348	2.973652	0.598346
Br	1.059004	0.275315	-0.153553	H	0.809240	4.524252	-0.040670
				C	-0.285473	3.202114	-2.036550
				H	-0.824239	3.231041	-2.983696
				H	0.654858	3.747524	-2.182943
8-ts-prime							
Pd	-1.867584	0.310032	0.520698				

H	-0.030299	2.164589	-1.806633	H	0.329765	2.945787	0.581865
Br	0.891468	0.43623	0.517376	H	0.908114	4.474483	-0.088262
9				C	-0.192222	3.142917	-2.081465
Pd	-1.614954	0.248415	0.694497	H	-0.738303	3.138587	-3.025360
P	-2.439518	2.711666	-0.388187	H	0.734790	3.705453	-2.250312
C	-3.627315	3.823853	0.658887	H	0.092493	2.123285	-1.817925
C	-3.392895	2.169748	-1.980245	Br	1.004869	0.338864	0.008984
C	-0.966736	3.833755	-0.942631	10			
C	-0.457102	-1.213087	4.452806	Pd	0.012237	1.267185	0.251796
C	-0.847158	-1.058266	3.117905	P	-1.143807	3.315679	0.433299
C	-1.335579	0.178327	2.684526	C	-1.710391	4.016353	2.128700
C	-1.474563	1.270820	3.532735	C	-2.703562	2.960319	-0.647472
C	-1.092571	1.095273	4.870637	C	-0.058877	4.619558	-0.470318
C	-0.585767	-0.128081	5.325575	C	0.875537	-0.157527	4.157546
H	-0.061369	-2.160171	4.811214	C	0.344986	-0.037830	2.853951
H	-1.859556	2.222991	3.188795	C	0.728184	1.080203	2.092518
H	-1.194951	1.926525	5.563447	C	1.665163	1.991327	2.593763
H	-0.294416	-0.232458	6.366994	C	2.192606	1.833444	3.878629
C	-2.728168	-2.801514	1.438695	C	1.784678	0.762826	4.675059
C	-3.561183	-0.476252	0.990030	H	0.574723	-1.001899	4.776201
C	-3.744998	-1.727147	1.836595	H	1.992317	2.829012	1.993216
H	-2.763038	-3.680922	2.094866	H	2.914973	2.554596	4.252717
H	-2.924270	-3.150568	0.416403	H	2.177091	0.641321	5.680848
H	-4.182680	0.349049	1.326208	C	-2.208565	-1.749275	3.459801
H	-3.766818	-0.696698	-0.064133	C	-2.157984	-1.218423	1.111293
H	-3.634122	-1.483637	2.898920	C	-3.079237	-1.057158	2.361067
H	-4.774502	-2.094541	1.708286	H	-2.251395	-1.286290	4.449984
Si	-1.034304	-1.971719	1.505508	H	-2.472573	-2.808459	3.567174
C	0.361444	-3.022086	0.835286	H	-2.156023	-0.389312	0.402879
H	0.251431	-3.170368	-0.243546	H	-2.386804	-2.138619	0.559248
H	1.334078	-2.565810	1.023275	H	-3.194498	0.005498	2.598994
H	0.319991	-4.006165	1.321402	H	-4.086593	-1.475453	2.242387
C	-4.807482	1.669252	-1.626962	Si	-0.708722	-1.501160	2.297326
H	-5.237898	1.207006	-2.524077	C	0.392843	-3.007745	2.047493
H	-4.802863	0.911927	-0.843622	H	-0.211012	-3.911251	1.902946
H	-5.480260	2.472863	-1.327028	H	1.026529	-2.872623	1.167387
C	-3.542485	3.243406	-3.072702	H	1.041705	-3.168869	2.916410
H	-2.587943	3.545765	-3.503943	O	0.815087	-0.509858	-0.362819
H	-4.147829	2.829883	-3.889575	C	2.150606	-0.584076	-0.819182
H	-4.051761	4.136819	-2.708670	C	2.277931	-1.898536	-1.611945
C	-2.639984	0.954691	-2.566685	H	2.054792	-2.755972	-0.967778
H	-2.632342	0.111378	-1.867548	H	1.568751	-1.908148	-2.447431
H	-3.160639	0.619012	-3.472401	H	3.287786	-2.030345	-2.017716
H	-1.608826	1.173382	-2.839396	C	2.490927	0.599342	-1.744497
C	-4.559552	2.900701	1.467806	H	1.790053	0.637007	-2.586995
H	-5.232438	3.522233	2.071505	H	2.413602	1.543313	-1.192720
H	-5.180826	2.259834	0.843829	H	3.507288	0.523705	-2.150212
H	-3.989300	2.270182	2.154343	C	3.140701	-0.604560	0.359359
C	-4.483249	4.818861	-0.145175	H	4.170042	-0.761099	0.014873
H	-5.201618	4.323813	-0.799550	H	3.103720	0.339389	0.909006
H	-5.058995	5.432952	0.559417	H	2.887271	-1.409123	1.056946
H	-3.880771	5.496114	-0.751029	C	-3.361003	4.198821	-1.276561
C	-2.827047	4.626560	1.703161	H	-4.265686	3.878382	-1.808121
H	-2.136546	3.999665	2.270994	H	-3.662240	4.936874	-0.531923
H	-2.263684	5.450914	1.266289	H	-2.715651	4.689449	-2.006583
H	-3.536297	5.062804	2.416902	C	-3.757750	2.214474	0.192711
C	-1.334042	5.253787	-1.407483	H	-4.539847	1.852185	-0.484983
H	-1.750235	5.866938	-0.607078	H	-3.335840	1.345127	0.699241
H	-0.416701	5.752333	-1.746920	H	-4.241872	2.851698	0.932783
H	-2.035314	5.259161	-2.242895	C	-2.289860	1.981959	-1.770121
C	0.012658	3.935168	0.246816	H	-1.554264	2.390568	-2.459583
H	-0.395700	4.484344	1.093436	H	-1.898846	1.042423	-1.361656

H	-3.182514	1.725225	-2.353226
C	1.358657	4.583936	0.136697
H	1.387418	4.849605	1.191951
H	1.809317	3.595618	0.011787
H	1.982501	5.307392	-0.402035
C	-0.595317	6.059359	-0.420020
H	0.051057	6.692523	-1.040460
H	-1.609895	6.145158	-0.809836
H	-0.579103	6.474202	0.589145
C	0.112613	4.201485	-1.944087
H	0.448346	3.164161	-2.034105
H	-0.793971	4.333046	-2.534867
H	0.885720	4.837754	-2.390679
C	-0.531234	4.680536	2.863192
H	0.314022	4.002730	2.978162
H	-0.192941	5.597573	2.380118
H	-0.874086	4.951700	3.868741
C	-2.844134	5.051647	2.021242
H	-3.772261	4.626010	1.639694
H	-3.054737	5.435439	3.026998
H	-2.573672	5.904053	1.396212
C	-2.171070	2.838335	3.011877
H	-1.374645	2.105140	3.148101
H	-2.440209	3.233628	3.998890
H	-3.045774	2.325209	2.617149

10-bp86d3

Pd	-0.010985	1.271151	0.265877
P	-1.136401	3.298771	0.439771
C	-1.705048	4.002512	2.140821
C	-2.701396	2.943320	-0.647462
C	-0.048756	4.608137	-0.468191
C	0.877093	-0.144146	4.169608
C	0.344238	-0.019584	2.858672
C	0.731429	1.105374	2.094394
C	1.682619	2.015660	2.594626
C	2.212251	1.851727	3.887237
C	1.794920	0.778377	4.689986
H	0.569683	-0.997059	4.789878
H	2.020964	2.856358	1.986883
H	2.946182	2.574126	4.262395
H	2.189593	0.655229	5.704274
C	-2.229868	-1.733265	3.430807
C	-2.142629	-1.194825	1.075837
C	-3.077150	-1.023288	2.319359
H	-2.284990	-1.278408	4.433662
H	-2.502510	-2.800878	3.522179
H	-2.109216	-0.352227	0.367967
H	-2.373714	-2.115274	0.508671
H	-3.175187	0.050047	2.560444
H	-4.100411	-1.422832	2.187113
Si	-0.704511	-1.488296	2.284363
C	0.410796	-2.999056	2.060650
H	-0.191042	-3.914518	1.920466
H	1.054771	-2.867924	1.176369
H	1.059065	-3.145877	2.942890
O	0.772199	-0.511313	-0.361319
C	2.119484	-0.570643	-0.819771
C	2.248753	-1.886995	-1.618560
H	2.032391	-2.753726	-0.969538
H	1.530205	-1.899207	-2.457164
H	3.265444	-2.012453	-2.032169
C	2.445550	0.625898	-1.740672

H	1.746465	0.654459	-2.596204
H	2.337082	1.570680	-1.176086
H	3.475817	0.576719	-2.139611
C	3.109429	-0.588145	0.364692
H	4.149299	-0.736494	0.020841
H	3.060285	0.362149	0.920694
H	2.857509	-1.402332	1.065311
C	-3.355414	4.183641	-1.284204
H	-4.260010	3.859510	-1.832369
H	-3.670947	4.924894	-0.534780
H	-2.697500	4.682906	-2.011373
C	-3.755926	2.199565	0.200100
H	-4.549293	1.835226	-0.478398
H	-3.328199	1.321712	0.708425
H	-4.238192	2.843356	0.949961
C	-2.273009	1.955748	-1.761800
H	-1.547351	2.374634	-2.470236
H	-1.850163	1.023636	-1.337577
H	-3.171251	1.661460	-2.336285
C	1.371753	4.562526	0.139242
H	1.404490	4.843081	1.200538
H	1.808371	3.555642	0.024390
H	2.011071	5.275511	-0.413828
C	-0.587369	6.050441	-0.414041
H	0.062557	6.691081	-1.039309
H	-1.611344	6.136873	-0.805443
H	-0.569359	6.467320	0.604480
C	0.116337	4.181388	-1.944016
H	0.450528	3.132701	-2.026989
H	-0.799357	4.313794	-2.538188
H	0.897396	4.816986	-2.400397
C	-0.518921	4.666254	2.871294
H	0.329476	3.976663	2.987480
H	-0.173629	5.587569	2.379630
H	-0.860662	4.944998	3.885254
C	-2.842101	5.038553	2.026853
H	-3.774080	4.608997	1.631679
H	-3.064977	5.422264	3.039972
H	-2.564727	5.900702	1.401842
C	-2.162145	2.815695	3.020231
H	-1.359915	2.071370	3.141621
H	-2.422703	3.205681	4.021712
H	-3.049818	2.305584	2.624109

10-m06

Pd	0.024626	1.255847	0.274263
P	-1.122302	3.337929	0.438252
C	-1.739607	4.040631	2.117293
C	-2.645694	2.961801	-0.681601
C	-0.039474	4.662549	-0.436669
C	0.866445	-0.187039	4.175520
C	0.344120	-0.066390	2.871967
C	0.734907	1.052507	2.126027
C	1.661171	1.965701	2.632365
C	2.174883	1.804638	3.918722
C	1.765851	0.730935	4.703511
H	0.564677	-1.039642	4.789540
H	1.988548	2.812687	2.034491
H	2.892708	2.527882	4.302928
H	2.152832	0.604894	5.712678
C	-2.187351	-1.768523	3.506322
C	-2.168424	-1.290069	1.169616
C	-3.031835	-1.036597	2.430479

H	-2.216496	-1.336334	4.512676
H	-2.475412	-2.826921	3.575224
H	-2.187000	-0.520876	0.390145
H	-2.426985	-2.253858	0.707227
H	-3.048813	0.041424	2.651700
H	-4.078213	-1.364759	2.353084
Si	-0.701550	-1.544391	2.332213
C	0.411413	-3.038152	2.101106
H	-0.182132	-3.959263	2.040578
H	0.991848	-2.940519	1.176852
H	1.115635	-3.140304	2.936882
O	0.811770	-0.555599	-0.319179
C	2.104373	-0.610606	-0.856651
C	2.227301	-1.945777	-1.595954
H	2.061358	-2.782499	-0.904517
H	1.475198	-2.011474	-2.393340
H	3.220058	-2.069805	-2.049897
C	2.345684	0.526097	-1.852577
H	1.565070	0.520495	-2.627896
H	2.313137	1.499181	-1.340155
H	3.322185	0.438196	-2.349969
C	3.170369	-0.549561	0.240018
H	4.180576	-0.692177	-0.168511
H	3.144543	0.422351	0.751049
H	2.990818	-1.328582	0.994639
C	-3.332193	4.179812	-1.298322
H	-4.205427	3.832590	-1.869940
H	-3.695805	4.888017	-0.546721
H	-2.687565	4.722085	-1.997927
C	-3.685359	2.174709	0.120798
H	-4.449677	1.805060	-0.577265
H	-3.252068	1.300480	0.622130
H	-4.202888	2.784726	0.866569
C	-2.186561	2.027895	-1.812893
H	-1.491268	2.490582	-2.515468
H	-1.726490	1.101613	-1.431169
H	-3.071615	1.718853	-2.387571
C	1.360253	4.640011	0.189224
H	1.371493	4.879112	1.255886
H	1.844616	3.664939	0.044484
H	1.978022	5.393750	-0.319721
C	-0.588236	6.088890	-0.383371
H	0.060613	6.730849	-0.997043
H	-1.601564	6.171707	-0.789562
H	-0.586386	6.509835	0.627513
C	0.158430	4.279078	-1.906797
H	0.502693	3.243214	-2.024131
H	-0.738781	4.424692	-2.516387
H	0.937548	4.931400	-2.325731
C	-0.590743	4.704974	2.880210
H	0.262011	4.031927	3.020097
H	-0.242204	5.632746	2.417258
H	-0.962571	4.968708	3.880399
C	-2.870996	5.061839	1.984744
H	-3.799243	4.627128	1.600425
H	-3.095402	5.456044	2.986476
H	-2.601508	5.915504	1.354192
C	-2.217377	2.875549	2.992068
H	-1.411125	2.157572	3.189892
H	-2.543414	3.284075	3.959373
H	-3.066711	2.333898	2.567401

10-m06I

Pd	0.024626	1.255847	0.274263
P	-1.122302	3.337929	0.438252
C	-1.739607	4.040631	2.117293
C	-2.645694	2.961801	-0.681601
C	-0.039474	4.662549	-0.436669
C	0.866445	-0.187039	4.175520
C	0.344120	-0.066390	2.871967
C	0.734907	1.052507	2.126027
C	1.661171	1.965701	2.632365
C	2.174883	1.804638	3.918722
C	1.765851	0.730935	4.703511
H	0.564677	-1.039642	4.789540
H	1.988548	2.812687	2.034491
H	2.892708	2.527882	4.302928
H	2.152832	0.604894	5.712678
C	-2.187351	-1.768523	3.506322
C	-2.168424	-1.290069	1.169616
C	-3.031835	-1.036597	2.430479
H	-2.216496	-1.336334	4.512676
H	-2.475412	-2.826921	3.575224
H	-2.187000	-0.520876	0.390145
H	-2.426985	-2.253858	0.707227
H	-3.048813	0.041424	2.651700
H	-4.078213	-1.364759	2.353084
Si	-0.701550	-1.544391	2.332213
C	0.411413	-3.038152	2.101106
H	-0.182132	-3.959263	2.040578
H	0.991848	-2.940519	1.176852
H	1.115635	-3.140304	2.936882
O	0.811770	-0.555599	-0.319179
C	2.104373	-0.610606	-0.856651
C	2.227301	-1.945777	-1.595954
H	2.061358	-2.782499	-0.904517
H	1.475198	-2.011474	-2.393340
H	3.220058	-2.069805	-2.049897
C	2.345684	0.526097	-1.852577
H	1.565070	0.520495	-2.627896
H	2.313137	1.499181	-1.340155
H	3.322185	0.438196	-2.349969
C	3.170369	-0.549561	0.240018
H	4.180576	-0.692177	-0.168511
H	3.144543	0.422351	0.751049
H	2.990818	-1.328582	0.994639
C	-3.332193	4.179812	-1.298322
H	-4.205427	3.832590	-1.869940
H	-3.695805	4.888017	-0.546721
H	-2.687565	4.722085	-1.997927
C	-3.685359	2.174709	0.120798
H	-4.449677	1.805060	-0.577265
H	-3.252068	1.300480	0.622130
H	-4.202888	2.784726	0.866569
C	-2.186561	2.027895	-1.812893
H	-1.491268	2.490582	-2.515468
H	-1.726490	1.101613	-1.431169
H	-3.071615	1.718853	-2.387571
C	1.360253	4.640011	0.189224
H	1.371493	4.879112	1.255886
H	1.844616	3.664939	0.044484
H	1.978022	5.393750	-0.319721
C	-0.588236	6.088890	-0.383371
H	0.060613	6.730849	-0.997043
H	-1.601564	6.171707	-0.789562
H	-0.586386	6.509835	0.627513

C	0.158430	4.279078	-1.906797
H	0.502693	3.243214	-2.024131
H	-0.738781	4.424692	-2.516387
H	0.937548	4.931400	-2.325731
C	-0.590743	4.704974	2.880210
H	0.262011	4.031927	3.020097
H	-0.242204	5.632746	2.417258
H	-0.962571	4.968708	3.880399
C	-2.870996	5.061839	1.984744
H	-3.799243	4.627128	1.600425
H	-3.095402	5.456044	2.986476
H	-2.601508	5.915504	1.354192
C	-2.217377	2.875549	2.992068
H	-1.411125	2.157572	3.189892
H	-2.543414	3.284075	3.959373
H	-3.066711	2.333898	2.567401

10-NEt2

Pd	-1.088802	0.377770	-0.172717
P	-2.501726	2.272269	-0.509128
C	-3.401708	3.228190	0.902092
C	-3.820357	1.677442	-1.786811
C	-1.322145	3.506794	-1.409899
C	-1.326274	-0.383082	4.029348
C	-1.488596	-0.598268	2.635799
C	-0.950550	0.408061	1.821101
C	-0.209438	1.480256	2.341057
C	-0.060857	1.639241	3.720045
C	-0.650912	0.707918	4.574076
H	-1.733483	-1.120273	4.715937
H	0.244209	2.205843	1.678001
H	0.501711	2.483695	4.111420
H	-0.567781	0.815724	5.653231
C	-3.535252	-2.787669	3.743914
C	-4.226190	-1.476856	1.938322
C	-4.474610	-1.604110	3.451975
H	-3.152716	-2.879040	4.771819
H	-4.045598	-3.736459	3.511931
H	-4.388561	-0.475797	1.528251
H	-4.906777	-2.158695	1.406531
H	-4.117735	-0.706984	3.975628
H	-5.527570	-1.741476	3.754043
Si	-2.371593	-2.329375	2.210673
C	-0.780124	-3.304876	2.926391
H	-0.953939	-4.383603	3.062995
H	0.153059	-3.193950	2.355923
H	-0.576791	-2.906580	3.928730
O	0.253600	-1.124595	-0.578009
C	1.655685	-1.003339	-0.598721
C	2.199691	-2.308142	-1.213457
H	1.883983	-3.164490	-0.608085
H	1.800991	-2.444098	-2.225363
H	3.294935	-2.309979	-1.272290
C	2.100591	0.189663	-1.465996
H	1.680562	0.097980	-2.474611
H	1.739186	1.127036	-1.031023
H	3.192403	0.253671	-1.554306
C	2.226157	-0.839757	0.820824
H	3.323221	-0.828829	0.816490
H	1.874891	0.093456	1.269499
H	1.891870	-1.663357	1.459430
C	-4.973652	0.982611	-1.040294
H	-5.607212	0.479614	-1.780521

H	-4.612118	0.221809	-0.346958
H	-5.610083	1.678231	-0.492830
C	-4.402408	2.765205	-2.702998
H	-3.654129	3.180370	-3.380014
H	-5.182751	2.309748	-3.325821
H	-4.861753	3.586347	-2.152156
C	-3.168611	0.588065	-2.664360
H	-2.755708	-0.216943	-2.052779
H	-3.940753	0.150693	-3.308959
H	-2.378872	0.964972	-3.310727
C	-3.976091	2.198319	1.892881
H	-4.404445	2.739711	2.745371
H	-4.769407	1.594268	1.457973
H	-3.203198	1.527245	2.268684
C	-4.536937	4.145580	0.412541
H	-5.366668	3.591908	-0.027667
H	-4.936251	4.686974	1.279275
H	-4.197871	4.890023	-0.309468
C	-2.407306	4.094724	1.697298
H	-1.567073	3.514519	2.077181
H	-2.029400	4.942883	1.126187
H	-2.941167	4.502563	2.564176
C	-1.916812	4.891827	-1.715914
H	-2.132674	5.463464	-0.812185
H	-1.178362	5.465806	-2.290229
H	-2.826738	4.840650	-2.314527
C	-0.052312	3.685457	-0.552062
H	-0.239662	4.144629	0.416505
H	0.439767	2.723864	-0.390275
H	0.644554	4.335085	-1.095967
C	-0.841498	2.877524	-2.733170
H	-1.617824	2.851415	-3.498241
H	-0.021114	3.490558	-3.125130
H	-0.452725	1.865415	-2.586263
N	-2.295202	-3.124462	0.571030
C	-1.581830	-4.367423	0.301184
H	-1.113098	-4.337686	-0.692256
H	-0.757509	-4.473642	1.000499
C	-2.457971	-5.626413	0.386522
H	-1.875035	-6.530199	0.165745
H	-2.882719	-5.733059	1.391847
H	-3.293255	-5.591540	-0.322490
C	-3.225551	-2.767919	-0.502305
H	-3.537196	-1.736255	-0.342051
H	-4.153794	-3.371470	-0.474056
C	-2.660432	-2.870071	-1.925202
H	-2.477300	-3.903794	-2.236191
H	-3.378883	-2.444561	-2.634613
H	-1.718237	-2.319066	-2.011727

10-NMe2

Pd	-1.109422	0.367238	-0.110237
P	-2.499982	2.263838	-0.516448
C	-3.394455	3.263464	0.868102
C	-3.825108	1.644110	-1.774596
C	-1.306281	3.461606	-1.443377
C	-1.307933	-0.432737	4.068148
C	-1.494983	-0.609811	2.672891
C	-0.990346	0.425660	1.876714
C	-0.274210	1.507622	2.408712
C	-0.110264	1.637241	3.789261
C	-0.652213	0.663315	4.628021
H	-1.673021	-1.203467	4.741843

H	0.153598	2.256445	1.754036	C	-0.835961	2.789742	-2.748779
H	0.433031	2.487876	4.194153	H	-1.611208	2.766567	-3.515313
H	-0.546146	0.742684	5.707684	H	0.001652	3.371071	-3.152505
C	-3.417963	-2.903941	3.769339	H	-0.476446	1.770937	-2.577729
C	-4.256236	-1.493474	2.096004	N	-2.477315	-3.097543	0.566212
C	-4.411529	-1.739939	3.608163	C	-1.625143	-4.147207	0.039424
H	-2.970971	-3.041660	4.765696	H	-0.850175	-3.763447	-0.648210
H	-3.907520	-3.856702	3.510549	H	-1.121772	-4.701349	0.828673
H	-4.472346	-0.467086	1.778955	C	-3.243144	-2.532731	-0.524798
H	-4.950252	-2.151297	1.549767	H	-3.739521	-1.614892	-0.222300
H	-4.056948	-0.868013	4.173847	H	-4.016087	-3.227397	-0.909852
H	-5.439740	-1.938141	3.957956	H	-2.220605	-4.877348	-0.537884
Si	-2.363854	-2.332608	2.204788	H	-2.594826	-2.292296	-1.384307
C	-0.699890	-3.302397	2.714379				
H	-0.831939	-4.389236	2.830309	10-OtBu			
H	0.143584	-3.141667	2.029525	Pd	-1.072223	0.196404	0.033039
H	-0.384711	-2.929987	3.697929	P	-2.531516	1.991349	-0.459089
O	0.210443	-1.185605	-0.368622	C	-3.470637	3.012959	0.876491
C	1.606705	-1.035095	-0.467172	C	-3.823907	1.188794	-1.639536
C	2.171117	-2.396584	-0.920342	C	-1.438580	3.203504	-1.483948
H	1.927589	-3.168910	-0.183231	C	-1.178983	-0.112396	4.276989
H	1.727481	-2.689633	-1.878609	C	-1.437638	-0.408842	2.915977
H	3.260864	-2.367498	-1.041607	C	-0.886072	0.496103	1.990064
C	1.979233	0.035587	-1.510838	C	-0.103551	1.587683	2.390420
H	1.534961	-0.215389	-2.481608	C	0.126867	1.839804	3.745288
H	1.592454	1.012815	-1.204034	C	-0.426898	0.985279	4.696807
H	3.064592	0.125178	-1.645100	H	-1.566663	-0.782349	5.037617
C	2.231801	-0.663766	0.890945	H	0.328523	2.250413	1.651590
H	3.327425	-0.641313	0.838984	H	0.731152	2.693642	4.042722
H	1.884065	0.319281	1.220060	H	-0.265522	1.160496	5.757916
H	1.936093	-1.392827	1.651895	C	-3.014697	-2.748815	4.364120
C	-4.973296	0.977453	-0.993654	C	-4.285014	-1.562865	2.813824
H	-5.604175	0.430956	-1.704575	C	-4.181096	-1.742887	4.337872
H	-4.605752	0.260385	-0.258264	H	-2.396530	-2.778389	5.275073
H	-5.613274	1.697753	-0.483558	H	-3.401234	-3.771142	4.222195
C	-4.410751	2.710961	-2.713140	H	-4.680284	-0.602078	2.461094
H	-3.664181	3.108133	-3.402865	H	-4.931349	-2.345980	2.388672
H	-5.194782	2.242308	-3.321439	H	-3.876107	-0.799357	4.809998
H	-4.865873	3.545890	-2.180110	H	-5.103660	-2.064891	4.851253
C	-3.187136	0.533464	-2.637836	Si	-2.346511	-2.101643	2.593773
H	-2.745966	-0.253896	-2.021778	C	-0.674479	-3.151583	2.628547
H	-3.973951	0.070780	-3.246199	H	-0.846402	-4.236834	2.583772
H	-2.423266	0.902770	-3.318845	H	-0.001645	-2.891208	1.803493
C	-3.972403	2.263963	1.887373	H	-0.137917	-2.964508	3.571716
H	-4.392807	2.829551	2.728071	O	0.299391	-1.320509	-0.258781
H	-4.771970	1.654369	1.472133	C	1.691122	-1.151035	-0.370173
H	-3.202311	1.597187	2.276399	C	2.270367	-2.500969	-0.839575
C	-4.524677	4.173689	0.354594	H	2.040558	-3.282358	-0.107291
H	-5.359775	3.613577	-0.066621	H	1.821258	-2.791584	-1.796101
H	-4.917429	4.743702	1.205748	H	3.358759	-2.459273	-0.969824
H	-4.181452	4.893518	-0.390154	C	2.037548	-0.065636	-1.407441
C	-2.398029	4.148521	1.640663	H	1.591091	-0.317278	-2.376996
H	-1.566907	3.575031	2.048887	H	1.632895	0.900954	-1.089710
H	-2.007024	4.972885	1.044274	H	3.120110	0.045904	-1.548772
H	-2.935643	4.591484	2.487753	C	2.319806	-0.779813	0.985972
C	-1.884383	4.844411	-1.788064	H	3.414404	-0.732698	0.926516
H	-2.102061	5.441013	-0.901046	H	1.953037	0.192504	1.325747
H	-1.136957	5.396805	-2.371877	H	2.047138	-1.521620	1.743562
H	-2.790520	4.784669	-2.391925	C	-4.902770	0.496610	-0.785248
C	-0.037408	3.645752	-0.584558	H	-5.516936	-0.127430	-1.444780
H	-0.223602	4.140353	0.366822	H	-4.462983	-0.154017	-0.027295
H	0.437442	2.681984	-0.385209	H	-5.573428	1.205826	-0.299515
H	0.673762	4.265420	-1.144717	C	-4.506640	2.138459	-2.638056

H	-3.807226	2.541242	-3.373151	C	-2.133899	-1.246170	1.090199
H	-5.263503	1.569154	-3.192754	C	-3.043077	-1.064343	2.334527
H	-5.016161	2.972732	-2.155059	H	-2.243889	-1.331518	4.424777
C	-3.120515	0.067093	-2.436443	H	-2.453010	-2.834089	3.502672
H	-2.658147	-0.668996	-1.772056	H	-2.135455	-0.434552	0.359503
H	-3.875476	-0.459066	-3.032992	H	-2.359786	-2.182107	0.563251
H	-2.360886	0.433865	-3.123623	H	-3.128607	0.002205	2.573372
C	-3.988771	2.049824	1.960117	H	-4.063446	-1.452478	2.219256
H	-4.470090	2.644000	2.746910	Si	-0.687760	-1.509459	2.276064
H	-4.727179	1.347355	1.582979	C	0.432483	-3.003529	2.069023
H	-3.179214	1.479630	2.413969	H	-0.157553	-3.908147	1.882503
C	-4.654144	3.826534	0.323474	H	1.117125	-2.857749	1.229581
H	-5.459689	3.194754	-0.052397	H	1.028652	-3.168021	2.974371
H	-5.070861	4.424710	1.143484	O	0.782717	-0.509260	-0.277056
H	-4.359184	4.517085	-0.467583	C	2.080929	-0.574183	-0.809107
C	-2.512903	3.989861	1.584375	C	2.186975	-1.900928	-1.570471
H	-1.642383	3.482803	2.000561	H	2.012034	-2.745359	-0.894819
H	-2.180480	4.804607	0.940590	H	1.433882	-1.942331	-2.365658
H	-3.058265	4.443415	2.420928	H	3.175553	-2.028257	-2.026781
C	-2.118453	4.519013	-1.897709	C	2.342051	0.579970	-1.784169
H	-2.355532	5.154815	-1.043510	H	1.589676	0.579774	-2.582337
H	-1.425260	5.082164	-2.535480	H	2.281536	1.540177	-1.256347
H	-3.032424	4.359611	-2.470896	H	3.332744	0.509380	-2.249698
C	-0.168686	3.527406	-0.670145	C	3.138879	-0.542451	0.299687
H	-0.369805	4.053998	0.260801	H	4.149635	-0.680652	-0.102430
H	0.383002	2.613679	-0.438317	H	3.108814	0.414501	0.830045
H	0.478967	4.169674	-1.279551	H	2.949031	-1.335512	1.031382
C	-0.946631	2.485790	-2.755980	C	-3.323837	4.178530	-1.281092
H	-1.733920	2.347784	-3.497750	H	-4.217563	3.841755	-1.821786
H	-0.169419	3.104831	-3.220131	H	-3.645530	4.916348	-0.543398
H	-0.499568	1.514388	-2.526558	H	-2.677759	4.676115	-2.007093
O	-2.529148	-2.359787	0.833107	C	-3.709083	2.207547	0.189189
C	-3.016786	-3.496132	0.133184	H	-4.482563	1.835751	-0.493998
C	-4.300858	-3.102105	-0.618685	H	-3.280611	1.341741	0.700253
H	-5.065862	-2.759812	0.085394	H	-4.205926	2.841016	0.925437
H	-4.096221	-2.291245	-1.320006	C	-2.231198	1.979255	-1.748763
H	-4.708473	-3.948704	-1.184639	H	-1.493832	2.386627	-2.438868
C	-1.944786	-3.923127	-0.882602	H	-1.839979	1.040029	-1.333628
H	-1.030109	-4.230519	-0.368498	H	-3.118568	1.711046	-2.335961
H	-2.289272	-4.759532	-1.503957	C	1.364190	4.583258	0.161117
H	-1.695824	-3.085264	-1.540711	H	1.390793	4.851502	1.217178
C	-3.345164	-4.684764	1.055702	H	1.816975	3.593886	0.037988
H	-2.457405	-5.044695	1.580262	H	1.989742	5.306003	-0.377577
H	-4.098695	-4.408225	1.799422	C	-0.576641	6.051324	-0.411070
H	-3.748340	-5.519454	0.470726	H	0.075584	6.677653	-1.032911
10-pbe0d3				H	-1.589137	6.137337	-0.809332
Pd	0.001670	1.278409	0.284064	H	-0.565516	6.476741	0.594609
P	-1.126286	3.323808	0.446412	C	0.136632	4.197085	-1.913225
C	-1.707582	4.030394	2.120880	H	0.477878	3.160011	-1.999064
C	-2.661266	2.957122	-0.641625	H	-0.765907	4.325576	-2.512770
C	-0.043675	4.617350	-0.449162	H	0.911907	4.834896	-2.355066
C	0.864500	-0.167875	4.153084	C	-0.540537	4.695683	2.858841
C	0.339813	-0.035507	2.852504	H	0.302623	4.015697	2.992167
C	0.715073	1.092065	2.105033	H	-0.192569	5.609230	2.373887
C	1.645508	1.998711	2.620837	H	-0.896271	4.975715	3.857930
C	2.169698	1.827769	3.902145	C	-2.835774	5.059218	1.998124
C	1.765371	0.749077	4.683765	H	-3.763428	4.630240	1.615885
H	0.566499	-1.022907	4.760083	H	-3.051264	5.449364	3.000795
H	1.972636	2.846063	2.030461	H	-2.563851	5.909054	1.368749
H	2.889663	2.547041	4.285636	C	-2.173899	2.866626	3.006675
H	2.156311	0.617225	5.689195	H	-1.380398	2.129394	3.151671
C	-2.191290	-1.771370	3.424409	H	-2.442174	3.272113	3.990253
				H	-3.052072	2.354243	2.615362

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Pd	0.014044	1.276384	0.259365
P	-1.145179	3.332996	0.428299
C	-1.739855	4.013698	2.112716
C	-2.677357	2.967653	-0.670360
C	-0.067325	4.650480	-0.448144
C	0.930266	-0.186250	4.123532
C	0.372872	-0.048067	2.837652
C	0.738686	1.078476	2.083811
C	1.679060	1.983018	2.584770
C	2.233170	1.807137	3.851680
C	1.848099	0.723848	4.635763
H	0.644985	-1.040263	4.737488
H	1.993143	2.832975	1.992029
H	2.961735	2.523800	4.221392
H	2.265382	0.583948	5.628680
C	-2.183432	-1.718102	3.486551
C	-2.158910	-1.244064	1.131882
C	-3.059186	-1.042357	2.386215
H	-2.208150	-1.231634	4.465617
H	-2.456916	-2.771636	3.618970
H	-2.173538	-0.444182	0.389187
H	-2.396885	-2.185516	0.621154
H	-3.161365	0.027277	2.600463
H	-4.070955	-1.453926	2.289983
Si	-0.702956	-1.506112	2.304852
C	0.378182	-3.021760	2.051294
H	-0.230902	-3.932103	2.013989
H	0.924774	-2.935569	1.107763
H	1.108881	-3.131961	2.860545
O	0.806693	-0.497883	-0.335776
C	2.129642	-0.596586	-0.797221
C	2.220256	-1.889217	-1.624250
H	1.975859	-2.757666	-1.002396
H	1.507131	-1.856754	-2.455659
H	3.224191	-2.037743	-2.038533
C	2.503694	0.596910	-1.693234
H	1.785606	0.689060	-2.517241
H	2.484077	1.529201	-1.114989
H	3.505801	0.486472	-2.124856
C	3.121955	-0.675455	0.374090
H	4.145077	-0.852967	0.021505
H	3.115378	0.256124	0.947878
H	2.846865	-1.489952	1.052738
C	-3.347471	4.197305	-1.300191
H	-4.246777	3.866271	-1.833827
H	-3.659971	4.932821	-0.556440
H	-2.706613	4.696742	-2.029348
C	-3.733909	2.200438	0.144344
H	-4.492082	1.822909	-0.551618
H	-3.306129	1.337861	0.661022
H	-4.249945	2.827995	0.872239
C	-2.240948	2.003406	-1.795437
H	-1.489938	2.415171	-2.467672
H	-1.864417	1.054472	-1.390729
H	-3.121072	1.755445	-2.400719
C	1.344552	4.628337	0.169029
H	1.363475	4.859753	1.233470
H	1.821795	3.655567	0.013947
H	1.955603	5.382679	-0.340856
C	-0.615457	6.084354	-0.392796
H	0.029848	6.724929	-1.006376

H	-1.628573	6.166671	-0.790053
H	-0.607718	6.497127	0.618042
C	0.132367	4.257951	-1.923905
H	0.493447	3.229052	-2.027552
H	-0.767223	4.381976	-2.528181
H	0.898487	4.917037	-2.348528
C	-0.574858	4.672133	2.872426
H	0.271067	3.993548	2.995209
H	-0.229240	5.596480	2.407123
H	-0.933370	4.931185	3.875478
C	-2.874041	5.045770	2.002446
H	-3.799831	4.617350	1.615260
H	-3.090983	5.426123	3.007916
H	-2.604631	5.902019	1.380945
C	-2.213315	2.834960	2.985156
H	-1.427359	2.087308	3.116644
H	-2.475749	3.225399	3.975643
H	-3.098295	2.339617	2.588266

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Pd	-2.028116	0.676512	0.190625
P	-2.499152	2.907918	-0.322321
C	-3.714261	3.824608	0.857381
C	-3.446222	2.480759	-1.958428
C	-1.013112	4.047793	-0.746968
C	-0.764027	-0.858448	3.803338
C	-1.236940	-0.646700	2.496174
C	-1.339676	0.680716	2.052633
C	-0.943554	1.752493	2.849156
C	-0.477541	1.509255	4.147664
C	-0.399850	0.204671	4.632500
H	-0.672127	-1.876850	4.173187
H	-0.967393	2.765215	2.486071
H	-0.176192	2.348603	4.769222
H	-0.044573	0.015173	5.641956
C	-3.160287	-3.025929	2.027353
C	-3.533372	-1.392986	0.406598
C	-4.188894	-1.954564	1.664765
H	-3.102365	-3.326179	3.082342
H	-3.332223	-3.938216	1.437041
H	-4.015747	-0.476431	0.029788
H	-3.606151	-2.121420	-0.416284
H	-4.211966	-1.179195	2.443163
H	-5.222177	-2.318710	1.543255
Si	-1.616158	-2.074854	1.293613
C	-0.330518	-3.436657	1.793839
H	-0.439707	-4.328319	1.162119
H	0.726867	-3.156732	1.785468
H	-0.572544	-3.760880	2.814605
O	-0.886395	-1.524021	-0.237724
C	0.455033	-1.514129	-0.772816
C	0.913965	-2.927625	-1.153796
H	1.109741	-3.551395	-0.282500
H	0.147399	-3.416712	-1.764578
H	1.835489	-2.877303	-1.744468
C	0.360252	-0.670168	-2.049543
H	-0.333711	-1.125902	-2.763796
H	-0.009757	0.327640	-1.801867
H	1.338542	-0.569934	-2.531717
C	1.436036	-0.840955	0.194279
H	2.439400	-0.802689	-0.244309
H	1.114448	0.184274	0.402543
H	1.502795	-1.373445	1.144740

C	-4.843643	1.907209	-1.652791
H	-5.262428	1.532278	-2.593956
H	-4.801850	1.067122	-0.958018
H	-5.541645	2.646190	-1.262937
C	-3.605063	3.653362	-2.938870
H	-2.651100	3.997713	-3.339394
H	-4.205974	3.307213	-3.788787
H	-4.122178	4.504587	-2.495316
C	-2.675154	1.341164	-2.666061
H	-2.653931	0.413083	-2.076031
H	-3.209298	1.088828	-3.589885
H	-1.653330	1.598825	-2.932639
C	-4.572615	2.752759	1.560749
H	-5.257611	3.257505	2.252572
H	-5.175409	2.160733	0.873563
H	-3.947207	2.067614	2.138957
C	-4.620463	4.837570	0.129601
H	-5.279813	4.380492	-0.605978
H	-5.260415	5.318672	0.879072
H	-4.046951	5.624720	-0.362598
C	-2.986575	4.601845	1.970555
H	-2.369002	3.959575	2.595317
H	-2.380617	5.427000	1.596161
H	-3.754636	5.036029	2.620684
C	-1.407038	5.494050	-1.094344
H	-1.866814	6.014102	-0.253074
H	-0.494557	6.043653	-1.355965
H	-2.083052	5.556856	-1.947091
C	-0.042349	4.064776	0.448681
H	-0.471621	4.509748	1.345644
H	0.311702	3.059615	0.687605
H	0.829394	4.669237	0.171538
C	-0.223228	3.443349	-1.920686
H	-0.759780	3.485705	-2.868139
H	0.698469	4.023647	-2.043553
H	0.065344	2.408817	-1.719852

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Pd	-2.071512	0.657118	0.189478
P	-2.512917	2.869352	-0.323480
C	-3.721756	3.794277	0.871133
C	-3.482267	2.445474	-1.956448
C	-1.038630	4.033106	-0.775479
C	-0.655397	-0.873373	3.768185
C	-1.190512	-0.654664	2.478504
C	-1.325564	0.676493	2.034446
C	-0.904398	1.757049	2.821835
C	-0.378873	1.511058	4.106360
C	-0.262854	0.198375	4.587123
H	-0.535760	-1.902960	4.127672
H	-0.952694	2.780289	2.459653
H	-0.060751	2.359716	4.722685
H	0.143118	0.010569	5.587379
C	-3.253433	-2.868423	2.070390
C	-3.511949	-1.365869	0.314765
C	-4.228802	-1.784024	1.598390
H	-3.210389	-3.073306	3.157094
H	-3.458765	-3.827505	1.553973
H	-3.958798	-0.489724	-0.209318
H	-3.553286	-2.188489	-0.430056
H	-4.232903	-0.938438	2.312929
H	-5.282488	-2.113005	1.474097
Si	-1.633737	-2.061944	1.273370

C	-0.462503	-3.538882	1.720797
H	-0.641839	-4.396643	1.044652
H	0.621263	-3.335328	1.712534
H	-0.727187	-3.891660	2.735816
O	-0.859884	-1.510057	-0.257297
C	0.522872	-1.484669	-0.710376
C	0.973221	-2.882217	-1.170817
H	1.077783	-3.582583	-0.329846
H	0.239815	-3.299800	-1.882438
H	1.949497	-2.821053	-1.683983
C	0.500712	-0.537279	-1.921291
H	-0.149925	-0.936863	-2.718372
H	0.093202	0.437165	-1.600327
H	1.512205	-0.383644	-2.336195
C	1.466855	-0.907268	0.358620
H	2.499172	-0.854515	-0.030442
H	1.150556	0.112572	0.635986
H	1.480938	-1.519745	1.273501
C	-4.882635	1.878696	-1.635725
H	-5.309545	1.481827	-2.575017
H	-4.841037	1.046984	-0.915610
H	-5.583128	2.633851	-1.253915
C	-3.645163	3.619617	-2.939704
H	-2.686137	3.973111	-3.345192
H	-4.249419	3.267103	-3.796627
H	-4.171957	4.475039	-2.492682
C	-2.707042	1.298610	-2.657910
H	-2.670780	0.370747	-2.048471
H	-3.252601	1.023468	-3.579857
H	-1.680024	1.562278	-2.938491
C	-4.571936	2.717902	1.585571
H	-5.250530	3.224528	2.296838
H	-5.191743	2.123784	0.900339
H	-3.930712	2.024101	2.154150
C	-4.636641	4.804554	0.142520
H	-5.300544	4.338926	-0.598041
H	-5.283968	5.286284	0.898871
H	-4.064734	5.601877	-0.355216
C	-2.979461	4.574839	1.976950
H	-2.358010	3.924557	2.606733
H	-2.364025	5.401008	1.592641
H	-3.746229	5.021788	2.635597
C	-1.453872	5.483621	-1.095108
H	-1.899041	5.995119	-0.228834
H	-0.545006	6.048458	-1.375056
H	-2.157683	5.552255	-1.937030
C	-0.043795	4.032224	0.404448
H	-0.457591	4.477394	1.320397
H	0.306082	3.012060	0.629794
H	0.836418	4.635880	0.115706
C	-0.272031	3.446274	-1.977493
H	-0.835267	3.491923	-2.920258
H	0.649543	4.040375	-2.117547
H	0.033623	2.404182	-1.792929

11-ts-m06

Pd	-2.196737	0.671001	0.311328
P	-2.575747	2.922154	-0.299238
C	-3.821903	3.860240	0.831357
C	-3.466305	2.478019	-1.954117
C	-1.082383	4.059824	-0.694109
C	-0.431108	-0.888372	3.642893
C	-1.075017	-0.622716	2.424360

C	-1.307694	0.706200	2.101492	H	-2.118265	5.549617	-1.941889
C	-0.914708	1.760910	2.916081	C	-0.145243	4.087313	0.515583
C	-0.277795	1.465585	4.124317	H	-0.598995	4.515464	1.413692
C	-0.036331	0.144702	4.488445	H	0.231951	3.084922	0.753907
H	-0.230307	-1.923709	3.924265	H	0.721298	4.714348	0.262610
H	-1.073997	2.795484	2.638265	C	-0.263020	3.469059	-1.842584
H	0.027342	2.281977	4.776837	H	-0.770380	3.520646	-2.810530
H	0.462860	-0.079312	5.429618	H	0.662082	4.054986	-1.933565
C	-3.216141	-2.673026	2.250009	H	0.029734	2.429900	-1.646210
C	-3.434919	-1.508424	0.294186				
C	-4.196283	-1.712894	1.595422	11-ts-m061			
H	-3.165826	-2.676334	3.349145	Pd	-2.077261	0.673754	0.211487
H	-3.412905	-3.705282	1.916383	P	-2.503214	2.906427	-0.293115
H	-3.830910	-0.761958	-0.425558	C	-3.711815	3.879065	0.838484
H	-3.458698	-2.452004	-0.282883	C	-3.437360	2.469449	-1.922350
H	-4.246670	-0.766346	2.157151	C	-1.003496	4.013932	-0.714872
H	-5.230651	-2.081803	1.492466	C	-0.714138	-0.898527	3.762800
Si	-1.620243	-2.031958	1.241718	C	-1.222987	-0.671825	2.472466
C	-0.562352	-3.582670	1.655048	C	-1.395844	0.660896	2.083115
H	-0.807149	-4.399878	0.959695	C	-1.058348	1.727993	2.909616
H	0.526299	-3.451857	1.631325	C	-0.558878	1.464792	4.188579
H	-0.837640	-3.940733	2.657494	C	-0.394129	0.152340	4.620152
O	-0.815315	-1.565152	-0.281862	H	-0.564198	-1.926150	4.095319
C	0.532764	-1.586480	-0.739563	H	-1.156185	2.752657	2.578403
C	0.946577	-2.988882	-1.183204	H	-0.299215	2.297921	4.838112
H	1.047197	-3.682167	-0.342765	H	-0.009092	-0.050851	5.616680
H	0.200689	-3.397213	-1.877950	C	-3.109863	-3.036500	2.022126
H	1.912055	-2.956161	-1.705601	C	-3.529086	-1.422470	0.429280
C	0.558675	-0.675949	-1.964412	C	-4.144139	-1.969824	1.703753
H	-0.130866	-1.048613	-2.733703	H	-3.011700	-3.350550	3.071055
H	0.242592	0.338579	-1.684963	H	-3.299977	-3.942527	1.428394
H	1.564340	-0.617487	-2.400791	H	-4.031741	-0.522323	0.029967
C	1.511468	-1.038532	0.295524	H	-3.607242	-2.172853	-0.374409
H	2.530622	-1.031358	-0.113807	H	-4.134397	-1.191132	2.481753
H	1.252507	-0.005194	0.567473	H	-5.185425	-2.324585	1.625344
H	1.527240	-1.639807	1.212418	Si	-1.599855	-2.084119	1.252779
C	-4.843367	1.870864	-1.662804	C	-0.296130	-3.426318	1.723017
H	-5.234432	1.452676	-2.600900	H	-0.382976	-4.308280	1.074489
H	-4.794433	1.051209	-0.935242	H	0.759645	-3.135115	1.725446
H	-5.575780	2.602798	-1.310662	H	-0.532097	-3.781420	2.735276
C	-3.644969	3.642488	-2.927467	O	-0.926052	-1.547141	-0.300348
H	-2.694144	4.004985	-3.331993	C	0.419666	-1.493409	-0.816533
H	-4.238543	3.284509	-3.781241	C	0.946794	-2.879752	-1.177035
H	-4.181478	4.489218	-2.489286	H	1.202627	-3.478396	-0.302222
C	-2.659556	1.376575	-2.662534	H	0.201256	-3.427782	-1.763108
H	-2.611105	0.440607	-2.083380	H	1.850879	-2.789211	-1.789676
H	-3.175945	1.129003	-3.601159	C	0.303930	-0.671320	-2.094732
H	-1.637724	1.665476	-2.915258	H	-0.361281	-1.158143	-2.816839
C	-4.697473	2.815165	1.533794	H	-0.115768	0.312296	-1.856727
H	-5.402938	3.342758	2.191557	H	1.281354	-0.526549	-2.567862
H	-5.288286	2.199887	0.849537	C	1.351637	-0.770126	0.148572
H	-4.093983	2.144331	2.158840	H	2.360982	-0.691773	-0.271690
C	-4.714105	4.856276	0.083614	H	0.983459	0.247238	0.335611
H	-5.376249	4.386034	-0.648623	H	1.429357	-1.282109	1.111958
H	-5.360781	5.351940	0.821882	C	-4.831875	1.913832	-1.613763
H	-4.139942	5.641474	-0.420074	H	-5.254538	1.528253	-2.549454
C	-3.114493	4.638799	1.943599	H	-4.790673	1.077737	-0.908996
H	-2.487951	4.002552	2.574936	H	-5.533643	2.653753	-1.228358
H	-2.517506	5.481204	1.581720	C	-3.568740	3.611985	-2.927875
H	-3.892371	5.058824	2.596094	H	-2.604738	3.937834	-3.325945
C	-1.471199	5.493558	-1.060748	H	-4.160652	3.253088	-3.779512
H	-1.961805	6.025639	-0.239870	H	-4.082762	4.485027	-2.519343
H	-0.550412	6.046423	-1.296498	C	-2.680744	1.309085	-2.592696

H	-2.679347	0.386070	-1.986617
H	-3.210601	1.039342	-3.515181
H	-1.650704	1.540916	-2.861967
C	-4.576784	2.850009	1.578167
H	-5.296011	3.384778	2.210987
H	-5.146127	2.193558	0.916745
H	-3.964783	2.215542	2.229364
C	-4.597534	4.862582	0.063824
H	-5.271176	4.386807	-0.649176
H	-5.226222	5.396071	0.787491
H	-4.011907	5.615799	-0.470737
C	-2.997546	4.703103	1.914730
H	-2.366946	4.104016	2.572156
H	-2.403839	5.526189	1.512423
H	-3.772358	5.152057	2.547685
C	-1.358358	5.449320	-1.107764
H	-1.825328	6.009328	-0.294587
H	-0.430025	5.974988	-1.364902
H	-2.013533	5.506649	-1.979740
C	-0.067851	4.039144	0.498434
H	-0.506533	4.513359	1.378603
H	0.258156	3.030351	0.773913
H	0.826659	4.615251	0.232172
C	-0.207606	3.369298	-1.850199
H	-0.718487	3.408849	-2.814719
H	0.736383	3.915902	-1.962965
H	0.043892	2.326375	-1.625676

11-ts-NEt2

Pd	-1.726689	0.490916	0.291647
P	-2.564432	2.594092	-0.326578
C	-3.727619	3.528412	0.890214
C	-3.623383	1.980121	-1.825902
C	-1.255419	3.837732	-1.006554
C	-0.472243	-0.623234	4.041036
C	-0.919399	-0.598916	2.705810
C	-0.988034	0.667702	2.124654
C	-0.576088	1.837486	2.758311
C	-0.129550	1.767263	4.086651
C	-0.092671	0.533223	4.733729
H	-0.407688	-1.579937	4.554824
H	-0.582499	2.789332	2.251611
H	0.182005	2.675653	4.597525
H	0.241685	0.467611	5.767348
C	-2.729698	-2.759404	3.003854
C	-3.562150	-1.309652	1.214952
C	-3.732265	-1.637318	2.700174
H	-2.402792	-2.771505	4.055721
H	-3.182718	-3.739462	2.815414
H	-4.115786	-0.392438	0.963526
H	-3.996202	-2.105453	0.593152
H	-3.450075	-0.750469	3.286082
H	-4.769150	-1.877463	3.018208
Si	-1.335085	-2.308625	1.675945
C	0.218986	-3.236699	2.445789
H	0.508701	-4.142777	1.902856
H	1.108885	-2.598307	2.506046
H	0.000407	-3.548990	3.476630
O	-0.496299	-1.327942	0.230671
C	0.774690	-1.307546	-0.419174
C	1.436371	-2.694598	-0.462948
H	1.865629	-2.967681	0.501187
H	0.702915	-3.454906	-0.731717

H	2.244939	-2.698234	-1.203428
C	0.528308	-0.834685	-1.860546
H	-0.094741	-1.554535	-2.401738
H	0.006305	0.126371	-1.846859
H	1.468154	-0.708957	-2.410829
C	1.717291	-0.319762	0.286527
H	2.701666	-0.299524	-0.197244
H	1.299670	0.691910	0.263931
H	1.854030	-0.603927	1.334083
C	-4.926706	1.318741	-1.336808
H	-5.410572	0.850411	-2.202631
H	-4.735237	0.533595	-0.604070
H	-5.640133	2.026430	-0.915436
C	-3.988651	3.046170	-2.871316
H	-3.116559	3.456249	-3.381439
H	-4.618815	2.577395	-3.637984
H	-4.557090	3.873318	-2.443323
C	-2.823819	0.848686	-2.514036
H	-2.659611	-0.005102	-1.840447
H	-3.420181	0.459708	-3.348802
H	-1.862825	1.164946	-2.912549
C	-4.434844	2.466936	1.756919
H	-5.078689	2.981073	2.481398
H	-5.062668	1.788207	1.181857
H	-3.709137	1.867780	2.312298
C	-4.773536	4.424374	0.201481
H	-5.470271	3.868479	-0.425085
H	-5.366407	4.923461	0.978273
H	-4.312740	5.203952	-0.407173
C	-2.934270	4.418652	1.865911
H	-2.193281	3.853733	2.430129
H	-2.444567	5.262039	1.378627
H	-3.644878	4.834177	2.590525
C	-1.811022	5.217528	-1.400605
H	-2.196393	5.772472	-0.544100
H	-0.994427	5.812490	-1.828962
H	-2.599344	5.157510	-2.151078
C	-0.154816	4.026170	0.054976
H	-0.515543	4.485422	0.974478
H	0.320549	3.073517	0.300273
H	0.615273	4.688481	-0.359091
C	-0.546194	3.222762	-2.227169
H	-1.185453	3.147060	-3.106688
H	0.296704	3.870933	-2.495927
H	-0.139561	2.234400	-1.999876
N	-1.729902	-3.641312	0.395093
C	-1.971509	-4.992668	0.863990
H	-1.341746	-5.730689	0.326283
H	-1.646391	-5.054423	1.907692
C	-3.420593	-5.511529	0.786317
H	-3.499259	-6.498622	1.259817
H	-4.116791	-4.835341	1.293115
H	-3.763054	-5.619921	-0.248633
C	-2.293626	-3.358730	-0.904422
H	-2.072097	-2.315815	-1.134437
H	-3.401270	-3.438167	-0.926348
C	-1.767137	-4.235991	-2.051878
H	-1.991175	-5.297901	-1.896602
H	-2.232086	-3.943220	-3.002781
H	-0.681562	-4.143985	-2.165140

11-ts-NMe2

Pd	-1.697597	0.512645	0.298129
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P	-2.562298	2.609074	-0.324095	H	-2.233303	3.866804	2.439095
C	-3.750190	3.522746	0.885534	H	-2.495196	5.272769	1.387152
C	-3.599475	1.981136	-1.832469	H	-3.699662	4.826782	2.588247
C	-1.267364	3.873870	-0.991627	C	-1.839612	5.246208	-1.387745
C	-0.480744	-0.577772	4.070052	H	-2.240164	5.794007	-0.533593
C	-0.905604	-0.566045	2.727221	H	-1.027885	5.853507	-1.807952
C	-0.984679	0.697419	2.139352	H	-2.620435	5.176716	-2.145246
C	-0.597620	1.875174	2.774754	C	-0.177341	4.075209	0.078328
C	-0.172560	1.817319	4.110440	H	-0.550766	4.527720	0.996128
C	-0.130623	0.586965	4.763971	H	0.308232	3.127884	0.324547
H	-0.414612	-1.530374	4.590900	H	0.586928	4.748423	-0.328839
H	-0.609424	2.824294	2.263309	C	-0.540025	3.270501	-2.207108
H	0.118299	2.732167	4.621923	H	-1.171805	3.181587	-3.090690
H	0.185536	0.530526	5.803770	H	0.292956	3.933163	-2.471263
C	-2.717105	-2.749105	2.999834	H	-0.117340	2.290255	-1.974229
C	-3.529210	-1.300105	1.213049	N	-1.641547	-3.630951	0.441499
C	-3.712249	-1.621917	2.697246	C	-1.953636	-4.955887	0.905892
H	-2.421734	-2.798629	4.060072	H	-1.569383	-5.736179	0.218623
H	-3.170808	-3.720596	2.762163	H	-1.505377	-5.150092	1.885439
H	-4.089507	-0.391445	0.947192	C	-2.239903	-3.395954	-0.841364
H	-3.952240	-2.106648	0.595443	H	-2.064374	-2.367098	-1.156900
H	-3.430233	-0.736782	3.285838	H	-3.340335	-3.564434	-0.866180
H	-4.752204	-1.859698	3.008689	H	-3.043655	-5.162610	1.007575
Si	-1.292484	-2.281026	1.709200	H	-1.824518	-4.063130	-1.624805
C	0.265146	-3.186972	2.496214	11-ts-OtBu			
H	0.517745	-4.133728	2.005377	Pd	-1.768670	0.574262	0.156259
H	1.170028	-2.566951	2.482691	P	-2.464702	2.748721	-0.406075
H	0.078371	-3.426595	3.552194	C	-3.727431	3.607078	0.771138
O	-0.464706	-1.310560	0.254292	C	-3.391892	2.280087	-2.042056
C	0.771572	-1.361836	-0.458065	C	-1.089313	4.023683	-0.867892
C	1.294145	-2.797319	-0.623770	C	-0.854658	-0.786253	3.922280
H	1.597177	-3.227307	0.330437	C	-1.199695	-0.675615	2.560929
H	0.522163	-3.439402	-1.050075	C	-1.194992	0.623335	2.050420
H	2.166107	-2.797344	-1.289050	C	-0.801707	1.743225	2.780078
C	0.513001	-0.774845	-1.854182	C	-0.460270	1.586731	4.131410
H	-0.205607	-1.390329	-2.405405	C	-0.503247	0.318081	4.707694
H	0.097714	0.232393	-1.756336	H	-0.851039	-1.772004	4.383797
H	1.436337	-0.711940	-2.441757	H	-0.743647	2.720327	2.329152
C	1.827509	-0.503670	0.258439	H	-0.166361	2.456075	4.715274
H	2.781602	-0.509938	-0.282225	H	-0.250584	0.185533	5.757895
H	1.481733	0.532800	0.336179	C	-3.118057	-2.768052	2.515182
H	2.004276	-0.875396	1.271856	C	-3.645417	-1.217376	0.707330
C	-4.897307	1.301424	-1.354915	C	-4.050675	-1.612217	2.129393
H	-5.366186	0.824690	-2.224351	H	-2.922539	-2.832530	3.597028
H	-4.700234	0.520650	-0.619265	H	-3.565523	-3.723522	2.227127
H	-5.624853	1.999022	-0.941066	H	-4.128584	-0.268233	0.430662
C	-3.971079	3.042697	-2.880039	H	-3.990262	-1.954451	-0.030105
H	-3.101191	3.465998	-3.382950	H	-3.851020	-0.758873	2.793657
H	-4.588259	2.565528	-3.652045	H	-5.124826	-1.850177	2.272824
H	-4.555181	3.860937	-2.455935	Si	-1.563962	-2.309736	1.402957
C	-2.777488	0.861157	-2.512197	C	-0.120631	-3.326852	2.255017
H	-2.610820	0.010137	-1.835782	H	0.251679	-4.150456	1.640346
H	-3.359375	0.463932	-3.353251	H	0.746389	-2.723123	2.546354
H	-1.816117	1.189231	-2.899901	H	-0.497494	-3.784640	3.180402
C	-4.451302	2.450306	1.744054	O	-0.618757	-1.338883	0.056028
H	-5.104717	2.955353	2.466339	C	0.711812	-1.363567	-0.464678
H	-5.069074	1.767195	1.163101	C	1.162288	-2.785672	-0.828596
H	-3.723252	1.856755	2.302245	H	1.244057	-3.422742	0.051631
C	-4.802372	4.405905	0.189668	H	0.448625	-3.243781	-1.517278
H	-5.486464	3.842348	-0.444056	H	2.143486	-2.753222	-1.317368
H	-5.408483	4.894699	0.962746	C	0.689851	-0.525676	-1.751625
H	-4.347451	5.193584	-0.412946	H	0.008925	-0.968788	-2.486124
C	-2.977313	4.422009	1.869230				

H	0.336335	0.484319	-1.522986	C	-0.602082	-0.853336	3.710385
H	1.687024	-0.452471	-2.200841	C	-1.160307	-0.615480	2.445536
C	1.704041	-0.725898	0.521212	C	-1.359309	0.712938	2.058341
H	2.717886	-0.709993	0.103508	C	-0.999311	1.773337	2.884151
H	1.406153	0.304265	0.739575	C	-0.449998	1.507678	4.141075
H	1.731770	-1.276031	1.464288	C	-0.254947	0.195177	4.559517
C	-4.748140	1.613983	-1.738582	H	-0.434491	-1.879480	4.031484
H	-5.150731	1.228563	-2.683285	H	-1.115420	2.799212	2.573510
H	-4.647258	0.767366	-1.058218	H	-0.174766	2.338887	4.785910
H	-5.488002	2.303674	-1.333420	H	0.171507	-0.010248	5.538222
C	-3.641048	3.439272	-3.020963	C	-3.171637	-2.851468	2.103613
H	-2.720014	3.857434	-3.428136	C	-3.462534	-1.401253	0.341502
H	-4.220363	3.053050	-3.869011	C	-4.169474	-1.806722	1.623883
H	-4.217681	4.249749	-2.573360	H	-3.112759	-3.028824	3.185753
C	-2.548112	1.193779	-2.750242	H	-3.367717	-3.819658	1.618848
H	-2.487163	0.270409	-2.157817	H	-3.924526	-0.559850	-0.207313
H	-3.049753	0.918906	-3.686490	H	-3.499348	-2.237618	-0.376672
H	-1.537098	1.509975	-2.995831	H	-4.194068	-0.957102	2.319968
C	-4.519667	2.488506	1.477655	H	-5.206403	-2.159004	1.505096
H	-5.223620	2.950188	2.181175	Si	-1.606742	-2.027625	1.245723
H	-5.096446	1.869944	0.791742	C	-0.414845	-3.474981	1.702276
H	-3.852211	1.833712	2.042839	H	-0.594145	-4.336911	1.045367
C	-4.700180	4.569939	0.064815	H	0.659649	-3.267943	1.683392
H	-5.341882	4.075227	-0.663508	H	-0.669096	-3.811751	2.715849
H	-5.358207	5.012347	0.823363	O	-0.854383	-1.516369	-0.289041
H	-4.183604	5.390707	-0.435173	C	0.480894	-1.533638	-0.797007
C	-3.022105	4.405669	1.883480	C	0.911300	-2.945093	-1.198042
H	-2.344438	3.787719	2.470775	H	1.068456	-3.594395	-0.336294
H	-2.479575	5.275227	1.511229	H	0.147038	-3.399560	-1.838148
H	-3.794855	4.776756	2.567347	H	1.848203	-2.907924	-1.765175
C	-1.597256	5.441206	-1.186304	C	0.436303	-0.673001	-2.058429
H	-2.052130	5.926006	-0.321489	H	-0.257587	-1.099407	-2.791225
H	-0.740548	6.057741	-1.486875	H	0.089301	0.332413	-1.803936
H	-2.316022	5.459823	-2.005573	H	1.425309	-0.593172	-2.522391
C	-0.084973	4.105417	0.297670	C	1.467592	-0.909603	0.187881
H	-0.522116	4.489459	1.218760	H	2.477308	-0.894021	-0.237519
H	0.362371	3.129759	0.501290	H	1.176641	0.122620	0.411765
H	0.722653	4.790169	0.011166	H	1.507202	-1.460365	1.130746
C	-0.278278	3.508374	-2.072055	C	-4.840420	1.885966	-1.622847
H	-0.835772	3.522854	-3.008256	H	-5.235152	1.476679	-2.560610
H	0.589524	4.165850	-2.202408	H	-4.808981	1.068291	-0.898502
H	0.100371	2.497679	-1.903654	H	-5.554286	2.631266	-1.272310
O	-1.839435	-3.511556	0.043776	C	-3.591891	3.605076	-2.916736
C	-2.357290	-4.816449	-0.078921	H	-2.632076	3.941969	-3.312528
C	-1.696391	-5.425283	-1.334183	H	-4.180448	3.238972	-3.767419
H	-2.073015	-6.432910	-1.549539	H	-4.116893	4.466035	-2.499866
H	-1.893113	-4.791935	-2.206680	C	-2.664285	1.313905	-2.588440
H	-0.611405	-5.488064	-1.199144	H	-2.667703	0.384267	-1.997380
C	-3.883338	-4.793812	-0.319035	H	-3.175374	1.058625	-3.525347
H	-4.269682	-5.799626	-0.525840	H	-1.632927	1.562601	-2.830376
H	-4.423570	-4.397029	0.543770	C	-4.623820	2.795927	1.565348
H	-4.114547	-4.157626	-1.180686	H	-5.326249	3.321994	2.223869
C	-2.041900	-5.748854	1.110804	H	-5.210031	2.176362	0.886214
H	-2.439405	-5.360506	2.049805	H	-4.009819	2.134130	2.183600
H	-2.479822	-6.740442	0.942879	C	-4.647666	4.833695	0.089925
H	-0.962579	-5.877562	1.229226	H	-5.302151	4.361989	-0.642317
11-ts-pbe0d3				H	-5.294613	5.332510	0.822112
Pd	-2.110505	0.686562	0.239748	H	-4.067800	5.610182	-0.413766
P	-2.534265	2.903661	-0.284381	C	-3.055499	4.645810	1.952244
C	-3.756973	3.842245	0.850858	H	-2.455453	4.022384	2.614413
C	-3.446768	2.457527	-1.915960	H	-2.440562	5.462968	1.572765
C	-1.045067	4.022880	-0.692052	H	-3.840384	5.097004	2.570855
				C	-1.420823	5.458186	-1.072240

H	-1.896384	5.999207	-0.252326
H	-0.497067	5.995585	-1.320652
H	-2.074475	5.511621	-1.944145
C	-0.103853	4.054948	0.517423
H	-0.547557	4.517012	1.399991
H	0.242256	3.051550	0.779437
H	0.775563	4.651833	0.246335
C	-0.235239	3.400764	-1.832204
H	-0.748317	3.430254	-2.794363
H	0.691467	3.976712	-1.941161
H	0.046501	2.368315	-1.606768

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Pd	-2.128523	0.671861	0.253675
P	-2.543877	2.916445	-0.280824
C	-3.736742	3.903253	0.852488
C	-3.478553	2.474488	-1.907061
C	-1.021819	3.990883	-0.697283
C	-0.644245	-0.885392	3.725310
C	-1.190396	-0.649521	2.454997
C	-1.405225	0.680053	2.084006
C	-1.080133	1.739655	2.922711
C	-0.542815	1.474451	4.183679
C	-0.328138	0.160991	4.589092
H	-0.461596	-1.909547	4.042710
H	-1.218887	2.762453	2.613818
H	-0.290943	2.302252	4.840970
H	0.091168	-0.046614	5.569566
C	-3.135373	-2.953816	2.068183
C	-3.464146	-1.456099	0.338460
C	-4.166775	-1.925290	1.607303
H	-3.076377	-3.148457	3.147263
H	-3.306898	-3.919191	1.568954
H	-3.942071	-0.595415	-0.162527
H	-3.497341	-2.256961	-0.417507
H	-4.226840	-1.097893	2.327128
H	-5.187554	-2.312281	1.468224
Si	-1.597268	-2.068535	1.240977
C	-0.345209	-3.463827	1.714127
H	-0.441310	-4.316308	1.028403
H	0.713382	-3.186388	1.745354
H	-0.614472	-3.842491	2.708697
O	-0.850862	-1.553152	-0.294071
C	0.481355	-1.515979	-0.807104
C	1.006145	-2.915814	-1.153383
H	1.255346	-3.500634	-0.267740
H	0.254790	-3.464467	-1.731460
H	1.911996	-2.835722	-1.764412
C	0.383545	-0.711499	-2.108044
H	-0.283623	-1.211204	-2.818922
H	-0.025084	0.280376	-1.898900
H	1.365039	-0.590343	-2.578545
C	1.431771	-0.793088	0.152848
H	2.436501	-0.727449	-0.279117
H	1.074752	0.225212	0.342825
H	1.509125	-1.308082	1.113812
C	-4.885316	1.924583	-1.600768
H	-5.293904	1.514481	-2.531419
H	-4.866160	1.112535	-0.870146
H	-5.584688	2.684181	-1.252607
C	-3.613459	3.622837	-2.917317
H	-2.650429	3.934552	-3.326334
H	-4.221319	3.268565	-3.758509

H	-4.110821	4.498868	-2.498307
C	-2.723267	1.311090	-2.591061
H	-2.724563	0.384732	-1.995630
H	-3.253180	1.058491	-3.516896
H	-1.694261	1.544988	-2.855503
C	-4.624350	2.887344	1.596938
H	-5.322733	3.440183	2.236410
H	-5.215961	2.256181	0.933484
H	-4.022898	2.235910	2.238236
C	-4.614610	4.903548	0.077541
H	-5.306500	4.428827	-0.616949
H	-5.221390	5.457341	0.803375
H	-4.018822	5.633927	-0.474423
C	-3.012290	4.720780	1.938127
H	-2.398556	4.109624	2.597783
H	-2.403705	5.531599	1.536773
H	-3.783828	5.181045	2.565578
C	-1.354915	5.437900	-1.094507
H	-1.807942	6.004225	-0.279368
H	-0.418822	5.944359	-1.358180
H	-2.015054	5.497323	-1.961187
C	-0.080433	4.004846	0.520842
H	-0.514713	4.478194	1.401491
H	0.239372	2.993695	0.787723
H	0.815074	4.578112	0.253513
C	-0.221717	3.339729	-1.835777
H	-0.725864	3.393969	-2.801649
H	0.727385	3.878151	-1.936879
H	0.017639	2.296299	-1.614041

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Pd	-3.485554	0.743088	1.061614
P	-2.916297	2.826958	-0.139334
C	-4.039496	4.209195	0.595261
C	-3.511360	2.414517	-1.922437
C	-1.116787	3.485074	-0.220497
C	0.109245	-0.350990	3.097309
C	-0.983750	-0.416652	2.205652
C	-2.048712	0.489457	2.403833
C	-2.043962	1.347625	3.516357
C	-0.955720	1.377928	4.390405
C	0.140834	0.541689	4.167815
H	0.951324	-1.024596	2.959962
H	-2.877799	2.021444	3.688062
H	-0.963277	2.059359	5.237995
H	0.998837	0.568373	4.834205
C	-2.779694	-2.464703	0.673044
C	-4.408670	-0.919031	1.878595
C	-3.682113	-2.259031	1.908875
H	-2.667881	-3.535011	0.446863
H	-3.250481	-2.013137	-0.207904
H	-4.840648	-0.676674	2.858001
H	-5.235815	-0.959562	1.143936
H	-3.084079	-2.329640	2.827595
H	-4.412981	-3.080390	1.973819
Si	-1.030595	-1.810591	0.929965
C	-0.047133	-3.239779	1.679518
H	-0.100235	-4.128612	1.042391
H	1.008149	-3.020329	1.865759
H	-0.499498	-3.502371	2.644336
O	-0.473573	-1.374787	-0.597328
C	0.856722	-1.396197	-1.166697
C	1.312779	-2.844887	-1.375709

H	1.489895	-3.355700	-0.428009	H	1.759550	0.974367	5.731738
H	0.555698	-3.402663	-1.936373	C	-2.283301	-1.864923	3.287297
H	2.246619	-2.867331	-1.947274	C	-1.924215	-1.496953	0.912684
C	0.737734	-0.707684	-2.529365	C	-3.029722	-1.351052	2.009564
H	-0.009636	-1.217833	-3.145638	H	-2.447506	-1.263271	4.186156
H	0.439387	0.336297	-2.419984	H	-2.548785	-2.901865	3.524713
H	1.696220	-0.736350	-3.057207	H	-1.822859	-0.644364	0.234780
C	1.835258	-0.642325	-0.261787	H	-2.053126	-2.402757	0.308110
H	2.822473	-0.583703	-0.732176	H	-3.298540	-0.298203	2.130667
H	1.483999	0.375231	-0.072471	H	-3.953047	-1.898175	1.784487
H	1.954841	-1.150514	0.699673	Si	-0.652698	-1.729459	2.301211
C	-5.032764	2.179105	-1.870077	C	0.396555	-3.294455	2.259107
H	-5.352665	1.740056	-2.822513	H	-0.229749	-4.178292	2.090079
H	-5.301438	1.472890	-1.075766	H	1.138481	-3.241996	1.456839
H	-5.602336	3.097735	-1.727660	H	0.931746	-3.435001	3.205771
C	-3.197865	3.455034	-3.007603	O	1.325447	-0.540471	0.426178
H	-2.124703	3.566346	-3.174956	C	2.608711	-0.711417	-0.199013
H	-3.640216	3.124548	-3.956413	C	2.383986	-1.828804	-1.228258
H	-3.611939	4.438221	-2.777953	H	2.020703	-2.736166	-0.735790
C	-2.897340	1.055163	-2.326182	H	1.640749	-1.518109	-1.970353
H	-3.105316	0.286749	-1.574211	H	3.316152	-2.070075	-1.751206
H	-3.349907	0.736433	-3.273434	C	3.084052	0.555182	-0.917628
H	-1.820917	1.089828	-2.472629	H	2.321517	0.895519	-1.626535
C	-5.347977	3.551520	1.087777	H	3.285316	1.366214	-0.214978
H	-5.939420	4.304377	1.623554	H	4.008072	0.355506	-1.472563
H	-5.968027	3.163784	0.281118	C	3.629972	-1.165719	0.851964
H	-5.136575	2.728981	1.780545	H	4.585893	-1.415720	0.379178
C	-4.384207	5.363373	-0.358919	H	3.809917	-0.383909	1.593318
H	-4.983827	5.033140	-1.208969	H	3.263061	-2.054118	1.375495
H	-4.978838	6.108177	0.185831	C	-3.295901	4.286440	-1.276225
H	-3.496748	5.869707	-0.741924	H	-4.168184	4.045069	-1.897137
C	-3.371403	4.792176	1.856326	H	-3.651083	4.882864	-0.434224
H	-3.098196	4.011012	2.570393	H	-2.634935	4.909001	-1.881227
H	-2.486193	5.389491	1.636719	C	-3.693371	2.087222	-0.159466
H	-4.093163	5.453026	2.351304	H	-4.450393	1.832949	-0.911111
C	-0.973359	4.927522	-0.732357	H	-3.269862	1.150623	0.211404
H	-1.403166	5.660290	-0.047189	H	-4.209502	2.588783	0.659836
H	0.094825	5.161195	-0.826625	C	-2.158943	2.192560	-2.078726
H	-1.428668	5.070148	-1.713968	H	-1.431738	2.732729	-2.682362
C	-0.478219	3.363348	1.179341	H	-1.717741	1.229869	-1.795298
H	-1.005243	3.913704	1.955447	H	-3.030131	1.988753	-2.713644
H	-0.415138	2.319417	1.488439	C	1.387974	4.445225	0.331544
H	0.542692	3.761835	1.126099	H	1.389328	4.508174	1.417742
C	-0.290971	2.553341	-1.121998	H	1.827940	3.486088	0.045928
H	-0.525607	2.667154	-2.181049	H	2.033680	5.246240	-0.049738
H	0.769959	2.800889	-0.996739	C	-0.547262	6.015693	-0.009994
H	-0.424572	1.509048	-0.835376	H	0.119275	6.748043	-0.482935
13-ts				H	-1.548654	6.175233	-0.413177
Pd	0.103509	1.180764	0.216330	H	-0.568407	6.242784	1.057098
P	-1.115915	3.160355	0.343265	C	0.199948	4.454178	-1.815340
C	-1.739695	3.596656	2.108056	H	0.557686	3.453679	-2.076336
C	-2.628922	2.974854	-0.831563	H	-0.695873	4.670729	-2.398000
C	-0.012901	4.603115	-0.296818	H	0.969928	5.170959	-2.125257
C	0.645569	-0.072874	4.202055	C	-0.553654	4.076311	2.967016
C	0.407947	-0.270296	2.832365	H	0.276318	3.366659	2.948983
C	1.105079	0.554626	1.924334	H	-0.185953	5.061147	2.675839
C	2.100947	1.441537	2.365279	H	-0.896006	4.154178	4.005942
C	2.324415	1.588226	3.737237	C	-2.849513	4.659422	2.157905
C	1.589272	0.849001	4.666699	H	-3.770259	4.321377	1.679428
H	0.092876	-0.673559	4.922484	H	-3.088540	4.865675	3.209017
H	2.650463	2.053763	1.663504	H	-2.550683	5.602662	1.699016
H	3.068970	2.305750	4.073557	C	-2.250184	2.304387	2.775993
				H	-1.484746	1.527166	2.777814

H	-2.502319	2.530132	3.819548	C	-0.525549	5.996314	0.016329
H	-3.145596	1.906594	2.304149	H	0.149629	6.736740	-0.452957
13-ts-bp86d3				H	-1.534686	6.165525	-0.389122
Pd	0.078243	1.179577	0.224505	H	-0.546115	6.215384	1.094809
P	-1.109338	3.134636	0.354193	C	0.206370	4.434169	-1.808470
C	-1.732580	3.571169	2.127178	H	0.566015	3.424804	-2.072746
C	-2.626741	2.956293	-0.827479	H	-0.701019	4.651385	-2.391054
C	0.003366	4.581149	-0.284852	H	0.980773	5.157251	-2.125497
C	0.619190	-0.015684	4.223357	C	-0.535889	4.040662	2.983428
C	0.394873	-0.233648	2.846709	H	0.291809	3.313256	2.966253
C	1.105643	0.578544	1.925626	H	-0.152732	5.028583	2.686361
C	2.115337	1.465679	2.360694	H	-0.877903	4.126160	4.031594
C	2.328304	1.632809	3.741443	C	-2.838888	4.642825	2.172203
C	1.571508	0.913543	4.681886	H	-3.766581	4.307167	1.683620
H	0.050561	-0.607708	4.952515	H	-3.085717	4.850116	3.230814
H	2.680091	2.068520	1.648237	H	-2.529998	5.593490	1.713278
H	3.082835	2.354768	4.074879	C	-2.249678	2.275190	2.789456
H	1.735066	1.057712	5.754678	H	-1.484703	1.483817	2.772390
C	-2.316046	-1.842859	3.239160	H	-2.487465	2.493828	3.847388
C	-1.886597	-1.474177	0.866943	H	-3.163122	1.889884	2.319406
C	-3.021032	-1.317796	1.937868	13-ts-m06			
H	-2.507253	-1.245632	4.146201	Pd	0.131166	1.166304	0.240801
H	-2.589106	-2.890524	3.461075	P	-1.115933	3.178799	0.354382
H	-1.747822	-0.609109	0.191032	C	-1.739153	3.657074	2.108100
H	-2.002401	-2.382531	0.248327	C	-2.632644	2.960237	-0.809089
H	-3.277882	-0.251915	2.055057	C	-0.034015	4.619025	-0.323152
H	-3.955452	-1.852074	1.684480	C	0.683812	-0.197355	4.194513
Si	-0.648679	-1.707804	2.296321	C	0.418970	-0.331729	2.825187
C	0.420429	-3.269122	2.307067	C	1.089600	0.540166	1.955734
H	-0.187300	-4.164693	2.086759	C	2.072452	1.424261	2.411073
H	1.219410	-3.197269	1.550466	C	2.320589	1.509411	3.781798
H	0.896850	-3.413027	3.293439	C	1.619749	0.714149	4.683326
O	1.298195	-0.551260	0.442981	H	0.156918	-0.846134	4.898265
C	2.582389	-0.704008	-0.213727	H	2.604766	2.077758	1.724465
C	2.341076	-1.835986	-1.229636	H	3.061483	2.222963	4.139903
H	1.991935	-2.747762	-0.716036	H	1.811894	0.787866	5.751366
H	1.574137	-1.535029	-1.964339	C	-2.286527	-1.881454	3.259395
H	3.271160	-2.078305	-1.773477	C	-1.932362	-1.510318	0.902945
C	3.014571	0.571621	-0.951145	C	-2.994908	-1.284694	2.011745
H	2.210187	0.904254	-1.631546	H	-2.436556	-1.325648	4.192338
H	3.232388	1.391099	-0.249017	H	-2.587060	-2.923667	3.433304
H	3.925962	0.385597	-1.547781	H	-1.803352	-0.686075	0.187917
C	3.630869	-1.134484	0.826337	H	-2.114882	-2.435115	0.338660
H	4.596263	-1.357326	0.339563	H	-3.152494	-0.207377	2.156046
H	3.795699	-0.342280	1.573728	H	-3.978362	-1.724108	1.794396
H	3.292754	-2.041328	1.355955	Si	-0.658224	-1.776884	2.275740
C	-3.287039	4.274552	-1.273333	C	0.370210	-3.348511	2.231226
H	-4.157573	4.037555	-1.914251	H	-0.277861	-4.234082	2.212624
H	-3.658089	4.869622	-0.425075	H	1.007430	-3.375874	1.339261
H	-2.611319	4.906913	-1.868829	H	1.020064	-3.421361	3.113151
C	-3.692646	2.068310	-0.151164	O	1.327722	-0.574312	0.388505
H	-4.458037	1.811423	-0.906932	C	2.616607	-0.718448	-0.195625
H	-3.262726	1.124014	0.221514	C	2.448529	-1.786488	-1.273860
H	-4.210544	2.574060	0.677217	H	2.071619	-2.721121	-0.839480
C	-2.145289	2.166925	-2.070312	H	1.732230	-1.447794	-2.034096
H	-1.416160	2.714007	-2.682358	H	3.404955	-2.000045	-1.769525
H	-1.688227	1.204018	-1.771701	C	3.121721	0.562970	-0.846724
H	-3.019868	1.942519	-2.709720	H	2.392328	0.931420	-1.582488
C	1.405823	4.398292	0.340604	H	3.295785	1.353094	-0.107798
H	1.409033	4.453866	1.436760	H	4.071738	0.380362	-1.367760
H	1.826288	3.421586	0.045998	C	3.601009	-1.207772	0.863885
H	2.071351	5.195187	-0.041724	H	4.572741	-1.452360	0.415251

H	3.766166	-0.449451	1.638655
H	3.212158	-2.111796	1.352100
C	-3.316950	4.247189	-1.270201
H	-4.199673	3.979472	-1.870083
H	-3.669133	4.865344	-0.436987
H	-2.677840	4.866208	-1.908986
C	-3.682463	2.079531	-0.125114
H	-4.446283	1.818185	-0.871381
H	-3.259950	1.138204	0.250831
H	-4.201091	2.584734	0.696301
C	-2.163527	2.172029	-2.040661
H	-1.448160	2.714727	-2.663522
H	-1.705651	1.213284	-1.753484
H	-3.037959	1.945737	-2.668365
C	1.361528	4.508913	0.303811
H	1.370834	4.625345	1.390022
H	1.826547	3.544343	0.060492
H	1.994860	5.303728	-0.116717
C	-0.582528	6.025183	-0.080616
H	0.087337	6.751468	-0.564364
H	-1.581104	6.170410	-0.506384
H	-0.620946	6.287826	0.981879
C	0.181049	4.438828	-1.828664
H	0.563269	3.439018	-2.075254
H	-0.718305	4.628906	-2.422846
H	0.938740	5.165492	-2.155261
C	-0.566044	4.175443	2.945688
H	0.276139	3.471378	2.958350
H	-0.202889	5.157036	2.624135
H	-0.911841	4.287754	3.983165
C	-2.855597	4.700717	2.140823
H	-3.782905	4.343268	1.680296
H	-3.088669	4.928382	3.191713
H	-2.573394	5.642596	1.659432
C	-2.229708	2.388470	2.814172
H	-1.454407	1.611479	2.846522
H	-2.488071	2.646000	3.851591
H	-3.124703	1.960517	2.357008

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Pd	0.070795	1.151330	0.223620
P	-1.117215	3.135126	0.358531
C	-1.783590	3.558185	2.105594
C	-2.597349	2.988788	-0.848239
C	0.002162	4.578332	-0.227644
C	0.674376	0.008557	4.210743
C	0.424504	-0.219139	2.850618
C	1.121678	0.578659	1.924746
C	2.145920	1.445808	2.329430
C	2.381295	1.619922	3.694069
C	1.636407	0.923453	4.644262
H	0.119815	-0.570843	4.950728
H	2.711613	2.024934	1.606778
H	3.147095	2.326903	4.007519
H	1.818947	1.070423	5.705158
C	-2.293011	-1.788993	3.257247
C	-1.855336	-1.547753	0.901384
C	-2.982108	-1.327104	1.944114
H	-2.500501	-1.164577	4.132438
H	-2.563891	-2.819404	3.515561
H	-1.750194	-0.761177	0.143919
H	-1.959050	-2.506128	0.377452
H	-3.225543	-0.260268	2.003974

H	-3.919022	-1.851533	1.715599
Si	-0.633990	-1.687205	2.335995
C	0.427004	-3.235301	2.404426
H	-0.171327	-4.136671	2.232263
H	1.212626	-3.201869	1.642542
H	0.916734	-3.340910	3.378952
O	1.298300	-0.599856	0.451526
C	2.547245	-0.730333	-0.239375
C	2.317856	-1.868250	-1.231411
H	2.034827	-2.787753	-0.708160
H	1.513484	-1.612381	-1.929593
H	3.224517	-2.072270	-1.812322
C	2.916665	0.539596	-0.995562
H	2.120951	0.804478	-1.703267
H	3.055074	1.385411	-0.314121
H	3.847910	0.405683	-1.559329
C	3.641263	-1.117756	0.751798
H	4.572174	-1.367129	0.230623
H	3.855844	-0.306271	1.452819
H	3.334057	-1.993213	1.335010
C	-3.240929	4.302546	-1.289827
H	-4.103429	4.077348	-1.930981
H	-3.611200	4.898439	-0.451066
H	-2.565371	4.929822	-1.876820
C	-3.672917	2.105766	-0.207961
H	-4.411257	1.847262	-0.977115
H	-3.254766	1.166137	0.174842
H	-4.214520	2.602424	0.600698
C	-2.113669	2.214391	-2.083988
H	-1.367697	2.744545	-2.677076
H	-1.689016	1.241423	-1.798052
H	-2.973158	2.019215	-2.738283
C	1.386372	4.396074	0.410138
H	1.385656	4.425734	1.500570
H	1.823969	3.438864	0.101714
H	2.045096	5.200364	0.057549
C	-0.522311	5.982603	0.071472
H	0.153987	6.718972	-0.382028
H	-1.519594	6.160268	-0.340536
H	-0.556595	6.200743	1.142094
C	0.237828	4.452258	-1.736064
H	0.589774	3.449641	-2.008380
H	-0.642701	4.688519	-2.337474
H	1.022975	5.163057	-2.022860
C	-0.612744	4.006099	2.986352
H	0.209100	3.281103	2.970618
H	-0.219158	4.989545	2.718002
H	-0.967389	4.074098	4.022492
C	-2.874815	4.627698	2.142836
H	-3.794230	4.303596	1.647497
H	-3.132502	4.832078	3.190409
H	-2.563214	5.574781	1.695594
C	-2.323792	2.276204	2.752222
H	-1.585273	1.467679	2.722291
H	-2.543308	2.483709	3.807731
H	-3.247624	1.918525	2.296775

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Pd	-1.134647	0.359515	-0.150134
P	-2.472102	2.261207	-0.417109
C	-3.153685	3.023349	1.217787
C	-3.965106	1.900059	-1.585867
C	-1.358132	3.584186	-1.274002

C	-1.251675	-0.867392	3.898561	H	-1.985862	5.454606	-0.307123
C	-1.213054	-1.122264	2.510931	H	-1.226401	5.649398	-1.882904
C	-0.478240	-0.187773	1.771182	H	-2.892590	5.081759	-1.778618
C	0.269437	0.849958	2.347463	C	0.014737	3.593319	-0.567042
C	0.202741	1.049174	3.729425	H	-0.027508	3.948129	0.460867
C	-0.573706	0.193719	4.511390	H	0.451438	2.591967	-0.563891
H	-1.808354	-1.551022	4.534693	H	0.687372	4.262077	-1.119635
H	0.855807	1.520708	1.732478	C	-1.071949	3.127448	-2.717668
H	0.749769	1.875331	4.177697	H	-1.936488	3.217002	-3.376460
H	-0.633711	0.331581	5.588162	H	-0.280850	3.763396	-3.133466
C	-3.382170	-3.304279	3.309024	H	-0.714859	2.092903	-2.743448
C	-3.912104	-1.806249	1.586980	N	-2.022909	-3.435679	0.203192
C	-4.283306	-2.080875	3.055534	C	-1.338821	-4.659823	-0.184871
H	-3.063865	-3.479297	4.348269	H	-0.608670	-4.474411	-0.990804
H	-3.892456	-4.223979	2.979385	H	-0.756768	-5.022487	0.658310
H	-3.980458	-0.757524	1.282454	C	-2.276633	-5.789668	-0.636955
H	-4.573510	-2.384765	0.924472	H	-1.705911	-6.691746	-0.892573
H	-3.967790	-1.243824	3.691861	H	-2.981737	-6.047294	0.162756
H	-5.358356	-2.232596	3.255653	H	-2.864289	-5.512513	-1.519224
Si	-2.113164	-2.770132	1.891949	C	-2.731508	-2.800667	-0.906882
C	-0.603913	-3.868689	2.605043	H	-3.026762	-1.801999	-0.583403
H	-0.839395	-4.940278	2.703930	H	-3.669261	-3.330873	-1.164772
H	0.349654	-3.794768	2.063485	C	-1.920731	-2.640924	-2.198772
H	-0.411205	-3.510968	3.625983	H	-1.654690	-3.598073	-2.659809
O	0.280186	-1.155493	0.295014	H	-2.509475	-2.080480	-2.934543
C	1.684321	-1.108597	0.027902	H	-0.997876	-2.086309	-2.005662
C	2.482997	-1.357977	1.316920	13-ts-NMe2			
H	2.364093	-0.538622	2.028309	Pd	-1.129810	0.353701	-0.125401
H	2.138303	-2.277672	1.799373	P	-2.466386	2.245733	-0.424086
H	3.550498	-1.465033	1.093445	C	-3.151144	3.027265	1.200657
C	1.931984	-2.272468	-0.947524	C	-3.954291	1.853176	-1.589565
H	1.602245	-3.215912	-0.503205	C	-1.360768	3.563813	-1.299511
H	1.374901	-2.118235	-1.877118	C	-1.233233	-0.884926	3.938811
H	2.997153	-2.357341	-1.193328	C	-1.215546	-1.134269	2.549775
C	2.126518	0.202642	-0.633102	C	-0.479890	-0.205055	1.802619
H	3.187239	0.158809	-0.908956	C	0.275616	0.830246	2.373603
H	1.541421	0.384349	-1.540721	C	0.223843	1.028140	3.756360
H	1.990933	1.053807	0.037152	C	-0.543207	0.171655	4.545968
C	-5.065548	1.166312	-0.797970	H	-1.785576	-1.566713	4.580565
H	-5.821552	0.813187	-1.510220	H	0.858824	1.499784	1.754596
H	-4.673956	0.291880	-0.274379	H	0.777015	1.853057	4.199276
H	-5.575971	1.805648	-0.077459	H	-0.589020	0.306504	5.623786
C	-4.588915	3.121789	-2.279309	C	-3.385473	-3.301498	3.379834
H	-3.902062	3.601808	-2.978707	C	-3.950241	-1.781079	1.684161
H	-5.459340	2.789960	-2.859948	C	-4.292143	-2.075974	3.156812
H	-4.936600	3.874414	-1.569684	H	-3.042479	-3.484504	4.409841
C	-3.484549	0.896056	-2.655142	H	-3.903021	-4.218954	3.055509
H	-3.079842	-0.002732	-2.183630	H	-4.018961	-0.726990	1.401224
H	-4.342604	0.600655	-3.272613	H	-4.628719	-2.344423	1.024813
H	-2.724260	1.300499	-3.321604	H	-3.965546	-1.245301	3.796003
C	-3.653445	1.870546	2.112319	H	-5.362587	-2.231641	3.376296
H	-3.954567	2.287600	3.081634	Si	-2.151637	-2.761041	1.937587
H	-4.515661	1.351280	1.698211	C	-0.645110	-3.910689	2.551852
H	-2.868310	1.133180	2.291487	H	-0.903396	-4.979677	2.612754
C	-4.281088	4.053527	1.036338	H	0.282702	-3.835147	1.968691
H	-5.186931	3.617908	0.612670	H	-0.398715	-3.603202	3.577740
H	-4.548641	4.455810	2.021878	O	0.263341	-1.175590	0.327859
H	-3.982535	4.896191	0.410645	C	1.666948	-1.127112	0.048366
C	-2.006468	3.695171	1.993702	C	2.473152	-1.393164	1.328954
H	-1.157289	3.022306	2.124020	H	2.366969	-0.578002	2.047294
H	-1.665046	4.620464	1.528274	H	2.124150	-2.313681	1.806681
H	-2.375881	3.953005	2.993863	H	3.537890	-1.507718	1.096303
C	-1.912843	5.017374	-1.304514				

C	1.905147	-2.277437	-0.944380	C	0.304144	0.894643	2.542982
H	1.617346	-3.232409	-0.496071	C	0.226429	1.191235	3.905991
H	1.306097	-2.128485	-1.848914	C	-0.545175	0.388011	4.744735
H	2.961384	-2.333638	-1.232819	H	-1.808674	-1.329030	4.875457
C	2.107801	0.190548	-0.601021	H	0.894911	1.523944	1.890798
H	3.168208	0.147142	-0.877910	H	0.768414	2.049443	4.296728
H	1.523026	0.381511	-1.506888	H	-0.602265	0.593439	5.810577
H	1.974824	1.036175	0.076189	C	-3.242218	-3.266337	3.870195
C	-5.042031	1.114808	-0.789050	C	-4.058121	-1.783187	2.258522
H	-5.797400	0.743974	-1.492860	C	-4.260389	-2.116830	3.747102
H	-4.636946	0.251994	-0.256796	H	-2.788736	-3.432066	4.860535
H	-5.556286	1.756756	-0.073498	H	-3.718571	-4.218974	3.587091
C	-4.594636	3.061686	-2.291529	H	-4.225559	-0.737405	1.986190
H	-3.914144	3.544997	-2.994928	H	-4.732230	-2.390467	1.634397
H	-5.461207	2.714630	-2.869050	H	-3.952481	-1.266959	4.369330
H	-4.951422	3.815278	-1.587561	H	-5.292780	-2.363517	4.049578
C	-3.468703	0.847825	-2.657135	Si	-2.200711	-2.623586	2.296350
H	-3.041943	-0.045358	-2.191725	C	-0.703525	-3.878831	2.577521
H	-4.330638	0.536849	-3.261316	H	-1.017388	-4.932280	2.522948
H	-2.726188	1.262835	-3.336796	H	0.128285	-3.748387	1.876806
C	-3.644672	1.887172	2.114426	H	-0.304315	-3.732179	3.592968
H	-3.946148	2.319033	3.077159	O	0.389290	-1.250397	0.704977
H	-4.505962	1.359136	1.709869	C	1.804980	-1.198160	0.488884
H	-2.856467	1.155733	2.305085	C	2.544493	-1.404374	1.819561
C	-4.284558	4.048232	1.006465	H	2.381824	-0.566036	2.499722
H	-5.190132	3.598058	0.597160	H	2.183643	-2.314398	2.309017
H	-4.548699	4.468054	1.985582	H	3.622434	-1.506399	1.650965
H	-3.995177	4.879864	0.362207	C	2.092495	-2.387932	-0.441257
C	-2.004549	3.713900	1.964653	H	1.773891	-3.324323	0.024898
H	-1.153588	3.044516	2.103750	H	1.549050	-2.270541	-1.384569
H	-1.665420	4.632853	1.485329	H	3.163501	-2.458948	-0.664923
H	-2.373173	3.985702	2.961350	C	2.272174	0.088797	-0.203502
C	-1.924232	4.993215	-1.347435	H	3.339337	0.024123	-0.448050
H	-2.000129	5.442579	-0.355729	H	1.714554	0.239124	-1.133776
H	-1.241816	5.622180	-1.933864	H	2.129717	0.967865	0.427153
H	-2.904462	5.045456	-1.822323	C	-4.900430	0.693491	-0.604507
C	0.013362	3.589627	-0.595529	H	-5.644117	0.189491	-1.234235
H	-0.028696	3.959600	0.427058	H	-4.418789	-0.067838	0.012915
H	0.454809	2.590571	-0.577794	H	-5.441665	1.384765	0.042917
H	0.681948	4.253184	-1.159155	C	-4.607343	2.472619	-2.343437
C	-1.075840	3.091425	-2.738287	H	-3.966162	2.917014	-3.106739
H	-1.942165	3.171755	-3.395900	H	-5.454474	2.008375	-2.865096
H	-0.287533	3.724972	-3.162923	H	-5.008481	3.275899	-1.722987
H	-0.716151	2.057648	-2.754100	C	-3.359396	0.294359	-2.470545
N	-2.152406	-3.408844	0.239770	H	-2.845215	-0.487791	-1.904565
C	-1.337136	-4.490692	-0.273494	H	-4.215649	-0.163049	-2.982272
H	-0.447595	-4.140022	-0.829795	H	-2.680253	0.666091	-3.236607
H	-0.991818	-5.152837	0.519001	C	-3.523876	1.903411	2.136160
C	-2.683999	-2.649359	-0.873382	H	-3.775883	2.434155	3.062883
H	-3.172450	-1.740196	-0.527636	H	-4.405499	1.341294	1.835031
H	-3.415137	-3.227396	-1.472804	H	-2.726175	1.193151	2.359098
H	-1.914202	-5.110389	-0.983986	C	-4.254418	3.892814	0.797152
H	-1.884888	-2.342780	-1.572593	H	-5.145547	3.364583	0.453869
13-ts-OtBu				H	-4.523865	4.405945	1.729482
Pd	-1.023723	0.177137	0.043246	H	-4.006164	4.659968	0.062240
P	-2.399741	1.993499	-0.449563	C	-1.943139	3.740935	1.740155
C	-3.082932	2.939296	1.083211	H	-1.074866	3.110468	1.942673
C	-3.882345	1.395424	-1.522014	H	-1.631150	4.604717	1.152114
C	-1.361304	3.236712	-1.497934	H	-2.304408	4.120466	2.703726
C	-1.237020	-0.700446	4.199141	C	-1.984402	4.628684	-1.692802
C	-1.206839	-1.039916	2.830932	H	-2.057355	5.186703	-0.757689
C	-0.426111	-0.187668	2.025612	H	-1.344159	5.212556	-2.366851
				H	-2.978032	4.585580	-2.141420

C	0.025722	3.389566	-0.837567
H	-0.010224	3.855415	0.145139
H	0.512065	2.416458	-0.733427
H	0.651381	4.021666	-1.480890
C	-1.092099	2.619216	-2.883578
H	-1.978264	2.592524	-3.518965
H	-0.343522	3.234170	-3.398217
H	-0.688146	1.605333	-2.801186
O	-2.231327	-2.851735	0.533978
C	-2.467357	-3.998895	-0.265066
C	-3.353878	-5.028753	0.457187
H	-2.862762	-5.408550	1.357508
H	-4.307872	-4.578742	0.749310
H	-3.567993	-5.885206	-0.192656
C	-3.196983	-3.508244	-1.526264
H	-2.572857	-2.787782	-2.064611
H	-3.432300	-4.334822	-2.207377
H	-4.131727	-3.007655	-1.252966
C	-1.141746	-4.657238	-0.686995
H	-0.496937	-3.913849	-1.165092
H	-0.609216	-5.064086	0.175291
H	-1.314104	-5.474119	-1.398718

13-ts-pbe0d3

Pd	0.098867	1.178134	0.242196
P	-1.106860	3.154845	0.360062
C	-1.736766	3.609971	2.104353
C	-2.602634	2.959097	-0.815342
C	-0.006977	4.579986	-0.288578
C	0.648623	-0.098124	4.196422
C	0.390826	-0.259012	2.829729
C	1.073968	0.581466	1.926483
C	2.072375	1.457269	2.379879
C	2.317449	1.567275	3.748746
C	1.598044	0.809114	4.669876
H	0.106986	-0.719423	4.909271
H	2.615322	2.088068	1.686890
H	3.069573	2.274988	4.090704
H	1.784942	0.907844	5.735272
C	-2.281745	-1.885756	3.258266
C	-1.921859	-1.499778	0.900037
C	-3.012217	-1.339790	1.996857
H	-2.454932	-1.317022	4.176856
H	-2.540765	-2.933056	3.455464
H	-1.819845	-0.657800	0.207271
H	-2.053100	-2.416543	0.312341
H	-3.246308	-0.279456	2.133439
H	-3.955838	-1.850664	1.768026
Si	-0.651208	-1.725055	2.284463
C	0.411984	-3.275612	2.250628
H	-0.204277	-4.164078	2.070926
H	1.165428	-3.214075	1.459645
H	0.933658	-3.411865	3.205260
O	1.299457	-0.524711	0.440286
C	2.566135	-0.680640	-0.198463
C	2.347772	-1.795914	-1.221401
H	2.002946	-2.708709	-0.724986
H	1.591161	-1.496061	-1.954710
H	3.277037	-2.024176	-1.755307
C	3.017596	0.584477	-0.920626
H	2.247668	0.909937	-1.629905
H	3.207851	1.401574	-0.220297
H	3.943026	0.398432	-1.478077

C	3.605250	-1.119700	0.832241
H	4.558727	-1.353280	0.346368
H	3.782283	-0.336439	1.573929
H	3.259892	-2.015354	1.358829
C	-3.264374	4.257854	-1.280468
H	-4.136526	4.004550	-1.897278
H	-3.621101	4.869553	-0.448932
H	-2.604485	4.871200	-1.897650
C	-3.668023	2.085585	-0.143390
H	-4.415555	1.818920	-0.900872
H	-3.248150	1.153319	0.246307
H	-4.196010	2.598863	0.662417
C	-2.128830	2.161310	-2.041542
H	-1.388712	2.684129	-2.646396
H	-1.704042	1.194188	-1.743066
H	-2.996350	1.958720	-2.682744
C	1.385580	4.430357	0.341030
H	1.387570	4.499042	1.428123
H	1.829684	3.470607	0.058665
H	2.029149	5.231298	-0.045209
C	-0.536485	5.991158	-0.024211
H	0.135599	6.713325	-0.505521
H	-1.536267	6.150247	-0.433846
H	-0.559886	6.235297	1.040003
C	0.213184	4.412398	-1.796615
H	0.576462	3.408881	-2.042977
H	-0.678297	4.620759	-2.390738
H	0.985235	5.126639	-2.108899
C	-0.557534	4.090103	2.959287
H	0.268904	3.373304	2.955156
H	-0.181122	5.070468	2.660450
H	-0.906581	4.181348	3.995353
C	-2.836592	4.673507	2.140146
H	-3.759940	4.335565	1.664470
H	-3.075470	4.889485	3.189644
H	-2.533569	5.612742	1.673782
C	-2.254256	2.334794	2.782417
H	-1.497631	1.545795	2.784383
H	-2.493559	2.572610	3.826735
H	-3.160946	1.944731	2.322467

13-ts-wb97xd

Pd	0.120142	1.167393	0.230425
P	-1.120397	3.165881	0.349489
C	-1.739754	3.623696	2.102359
C	-2.629778	2.968781	-0.814007
C	-0.019530	4.590607	-0.308157
C	0.638710	-0.117760	4.184489
C	0.393381	-0.281808	2.815962
C	1.082830	0.562248	1.922048
C	2.067126	1.447110	2.385341
C	2.299884	1.558646	3.755672
C	1.576851	0.795109	4.667763
H	0.093147	-0.738760	4.893788
H	2.614607	2.080375	1.698532
H	3.042949	2.271023	4.105032
H	1.750424	0.895977	5.734537
C	-2.271111	-1.891905	3.268510
C	-1.939535	-1.514713	0.904387
C	-3.011634	-1.318206	2.019179
H	-2.422886	-1.330490	4.194816
H	-2.548195	-2.936213	3.454487
H	-1.846791	-0.693183	0.187690

H	-2.100019	-2.444496	0.345555	C	-2.698171	3.018427	-0.955317
H	-3.207047	-0.251203	2.161297	C	-0.162857	4.812438	-0.608790
H	-3.973285	-1.799831	1.807314	C	0.721657	-0.651741	4.497325
Si	-0.655643	-1.745850	2.273897	C	0.708397	-0.875820	3.109910
C	0.408153	-3.295132	2.218303	C	1.572133	-0.097100	2.321860
H	-0.207441	-4.184348	2.041147	C	2.414422	0.866003	2.884464
H	1.151732	-3.227959	1.418360	C	2.415502	1.049153	4.267414
H	0.941898	-3.435316	3.165523	C	1.568652	0.292181	5.079620
O	1.333869	-0.531248	0.419776	H	0.054493	-1.227448	5.133149
C	2.614193	-0.697228	-0.187797	H	3.040905	1.480441	2.251798
C	2.408225	-1.794571	-1.238662	H	3.070162	1.797357	4.705039
H	2.036908	-2.710674	-0.768114	H	1.563229	0.442499	6.155135
H	1.675857	-1.470066	-1.985789	C	-2.052789	-2.305373	3.389345
H	3.348045	-2.026618	-1.751611	C	-1.770174	-1.334352	1.195456
C	3.114124	0.573629	-0.878942	C	-2.709395	-1.247047	2.442374
H	2.380103	0.920964	-1.615006	H	-2.078949	-2.064541	4.455605
H	3.291589	1.378320	-0.161409	H	-2.508038	-3.293878	3.253415
H	4.057636	0.377755	-1.400753	H	-1.540328	-0.380474	0.704686
C	3.619489	-1.171228	0.867435	H	-2.154116	-2.035991	0.445335
H	4.580281	-1.417807	0.403188	H	-2.629808	-0.252703	2.891980
H	3.793058	-0.399976	1.622589	H	-3.769864	-1.425823	2.227004
H	3.241665	-2.065531	1.373504	Si	-0.476369	-2.123042	2.336116
C	-3.301592	4.272352	-1.269272	C	0.409219	-3.695794	1.800605
H	-4.190164	4.022023	-1.862553	H	-0.321474	-4.468146	1.533824
H	-3.632047	4.889568	-0.431179	H	1.046247	-3.523893	0.928215
H	-2.653051	4.879685	-1.904129	H	1.039320	-4.090438	2.606249
C	-3.690246	2.089431	-0.128044	O	1.475821	-0.275397	0.943578
H	-4.445381	1.816499	-0.874475	C	2.648657	-0.632041	0.102109
H	-3.261941	1.160618	0.261387	C	1.997592	-1.297753	-1.106248
H	-4.210384	2.604511	0.681424	H	1.447971	-2.194822	-0.810311
C	-2.177177	2.172807	-2.056900	H	1.298297	-0.601718	-1.582284
H	-1.459547	2.705734	-2.679501	H	2.760844	-1.579920	-1.837113
H	-1.734362	1.210271	-1.771954	C	3.386468	0.633833	-0.332529
H	-3.057013	1.962582	-2.677263	H	2.664982	1.371761	-0.701807
C	1.384894	4.442978	0.311686	H	3.963889	1.079759	0.480229
H	1.397524	4.500763	1.399136	H	4.083480	0.389312	-1.140626
H	1.835883	3.490282	0.017003	C	3.558357	-1.592486	0.859073
H	2.020973	5.251401	-0.069765	H	4.369383	-1.911831	0.197762
C	-0.545780	6.008974	-0.044502	H	4.007318	-1.116436	1.734558
H	0.119031	6.728907	-0.537847	H	3.013161	-2.481093	1.186488
H	-1.550733	6.164216	-0.442883	C	-3.454782	4.274770	-1.415774
H	-0.556081	6.258104	1.018612	H	-4.348264	3.967691	-1.974898
C	0.190871	4.423188	-1.823701	H	-3.790567	4.890943	-0.579943
H	0.533984	3.414454	-2.076645	H	-2.859161	4.900319	-2.083136
H	-0.701379	4.651515	-2.409038	C	-3.678296	2.107779	-0.192809
H	0.971753	5.124638	-2.140657	H	-4.463847	1.784551	-0.886988
C	-0.551214	4.100307	2.956450	H	-3.183868	1.210173	0.188252
H	0.270035	3.378113	2.949262	H	-4.171123	2.616165	0.636489
H	-0.170119	5.077695	2.655062	C	-2.253802	2.211284	-2.194195
H	-0.893865	4.196735	3.993537	H	-1.612418	2.775754	-2.869489
C	-2.840335	4.694131	2.149525	H	-1.714079	1.307730	-1.893584
H	-3.771592	4.351516	1.693084	H	-3.145795	1.911396	-2.758995
H	-3.060598	4.920170	3.200365	C	1.266692	4.795883	-0.025041
H	-2.545567	5.628080	1.667554	H	1.300977	5.000178	1.043859
C	-2.261632	2.348868	2.792870	H	1.744079	3.826306	-0.196962
H	-1.512648	1.553011	2.788563	H	1.860424	5.569733	-0.528574
H	-2.486021	2.588442	3.839517	C	-0.776785	6.204046	-0.382406
H	-3.177721	1.965063	2.346928	H	-0.166299	6.951510	-0.905761
				H	-1.793680	6.285703	-0.769939
				H	-0.790009	6.484535	0.672429
				C	0.007575	4.586624	-2.123092
				H	0.403136	3.589060	-2.338216
				H	-0.918691	4.724239	-2.682224
14							
Pd	0.143558	1.491892	0.349440				
P	-1.138088	3.324823	0.143259				
C	-1.734021	3.836082	1.907560				

H	0.728132	5.319630	-2.506289
C	-0.542597	4.423414	2.687444
H	0.330034	3.764932	2.636203
H	-0.256108	5.418499	2.344877
H	-0.828829	4.514572	3.742501
C	-2.903867	4.831552	1.966086
H	-3.827986	4.411323	1.564906
H	-3.098153	5.089380	3.015471
H	-2.693491	5.761485	1.435835
C	-2.126987	2.550790	2.668512
H	-1.288427	1.848250	2.697292
H	-2.389531	2.819332	3.700064
H	-2.982095	2.036336	2.235140

15-ts

Pd	-1.157092	0.357493	-0.210567
C	1.530247	0.288307	3.014808
C	0.723610	-0.282384	2.013513
C	-0.516334	0.329428	1.712803
C	-0.941426	1.446255	2.458089
C	-0.114909	2.003970	3.435957
C	1.127880	1.427148	3.714902
H	2.489056	-0.165838	3.254540
H	-1.920097	1.881217	2.271505
H	-0.446103	2.880031	3.988437
H	1.767158	1.850841	4.484719
C	-0.379147	-2.862139	0.892467
C	-2.097068	-1.017999	1.292887
C	-1.496390	-2.320491	1.804916
H	-0.165195	-3.911108	1.136768
H	-0.713879	-2.843527	-0.151127
H	-2.737145	-0.526871	2.024983
H	-2.701951	-1.236981	0.404836
H	-1.118441	-2.190837	2.826823
H	-2.309993	-3.058674	1.872585
Si	1.203689	-1.860843	1.116605
C	2.396623	-2.841336	2.196072
H	2.733003	-3.743598	1.672004
H	3.286168	-2.281342	2.498304
H	1.882089	-3.164166	3.109932
O	1.831645	-1.617758	-0.419623
C	2.906695	-0.766443	-0.877911
C	4.198946	-1.069376	-0.114200
H	4.112034	-0.790702	0.939853
H	4.445630	-2.133931	-0.175069
H	5.031096	-0.498985	-0.540019
C	3.076506	-1.107244	-2.359561
H	3.335654	-2.164490	-2.478927
H	2.146340	-0.920315	-2.902351
H	3.869996	-0.503076	-2.810313
C	2.510034	0.702885	-0.704345
H	3.213722	1.356458	-1.230655
H	1.506537	0.866414	-1.105461
H	2.496943	0.990394	0.349725
P	-2.002540	0.900143	-2.403395
C	-3.795299	1.572930	-2.175527
C	-2.059551	-0.618680	-3.584244
C	-0.948282	2.282985	-3.227522
C	-3.727633	2.967720	-1.524070
H	-4.742315	3.260083	-1.227493
H	-3.109721	2.957450	-0.620566
H	-3.353508	3.739484	-2.196903
C	-4.528131	0.683174	-1.148238

H	-3.996080	0.677267	-0.193403
H	-5.528807	1.100745	-0.979472
H	-4.655129	-0.348351	-1.472341
C	-4.639239	1.657478	-3.457627
H	-5.596161	2.141736	-3.224012
H	-4.156575	2.243051	-4.241038
H	-4.870547	0.670224	-3.863207
C	-3.149866	-1.588180	-3.091903
H	-4.159332	-1.212482	-3.262611
H	-3.055208	-2.527971	-3.649175
H	-3.035320	-1.822003	-2.029357
C	-0.720073	-1.371682	-3.436972
H	0.110637	-0.852293	-3.910815
H	-0.463896	-1.531060	-2.385330
H	-0.809112	-2.352510	-3.920556
C	-2.308660	-0.309041	-5.068473
H	-2.346896	-1.253297	-5.627064
H	-3.255509	0.207197	-5.233459
H	-1.510460	0.291761	-5.507736
C	-0.496420	3.242624	-2.103846
H	0.180313	3.994336	-2.529772
H	-1.321176	3.773860	-1.631391
H	0.047039	2.702458	-1.321435
C	0.342291	1.673615	-3.806055
H	0.856717	1.039359	-3.083171
H	0.166128	1.097096	-4.714884
H	1.023426	2.491924	-4.069659
C	-1.636462	3.086074	-4.343887
H	-0.912803	3.794713	-4.767057
H	-1.984377	2.449201	-5.159705
H	-2.484112	3.671069	-3.983401

16

Pd	-0.493023	0.794091	-0.393849
C	0.366377	0.905117	1.770110
C	-0.121419	-0.414928	1.555567
C	-1.456002	-0.710622	1.996009
C	-2.189506	0.267484	2.670159
C	-1.687681	1.561798	2.869868
C	-0.423667	1.892306	2.399111
H	1.406637	1.136101	1.565103
H	-3.184786	0.021202	3.031983
H	-2.291564	2.302060	3.387280
H	-0.018285	2.889027	2.548531
C	-0.064786	-3.334197	0.915958
C	-2.109098	-2.058286	1.746714
C	-1.206197	-3.284124	1.945583
H	0.530711	-4.248263	1.035789
H	-0.488071	-3.365890	-0.096812
H	-2.988484	-2.141114	2.394207
H	-2.487534	-2.077641	0.714662
H	-0.799636	-3.272729	2.966141
H	-1.823714	-4.188225	1.871605
Si	1.040768	-1.826853	1.064850
C	2.262616	-2.018428	2.483737
H	2.912952	-2.889740	2.353664
H	2.894997	-1.133775	2.612350
H	1.702918	-2.155305	3.417317
O	1.788580	-1.668360	-0.420129
C	3.047629	-1.110042	-0.858457
C	4.194129	-2.017239	-0.402433
H	4.295739	-2.017025	0.685354
H	4.020582	-3.045569	-0.735621

H	5.142697	-1.674399	-0.828890	H	2.201861	2.604286	2.017731
C	2.966053	-1.087107	-2.385489	H	3.154567	2.259974	4.253501
H	2.774279	-2.092891	-2.772869	H	2.356894	0.362653	5.672522
H	2.153314	-0.433124	-2.707711	C	-2.146106	-1.760790	3.702794
H	3.902445	-0.720915	-2.818081	C	-1.974955	-1.230209	0.950687
C	3.224078	0.311009	-0.321764	C	-3.366696	-1.585838	1.521292
H	4.132153	0.763875	-0.733510	H	-1.937823	-1.262617	4.655008
H	2.365194	0.929155	-0.604424	H	-2.293069	-2.826789	3.922720
H	3.316788	0.314466	0.768694	H	-1.921468	-0.168916	0.687801
P	-1.659220	1.247440	-2.343037	H	-1.733516	-1.790262	0.042090
C	-3.381579	1.983008	-1.871782	H	-4.176990	-1.103071	0.960137
C	-1.955695	-0.378550	-3.339000	H	-3.528924	-2.669347	1.439419
C	-0.762604	2.512009	-3.488106	Si	-0.779884	-1.559958	2.382160
C	-3.199086	3.441020	-1.409544	C	0.213253	-3.144385	2.135601
H	-4.140833	3.783203	-0.963227	H	-0.456388	-4.002535	2.001091
H	-2.420979	3.523168	-0.644560	H	0.836845	-3.060017	1.240347
H	-2.963903	4.122899	-2.227457	H	0.868463	-3.358274	2.987528
C	-3.901448	1.224597	-0.631612	O	1.075317	-0.532936	-0.441862
H	-3.183027	1.292582	0.189791	C	2.457330	-0.629906	-0.720227
H	-4.843487	1.686376	-0.308417	C	2.619783	-1.718099	-1.798676
H	-4.099550	0.170202	-0.816509	H	2.207371	-2.668599	-1.442838
C	-4.451159	1.945382	-2.975171	H	2.081242	-1.433253	-2.709817
H	-5.355415	2.450137	-2.610745	H	3.673021	-1.877572	-2.057977
H	-4.136062	2.458855	-3.885185	C	3.022560	0.697388	-1.256986
H	-4.739100	0.926458	-3.240019	H	2.454600	1.022409	-2.136716
C	-2.968819	-1.253152	-2.576638	H	2.949187	1.478995	-0.493834
H	-3.984963	-0.858719	-2.608474	H	4.076149	0.603676	-1.547666
H	-2.991466	-2.244772	-3.044945	C	3.241654	-1.043960	0.539344
H	-2.675353	-1.388255	-1.531180	H	4.308161	-1.178931	0.321432
C	-0.636700	-1.178544	-3.339594	H	3.144608	-0.283075	1.318252
H	0.150360	-0.708584	-3.926009	H	2.854551	-1.986872	0.939030
H	-0.262450	-1.313982	-2.321270	C	-3.262290	4.088658	-1.180500
H	-0.824630	-2.168459	-3.774744	H	-4.173816	3.790810	-1.713404
C	-2.442214	-0.201073	-4.785905	H	-3.549891	4.822076	-0.425627
H	-2.627026	-1.190872	-5.223289	H	-2.611723	4.577763	-1.906397
H	-3.373590	0.363794	-4.850542	C	-3.711342	2.098776	0.250507
H	-1.699674	0.293511	-5.414874	H	-4.494361	1.771537	-0.443815
C	-0.145384	3.606138	-2.590136	H	-3.326145	1.208653	0.747624
H	0.470320	4.267521	-3.213104	H	-4.186667	2.737843	0.994615
H	-0.886417	4.225515	-2.087461	C	-2.228642	1.858841	-1.702140
H	0.496402	3.159797	-1.823818	H	-1.459371	2.253133	-2.363564
C	0.430421	1.816179	-4.167541	H	-1.884469	0.898501	-1.303802
H	1.064862	1.306992	-3.437324	H	-3.116088	1.654612	-2.313273
H	0.129420	1.099575	-4.932559	C	1.430133	4.452474	0.250619
H	1.042362	2.580426	-4.662166	H	1.456378	4.686961	1.313054
C	-1.631133	3.171644	-4.571155	H	1.887274	3.472065	0.097201
H	-0.996949	3.819449	-5.190513	H	2.047312	5.196699	-0.267192
H	-2.098229	2.441936	-5.234586	C	-0.528828	5.927176	-0.272428
H	-2.416898	3.801239	-4.149972	H	0.113979	6.576879	-0.879390
17				H	-1.544970	6.021202	-0.655615
Pd	0.184319	1.162311	0.272532	H	-0.507966	6.315958	0.747298
P	-1.059275	3.154975	0.516083	C	0.191020	4.101379	-1.837921
C	-1.623522	3.801852	2.231006	H	0.542638	3.069925	-1.942514
C	-2.628116	2.828694	-0.567734	H	-0.716018	4.226678	-2.429087
C	0.012851	4.491256	-0.356790	H	0.955559	4.755599	-2.273287
C	0.974874	-0.341481	4.174215	C	-0.437457	4.425187	2.989125
C	0.412553	-0.177717	2.887787	H	0.407037	3.740415	3.065536
C	0.847815	0.922056	2.126934	H	-0.100840	5.363305	2.546349
C	1.841858	1.778639	2.617121	H	-0.772351	4.650083	4.008706
C	2.388326	1.580881	3.888038	C	-2.744427	4.854045	2.158782
C	1.946048	0.520295	4.679172	H	-3.675168	4.455925	1.755050
H	0.647146	-1.175593	4.792605	H	-2.956564	5.200524	3.177733
				H	-2.459332	5.726682	1.569446

C	-2.099317	2.596810	3.068470	H	-1.582972	1.485093	-2.785853
H	-1.308821	1.854006	3.185373	C	-4.878696	2.921279	1.525185
H	-2.374051	2.958143	4.066892	H	-5.596384	3.516204	2.103356
H	-2.973901	2.104061	2.649224	H	-5.446443	2.308114	0.826518
C	-3.403996	-1.187989	3.009255	H	-4.356055	2.254978	2.216018
H	-4.332896	-1.523020	3.487883	C	-4.662652	4.881502	-0.048421
H	-3.387450	-0.092884	3.081736	H	-5.303977	4.398395	-0.784728
18-ts				H	-5.313877	5.477538	0.602132
Pd	-2.506334	0.570227	0.621130	H	-3.998239	5.574332	-0.567777
P	-2.618339	2.806325	-0.147027	C	-3.223443	4.697866	1.956747
C	-3.890859	3.882621	0.833059	H	-2.703870	4.070516	2.679403
C	-3.403580	2.337609	-1.853535	H	-2.536025	5.459908	1.590920
C	-1.020905	3.821354	-0.459441	H	-4.019822	5.217098	2.502411
C	-0.341054	-0.815909	3.850537	C	-1.282056	5.262581	-0.933062
C	-1.117115	-0.649133	2.689963	H	-1.771244	5.874084	-0.174141
C	-1.523077	0.641611	2.349229	H	-0.314912	5.731323	-1.152299
C	-1.218235	1.740459	3.150846	H	-1.879798	5.304338	-1.843739
C	-0.458460	1.550227	4.311424	C	-0.179175	3.852526	0.829932
C	-0.007113	0.274898	4.655601	H	-0.680871	4.337618	1.665519
H	-0.003629	-1.811418	4.130287	H	0.112085	2.846393	1.137544
H	-1.546727	2.733207	2.893494	H	0.735933	4.419983	0.623394
H	-0.222085	2.405848	4.938960	C	-0.154422	3.107479	-1.512492
H	0.592192	0.130971	5.550947	H	-0.559634	3.191508	-2.521302
C	-3.300470	-2.512575	2.906922	H	0.832295	3.584765	-1.519489
C	-3.580528	-1.541259	0.479517	H	-0.007307	2.051663	-1.272016
C	-4.843038	-1.417126	1.334305	C	-4.419934	-1.490463	2.810509
H	-2.873735	-2.571266	3.916377	H	-4.031998	-0.505146	3.108138
H	-3.680925	-3.517233	2.661944	H	-5.274761	-1.708087	3.466453
H	-3.663196	-1.022340	-0.489474	19			
H	-3.449997	-2.581389	0.141896	Pd	-3.210234	0.501481	0.626719
H	-5.366674	-0.476306	1.126237	P	-2.734996	2.827116	-0.257467
H	-5.554430	-2.228816	1.118738	C	-3.708410	4.209469	0.672340
Si	-1.800513	-2.100091	1.670724	C	-3.463429	2.691688	-2.038353
C	-0.883078	-3.730110	2.142354	C	-0.893546	3.355407	-0.379778
H	0.204350	-3.682128	2.040910	C	-0.501309	-0.288163	3.901379
H	-1.108212	-4.027169	3.173168	C	-1.266194	-0.563724	2.745709
H	-1.225809	-4.550806	1.497511	C	-2.308909	0.335515	2.410003
O	-1.040409	-1.884423	0.080994	C	-2.641161	1.357001	3.316280
C	0.304569	-1.964811	-0.402683	C	-1.889383	1.586601	4.470695
C	0.653654	-3.406180	-0.806840	C	-0.784157	0.782803	4.748458
H	0.721949	-4.069632	0.056860	H	0.326395	-0.943464	4.158280
H	-0.114223	-3.800253	-1.481653	H	-3.485766	2.003865	3.113258
H	1.615324	-3.438799	-1.331695	H	-2.164935	2.398615	5.139513
C	0.330814	-1.082940	-1.660713	H	-0.170631	0.966109	5.626398
H	-0.406729	-1.435408	-2.389632	C	-2.580888	-3.307088	2.512738
H	0.083765	-0.051573	-1.396551	C	-4.043252	-1.376283	0.687910
H	1.317867	-1.092792	-2.136254	C	-4.742989	-2.045254	1.862499
C	1.327645	-1.415141	0.601368	H	-2.224581	-3.945172	3.333264
H	2.332299	-1.431674	0.164066	H	-2.842424	-3.996261	1.697939
H	1.086462	-0.381405	0.865343	H	-4.794293	-1.135617	-0.089452
H	1.355162	-2.001435	1.522372	H	-3.303990	-2.046195	0.240287
C	-4.819318	1.771389	-1.610983	H	-5.500486	-1.373544	2.288605
H	-5.180634	1.342090	-2.552405	H	-5.299298	-2.916475	1.474454
H	-4.821986	0.973007	-0.862420	Si	-1.062132	-2.285281	2.006928
H	-5.538429	2.530313	-1.304239	C	0.439339	-3.139345	2.772104
C	-3.485912	3.478603	-2.880354	H	1.387074	-2.622414	2.593175
H	-2.498254	3.804470	-3.210694	H	0.321836	-3.253854	3.855550
H	-4.015112	3.103247	-3.765202	H	0.526508	-4.147801	2.350247
H	-4.032557	4.347235	-2.515341	O	-0.953922	-2.369031	0.338783
C	-2.585693	1.188920	-2.490102	C	0.098082	-1.936895	-0.551267
H	-2.493668	0.316132	-1.838107	C	1.022407	-3.128089	-0.816927
H	-3.114681	0.860413	-3.392531	H	1.531613	-3.440388	0.099461

H	0.446489	-3.977575	-1.198210
H	1.785072	-2.868412	-1.558967
C	-0.611803	-1.505846	-1.835610
H	-1.188571	-2.340046	-2.248972
H	-1.301117	-0.686219	-1.620235
H	0.106099	-1.173020	-2.592197
C	0.881520	-0.762824	0.041245
H	1.600158	-0.378591	-0.689466
H	0.203117	0.045768	0.316043
H	1.441900	-1.062246	0.931509
C	-4.999008	2.599404	-1.943083
H	-5.390355	2.314531	-2.927115
H	-5.316040	1.832600	-1.228610
H	-5.469851	3.544334	-1.671451
C	-3.087979	3.827841	-3.002361
H	-2.020592	3.838533	-3.230071
H	-3.619841	3.678711	-3.951003
H	-3.365151	4.810961	-2.621353
C	-3.008315	1.350115	-2.653396
H	-3.326952	0.494111	-2.048418
H	-3.478700	1.242374	-3.638877
H	-1.932751	1.276959	-2.795098
C	-5.028559	3.591269	1.183228
H	-5.514613	4.304859	1.859748
H	-5.732441	3.370433	0.382092
H	-4.852908	2.664206	1.735610
C	-4.030644	5.467483	-0.152482
H	-4.702494	5.263875	-0.987413
H	-4.537258	6.191790	0.498326
H	-3.133772	5.951573	-0.543540
C	-2.919957	4.656437	1.918955
H	-2.620722	3.818494	2.547613
H	-2.030627	5.234723	1.669205
H	-3.568600	5.305703	2.519525
C	-0.639922	4.828382	-0.739628
H	-1.006974	5.519439	0.020064
H	0.442843	4.987816	-0.824538
H	-1.087152	5.104145	-1.696267
C	-0.229821	3.029526	0.976806
H	-0.584702	3.659864	1.790780
H	-0.393490	1.988531	1.264355
H	0.851329	3.190808	0.884054
C	-0.188628	2.477519	-1.430514
H	-0.458851	2.747085	-2.452805
H	0.894077	2.621643	-1.332552
H	-0.392881	1.417029	-1.280753
C	-3.830802	-2.542579	2.991727
H	-3.523377	-1.690255	3.606346
H	-4.426245	-3.193570	3.646088

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Pd	-0.051959	1.053515	0.081591
P	-1.163801	3.116381	0.356560
C	-1.572930	3.781854	2.105441
C	-2.813590	2.836433	-0.608981
C	-0.118055	4.416061	-0.601986
C	1.221246	-0.333994	3.906549
C	0.485709	-0.192832	2.707892
C	0.856226	0.850364	1.838555
C	1.948687	1.672885	2.142548
C	2.664633	1.498023	3.330035
C	2.294139	0.495393	4.225984
H	0.950342	-1.125304	4.603522

H	2.251364	2.458666	1.464610
H	3.505544	2.151288	3.549188
H	2.837822	0.356157	5.156281
C	-1.966420	-1.691444	3.930436
C	-2.183713	-1.206607	1.174458
C	-3.489239	-1.494834	1.950796
H	-1.605417	-1.196186	4.837576
H	-2.113523	-2.751034	4.180342
H	-2.127093	-0.152020	0.885036
H	-2.101511	-1.789759	0.252110
H	-4.353255	-0.983987	1.506673
H	-3.706165	-2.571148	1.911525
Si	-0.802041	-1.550392	2.422118
C	0.123535	-3.162308	2.106278
H	-0.577935	-3.994808	1.973561
H	0.732041	-3.084405	1.200409
H	0.788825	-3.413316	2.940467
O	0.713497	-0.714108	-0.588962
C	-3.451021	4.110141	-1.189191
H	-4.402627	3.834848	-1.660532
H	-3.670712	4.853664	-0.421241
H	-2.836457	4.579385	-1.957822
C	-3.864084	2.147715	0.283054
H	-4.705311	1.854419	-0.356208
H	-3.481060	1.240489	0.750222
H	-4.263502	2.801721	1.058258
C	-2.520844	1.843251	-1.756750
H	-1.786534	2.204815	-2.474415
H	-2.181471	0.874570	-1.370914
H	-3.453201	1.658134	-2.303849
C	1.339428	4.333957	-0.106864
H	1.456478	4.555921	0.952227
H	1.753856	3.342936	-0.306721
H	1.934663	5.066110	-0.665740
C	-0.609035	5.867500	-0.478728
H	0.006576	6.499383	-1.130959
H	-1.647607	5.992758	-0.785393
H	-0.501621	6.252448	0.536968
C	-0.059393	4.022119	-2.091336
H	0.265765	2.984771	-2.219541
H	-1.003215	4.163733	-2.617277
H	0.683336	4.661741	-2.582569
C	-0.307476	4.352129	2.772869
H	0.511898	3.632281	2.786523
H	0.034574	5.276427	2.305523
H	-0.554922	4.588302	3.814638
C	-2.654945	4.876252	2.118926
H	-3.627544	4.512111	1.786888
H	-2.776264	5.228008	3.150837
H	-2.384159	5.739244	1.508935
C	-2.031634	2.593425	2.975473
H	-1.258032	1.827035	3.042689
H	-2.227982	2.963781	3.988974
H	-2.946774	2.128598	2.615364
C	-3.292966	-1.081864	3.422600
H	-4.151735	-1.381695	4.036617
H	-3.231597	0.012350	3.478750
C	2.097155	-0.948905	-0.574208
C	2.398422	-2.279233	-1.283527
C	2.908990	0.181791	-1.227244
H	2.454335	-1.048646	0.469471
C	3.900021	-2.595834	-1.299323
H	2.023165	-2.210036	-2.315112

H	1.839012	-3.085607	-0.794316	C	-3.090951	4.629620	1.726112
C	4.413487	-0.118529	-1.245507	H	-2.616606	3.989021	2.469142
H	2.541637	0.314517	-2.256160	H	-2.351933	5.331332	1.340843
H	2.708243	1.118015	-0.693281	H	-3.852856	5.217273	2.251259
C	4.705470	-1.456635	-1.936846	C	-1.139756	4.985837	-1.196009
H	4.083136	-3.537339	-1.831656	H	-1.581661	5.655303	-0.456869
H	4.247277	-2.747838	-0.267372	H	-0.154374	5.393327	-1.453143
H	4.958712	0.694585	-1.740560	H	-1.752727	5.018566	-2.096916
H	4.784222	-0.159443	-0.211302	C	-0.081061	3.610076	0.615729
H	5.778752	-1.680528	-1.898246	H	-0.552815	4.149051	1.435833
H	4.437583	-1.377727	-3.000241	H	0.175706	2.607723	0.962470
21-ts				H	0.852295	4.131973	0.373480
Pd	-2.634146	0.464621	0.678487	C	-0.122570	2.753410	-1.686995
P	-2.583436	2.633496	-0.282519	H	-0.533308	2.812475	-2.694958
C	-3.802260	3.821828	0.624297	H	0.886568	3.179833	-1.723321
C	-3.383272	2.094832	-1.965488	H	-0.027914	1.705251	-1.399046
C	-0.940827	3.556663	-0.660304	C	-4.493692	-1.355256	3.025248
C	-0.219291	-0.881263	3.755412	H	-4.054180	-0.365919	3.220975
C	-1.103773	-0.732973	2.672724	H	-5.320999	-1.485107	3.737065
C	-1.499452	0.557558	2.314526	C	0.157880	-2.136639	0.023664
C	-1.096102	1.673885	3.044467	C	0.599844	-3.318381	-0.844188
C	-0.233395	1.502212	4.134527	C	0.604059	-0.812358	-0.604471
C	0.221298	0.228788	4.479914	H	0.659634	-2.223152	1.000372
H	0.112324	-1.876461	4.043024	C	2.112811	-3.299394	-1.101519
H	-1.422451	2.666761	2.782641	H	0.058289	-3.259177	-1.799136
H	0.082012	2.372109	4.705095	H	0.299376	-4.256912	-0.364361
H	0.903522	0.100786	5.316325	C	2.116154	-0.779073	-0.855916
C	-3.410748	-2.413352	3.152344	H	0.066167	-0.685499	-1.554041
C	-3.766110	-1.587928	0.669743	H	0.294660	0.009204	0.049169
C	-4.986839	-1.381383	1.569448	C	2.561180	-1.967628	-1.718158
H	-2.930821	-2.404959	4.139234	H	2.396739	-4.136053	-1.751363
H	-3.844585	-3.416494	3.016234	H	2.641038	-3.450163	-0.149165
H	-3.865673	-1.124837	-0.327162	H	2.399077	0.167712	-1.332212
H	-3.676785	-2.649635	0.386365	H	2.643736	-0.814151	0.107894
H	-5.508171	-0.450094	1.317936	H	3.650008	-1.957415	-1.850717
H	-5.717833	-2.194971	1.447708	H	2.120159	-1.868492	-2.720344
Si	-1.972802	-2.186241	1.812788	22			
C	-1.148981	-3.867015	2.285984	Pd	-3.195641	0.437308	0.696293
H	-1.679138	-4.677849	1.765885	P	-2.475228	2.643488	-0.267096
H	-0.093866	-3.955956	2.008475	C	-3.375141	4.169002	0.489745
H	-1.234436	-4.078019	3.358527	C	-3.127920	2.392139	-2.061424
O	-1.252857	-2.142363	0.187527	C	-0.594301	3.021491	-0.335305
C	-4.830376	1.621413	-1.713087	C	-0.527864	-0.332804	3.984827
H	-5.206727	1.173796	-2.640037	C	-1.330391	-0.621069	2.856973
H	-4.886313	0.853569	-0.934531	C	-2.317618	0.325565	2.487337
H	-5.507053	2.433723	-1.448592	C	-2.571866	1.414282	3.338634
C	-3.400924	3.178379	-3.056564	C	-1.786534	1.655680	4.467651
H	-2.396980	3.445817	-3.389221	C	-0.727984	0.799694	4.773065
H	-3.933133	2.776090	-3.927532	H	0.258782	-1.026460	4.268322
H	-3.917162	4.087735	-2.749803	H	-3.376506	2.102324	3.108792
C	-2.623830	0.868132	-2.525192	H	-1.998019	2.517884	5.095735
H	-2.578845	0.033556	-1.820145	H	-0.089033	0.992012	5.630609
H	-3.164844	0.515081	-3.411136	C	-2.866497	-3.271985	2.818931
H	-1.606240	1.095880	-2.832465	C	-4.192805	-1.356763	0.858821
C	-4.859234	2.955329	1.341604	C	-4.934716	-1.907941	2.069019
H	-5.545235	3.620932	1.879776	H	-2.557482	-3.872858	3.685069
H	-5.454803	2.349642	0.660189	H	-3.175622	-3.997714	2.053564
H	-4.391809	2.287149	2.069506	H	-4.929142	-1.098923	0.073253
C	-4.505851	4.827506	-0.304820	H	-3.513859	-2.106931	0.443760
H	-5.164534	4.347204	-1.028248	H	-5.649586	-1.165180	2.448763
H	-5.130836	5.484064	0.312614	H	-5.544740	-2.765104	1.733888
H	-3.800261	5.461043	-0.844762	Si	-1.284843	-2.398769	2.240158

C	0.161605	-3.314590	3.038163	Br	1.596342	-1.611722	0.000000
H	0.204232	-4.332613	2.631609				
H	1.133361	-2.846892	2.854216	HNEt2_b3_n			
H	0.031604	-3.404456	4.122492	N	-1.397645	1.386590	-1.129647
O	-1.190225	-2.611004	0.576423	C	-1.979170	2.710969	-1.375052
C	-4.668820	2.439051	-2.054725	H	-2.991179	2.701872	-0.953151
H	-5.028536	2.081072	-3.026940	H	-1.423902	3.509841	-0.848366
H	-5.093255	1.784777	-1.286657	C	-2.062086	3.071139	-2.856153
H	-5.067761	3.444011	-1.915060	H	-2.608360	4.012112	-2.985851
C	-2.607344	3.380488	-3.116690	H	-1.069881	3.204487	-3.298207
H	-1.529874	3.297602	-3.268063	H	-2.583553	2.288332	-3.417694
H	-3.087410	3.157489	-4.078339	C	0.050728	1.292484	-1.377027
H	-2.837428	4.417825	-2.869018	H	0.535545	2.280589	-1.296278
C	-2.764398	0.953477	-2.493507	H	0.489364	0.670849	-0.587982
H	-3.205117	0.206912	-1.820494	C	0.388899	0.663119	-2.728760
H	-3.176704	0.770827	-3.493547	H	0.003309	1.255078	-3.563775
H	-1.694372	0.769145	-2.539234	H	1.475232	0.577016	-2.851058
C	-4.764232	3.700260	0.975586	H	-0.044119	-0.340461	-2.802357
H	-5.231880	4.512942	1.544943	H	-1.563474	1.164373	-0.152463
H	-5.437739	3.445042	0.158905	NEt2_b3_n			
H	-4.687526	2.827611	1.630328	N	-1.414706	1.392570	-1.047527
C	-3.547540	5.365667	-0.460191	C	-1.885519	2.688379	-1.408015
H	-4.188597	5.136433	-1.312244	H	-2.846363	2.888553	-0.887593
H	-4.023329	6.186809	0.091209	H	-1.206701	3.526190	-1.068398
H	-2.593460	5.735562	-0.839606	C	-2.173798	2.998566	-2.908297
C	-2.619853	4.663297	1.739488	H	-2.706639	3.954589	-3.039513
H	-2.421512	3.863320	2.452531	H	-1.252158	3.053822	-3.499301
H	-1.676349	5.152393	1.497044	H	-2.792782	2.200212	-3.339725
H	-3.247724	5.407782	2.243869	C	-0.018684	1.227811	-1.288783
C	-0.210926	4.436847	-0.798525	H	0.588584	2.149984	-1.056231
H	-0.547414	5.213369	-0.110589	H	0.392447	0.451794	-0.605514
H	0.883457	4.504278	-0.849827	C	0.442189	0.779588	-2.707697
H	-0.599761	4.667790	-1.791957	H	0.258707	1.551704	-3.463735
C	-0.015955	2.756441	1.072381	H	1.516638	0.534262	-2.737593
H	-0.410189	3.423258	1.837315	H	-0.118033	-0.114010	-3.013436
H	-0.203162	1.728152	1.391092				
H	1.070337	2.905291	1.033704	NMe2_b3_n			
C	0.093932	2.009069	-1.266782	N	-1.380038	1.461622	-0.760930
H	-0.121676	2.181393	-2.321983	C	-1.859338	2.660864	-1.348285
H	1.178452	2.104008	-1.136962	H	-2.896105	2.887211	-1.038971
H	-0.179024	0.984482	-1.014361	H	-1.271095	3.601590	-1.108601
C	-4.060193	-2.388836	3.234104	C	-0.051771	1.261333	-1.217045
H	-3.695458	-1.519626	3.791513	H	0.689080	2.084023	-0.967691
H	-4.700897	-2.949826	3.927941	H	0.394600	0.340598	-0.798733
C	-0.381962	-1.856235	-0.333955	H	-1.881072	2.684437	-2.482643
C	1.110814	-2.019278	-0.031014	H	0.079291	1.164824	-2.340353
C	-0.722365	-2.333534	-1.745632				
H	-0.657726	-0.796971	-0.238546	Pd_2PtBu3_b3_n			
C	1.998590	-1.373947	-1.104081	Pd	-3.616806	-0.585544	-0.094679
H	1.328036	-3.093939	0.032891	P	-1.274161	-0.596183	-0.085704
H	1.336128	-1.584458	0.948759	P	-5.959450	-0.574521	-0.103731
C	0.165506	-1.679030	-2.811643	C	-0.583650	1.200456	-0.174509
H	-0.587402	-3.423453	-1.773225	C	-0.606195	-1.419168	1.523551
H	-1.781580	-2.135299	-1.946104	C	-0.596582	-1.582789	-1.596347
C	1.652812	-1.888849	-2.505731	C	-6.627221	0.248594	-1.713003
H	3.052637	-1.567343	-0.872619	C	-6.636917	0.412154	1.406914
H	1.867865	-0.285122	-1.077604	C	-6.650276	-2.371037	-0.014938
H	-0.085749	-2.081959	-3.799703	C	-0.808664	1.897685	1.180945
H	-0.041245	-0.602286	-2.851305	H	-0.591600	2.966116	1.060514
H	2.270360	-1.384062	-3.258343	H	-1.847375	1.806512	1.512292
H	1.889240	-2.960456	-2.567798	H	-0.154299	1.523069	1.969176
				C	0.899611	1.335462	-0.555989
Br_b3_n							

H	1.102319	0.987679	-1.570716	C	-5.749278	-0.240822	-2.885437
H	1.182817	2.395522	-0.516781	H	-5.856220	-1.304174	-3.092769
H	1.558616	0.796419	0.127047	H	-6.036434	0.304287	-3.793726
C	-1.444993	1.985335	-1.188340	H	-4.692151	-0.042114	-2.681092
H	-2.505064	1.925383	-0.921275				
H	-1.141223	3.039831	-1.167119	Prod			
H	-1.337012	1.633682	-2.213080	C	-1.028568	-2.998363	-0.140470
C	-1.484087	-0.929770	2.696029	C	0.355219	-2.962573	0.020362
H	-1.196810	-1.474805	3.604325	C	1.056336	-1.747289	0.125437
H	-1.377220	0.133603	2.903297	C	0.330921	-0.536250	0.056248
H	-2.541214	-1.128580	2.491780	C	-1.061415	-0.583009	-0.111369
C	0.873593	-1.161188	1.850802	C	-1.739097	-1.797375	-0.204801
H	1.079449	-0.108527	2.053030	H	-1.548378	-3.949211	-0.218798
H	1.141128	-1.721070	2.756552	H	0.904557	-3.900993	0.060177
H	1.541793	-1.491805	1.053554	H	-1.618752	0.348893	-0.173532
C	-0.834116	-2.941294	1.448233	H	-2.817876	-1.806458	-0.335857
H	-0.630550	-3.370651	2.436997	C	1.004994	0.820412	0.168518
H	-1.870002	-3.181337	1.190842	H	0.360832	1.567561	-0.308058
H	-0.171103	-3.439238	0.739513	H	1.060764	1.106026	1.230104
C	0.878659	-2.005500	-1.519301	C	2.418277	0.905861	-0.426688
H	1.066284	-2.710389	-0.707540	H	2.731998	1.957210	-0.426723
H	1.155150	-2.509727	-2.454522	H	2.384905	0.591602	-1.478436
H	1.552708	-1.156017	-1.395093	C	3.436763	0.049782	0.347959
C	-0.807963	-0.752254	-2.876179	H	3.492598	0.404396	1.387194
H	-0.139701	0.106857	-2.944678	H	4.441110	0.167722	-0.072744
H	-0.602317	-1.392212	-3.743037	Si	2.916453	-1.760897	0.356826
H	-1.841106	-0.402554	-2.961112	C	3.365906	-2.594141	1.980361
C	-1.481419	-2.836106	-1.769669	H	3.017495	-3.631651	2.014206
H	-1.198164	-3.342906	-2.701108	H	4.445326	-2.590246	2.166498
H	-1.377131	-3.556435	-0.959995	H	2.886807	-2.056388	2.807880
H	-2.537373	-2.554150	-1.835287	O	3.470025	-2.610942	-0.977057
C	-8.112126	0.834981	1.329896	C	4.761189	-3.194925	-1.263240
H	-8.388563	1.339217	2.265129	C	4.867586	-4.542724	-0.543082
H	-8.299711	1.539896	0.518149	H	5.782063	-5.066475	-0.840646
H	-8.786242	-0.014450	1.205689	H	4.890798	-4.413251	0.542144
C	-5.751968	1.665393	1.580226	H	4.011121	-5.175173	-0.797895
H	-4.696038	1.383345	1.645836	C	5.894654	-2.258060	-0.836402
H	-5.856197	2.385730	0.770551	H	5.819176	-1.296386	-1.352501
H	-6.035171	2.172220	2.511665	H	5.879734	-2.077293	0.243427
C	-6.425588	-0.418412	2.686733	H	6.864453	-2.701688	-1.083770
H	-7.093889	-1.277496	2.755207	C	4.784345	-3.398362	-2.779192
H	-5.392463	-0.768162	2.771670	H	5.724960	-3.859375	-3.096677
H	-6.631214	0.221537	3.553603	H	3.959085	-4.047783	-3.088394
C	-8.133584	-2.505764	0.366456	H	4.677681	-2.438115	-3.293979
H	-8.416973	-3.565777	0.327290				
H	-8.336293	-2.157887	1.381151	PtBu			
H	-8.792452	-1.966645	-0.316651	3_b3_			
C	-6.425297	-3.068346	-1.370357	n			
H	-5.386551	-2.977354	-1.701647	P	-5.953181	-0.578455	-0.102266
H	-6.642542	-4.136738	-1.249902	C	-6.647282	0.241634	-1.708631
H	-7.079556	-2.693649	-2.158637	C	-6.655084	0.407781	1.403866
C	-5.789142	-3.156031	0.998981	C	-6.668832	-2.370543	-0.011685
H	-5.897134	-2.804318	2.023700	C	-8.128243	0.838898	1.331292
H	-6.093095	-4.210474	0.977778	H	-8.400687	1.356117	2.261449
H	-4.729040	-3.096274	0.731988	H	-8.317937	1.533924	0.511607
C	-8.107005	-0.009243	-2.040387	H	-8.805605	-0.009922	1.219531
H	-8.374420	0.550709	-2.946129	C	-5.764440	1.658949	1.572222
H	-8.312934	-1.061876	-2.242687	H	-4.706870	1.385555	1.646988
H	-8.775241	0.321387	-1.243175	H	-5.868527	2.377225	0.760405
C	-6.399172	1.770697	-1.637605	H	-6.042318	2.174293	2.500756
H	-6.602610	2.200109	-2.626371	C	-6.451417	-0.415952	2.690227
H	-7.062206	2.268674	-0.928928	H	-7.120748	-1.274410	2.758157
H	-5.363288	2.010639	-1.380112	H	-5.420332	-0.768866	2.791298

H	-6.662992	0.227010	3.553898	H	-4.445839	1.264097	0.174933
C	-8.149061	-2.514103	0.377961	H	-4.305120	0.229656	-1.257104
H	-8.428276	-3.576431	0.352888	C	-1.510367	-1.452673	-0.404382
H	-8.351341	-2.154991	1.388835	H	-1.818365	-1.770900	-1.406464
H	-8.813134	-1.986064	-0.309028	H	-0.418655	-1.526461	-0.348011
C	-6.452941	-3.074667	-1.365718	H	-1.922357	-2.172098	0.314183
H	-5.416877	-2.992995	-1.709129	C	-1.695293	0.680159	1.784287
H	-6.673382	-4.142457	-1.242597	H	-0.611049	0.653478	1.946643
H	-7.110143	-2.699917	-2.151629	H	-2.047082	1.680100	2.065705
C	-5.798968	-3.150359	1.000217	H	-2.150056	-0.038757	2.477327
H	-5.906474	-2.798089	2.025109	N	-1.401525	1.405179	-1.138439
H	-6.094564	-4.207403	0.985840	C	-1.989472	2.725563	-1.364605
H	-4.737993	-3.098117	0.734598	H	-3.016890	2.718211	-0.986471
C	-8.124343	-0.019864	-2.045745	H	-1.452807	3.495304	-0.782913
H	-8.389645	0.530580	-2.958812	C	-2.017732	3.152052	-2.834009
H	-8.329051	-1.074567	-2.238220	H	-2.511817	4.125309	-2.939350
H	-8.796587	0.317185	-1.254461	H	-1.008112	3.247719	-3.246333
C	-6.429150	1.766132	-1.640293	H	-2.564140	2.419734	-3.438543
H	-6.632929	2.191958	-2.630937	C	0.043289	1.317106	-1.387248
H	-7.097971	2.262070	-0.935469	H	0.470937	2.329247	-1.372509
H	-5.396970	2.021892	-1.381384	H	0.537593	0.779606	-0.565914
C	-5.763321	-0.247754	-2.877955	C	0.406748	0.627967	-2.704750
H	-5.866611	-1.312301	-3.082506	H	-0.022851	1.155545	-3.561713
H	-6.048522	0.289721	-3.791544	H	1.495476	0.591412	-2.836100
H	-4.704943	-0.041739	-2.687428	H	0.029331	-0.399505	-2.720657

tBuO_b3_n

C	-4.149147	0.671189	-0.046490
C	-3.659935	1.365592	1.261357
H	-2.561936	1.384049	1.275380
H	-4.000998	2.409468	1.269114
H	-4.004171	0.887973	2.190887
C	-3.660010	-0.810895	0.004055
H	-4.001907	-1.374004	0.885492
H	-4.007305	-1.341868	-0.892306
H	-2.562229	-0.834290	-0.009225
C	-5.708486	0.643790	-0.003240
H	-6.091888	1.672754	-0.019300
H	-6.090216	0.140720	-0.901599
H	-6.131956	0.136508	0.876476
O	-3.690397	1.315310	-1.153507

tBuOH_b3_n

C	-4.178943	0.624150	0.030667
C	-3.653944	1.370460	1.261076
H	-2.557459	1.382462	1.265517
H	-4.007632	2.406696	1.259184
H	-3.988034	0.892797	2.188181
C	-3.656182	-0.815785	0.001770
H	-3.994733	-1.379168	0.877831
H	-4.007742	-1.331683	-0.897710
H	-2.559724	-0.827850	-0.002322
C	-5.705597	0.650994	-0.014345
H	-6.070426	1.683271	-0.028326
H	-6.071346	0.144854	-0.913806
H	-6.127022	0.147302	0.860721
O	-3.753148	1.312684	-1.164221
H	-2.784720	1.324125	-1.156437

TMSNEt2_b3_n

Si	-2.133297	0.282129	-0.011880
C	-4.006476	0.336652	-0.208088
H	-4.459430	-0.490934	0.351781

TMSOtBu_b3_n

Si	-2.266990	0.192986	0.159644
C	-4.110263	0.045702	-0.194713
H	-4.492406	-0.902628	0.203927
H	-4.689644	0.853534	0.263141
H	-4.311515	0.054975	-1.272254
C	-1.384363	-1.327113	-0.499698
H	-1.513313	-1.423668	-1.583912
H	-0.308696	-1.286939	-0.293245
H	-1.779524	-2.238893	-0.035875
C	-2.000719	0.329844	2.017768
H	-0.937694	0.406799	2.271031
H	-2.517206	1.191928	2.453036
H	-2.393533	-0.568793	2.510613
O	-1.570471	1.458387	-0.693331
C	-1.627391	2.887660	-0.500553
C	-3.043246	3.337687	-0.128963
H	-3.762794	3.017387	-0.888472
H	-3.351481	2.929533	0.838635
H	-3.086131	4.429243	-0.056387
C	-1.215909	3.494759	-1.843780
H	-1.197946	4.587894	-1.790043
H	-0.217812	3.146228	-2.128123
H	-1.919785	3.198133	-2.628176
C	-0.627169	3.282313	0.590673
H	-0.914319	2.865433	1.559741
H	0.372463	2.913651	0.338993
H	-0.576442	4.371504	0.692384

