

# Supplementary Materials

## Reduction of Bromo- and Iodo-2,6-bis(diphenylphosphanylmethyl)benzene with Magnesium and Calcium

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### Content:

Table S1: Crystal data and refinement details for the X-ray structure determinations of the compounds **1a**, **2**, **3a**, **3b**, and **4**.

Cartesian coordinates of calculated structures

**Table S1.** Crystal data and refinement details for the X-ray structure determinations of the compounds **1a**, **2**, **3a**, **3b**, and **4**.

Compound	<b>1a</b>	<b>2</b>	<b>3a</b>	<b>3b</b>	<b>4</b>
formula	C <sub>32</sub> H <sub>27</sub> BrP <sub>2</sub>	C <sub>64</sub> H <sub>54</sub> MgP <sub>4</sub>	C <sub>48</sub> H <sub>68</sub> Br <sub>2</sub> Ca <sub>2</sub> O <sub>10</sub> P <sub>2</sub>	C <sub>56</sub> H <sub>88</sub> Ca <sub>2</sub> I <sub>2</sub> O <sub>12</sub> P <sub>2</sub>	C <sub>12</sub> H <sub>28</sub> Br <sub>2</sub> CaO <sub>5</sub>
fw (g·mol <sup>-1</sup> )	553.39	971.26	1106.94	1349.16	452.24
<i>T</i> /°C	-140(2)	-140(2)	-140(2)	-140(2)	-140(2)
crystal system	triclinic	monoclinic	monoclinic	monoclinic	orthorhombic
space group	P $\bar{1}$	P 2 <sub>1</sub> /c	P 2 <sub>1</sub> /n	P 2 <sub>1</sub> /n	P bcn
<i>a</i> /Å	9.3025(3)	12.4695(2)	11.3347(4)	12.3778(3)	11.4609(3)
<i>b</i> /Å	10.1879(4)	20.0948(3)	19.4430(8)	17.8753(4)	11.5457(3)
<i>c</i> /Å	15.2499(6)	20.8722(3)	12.3105(4)	14.3016(3)	14.2003(3)
$\alpha$ /°	104.318(2)	90	90	90	90
$\beta$ /°	106.891(2)	90.828(1)	101.618(2)	103.851(1)	90
$\gamma$ /°	95.661(2)	90	90	90	90
<i>V</i> /Å <sup>3</sup>	1317.12(8)	5229.44(14)	2657.41(17)	3072.31(12)	1879.04(8)
<i>Z</i>	2	4	2	2	4
$\rho$ (g·cm <sup>-3</sup> )	1.395	1.234	1.383	1.458	1.599
$\mu$ (cm <sup>-1</sup> )	17.01	1.97	18.3	12.99	46
measured data	14817	34467	15087	17438	8358
data with <i>I</i> > 2σ( <i>I</i> )	5142	10279	4113	6320	1974
unique data ( <i>R</i> <sub>int</sub> )	5981/0.0318	11953/0.0528	5811/0.0421	6997/0.0214	2138/0.0234
w <i>R</i> <sub>2</sub> (all data, on <i>F</i> <sup>2</sup> ) <sup>a)</sup>	0.0863	0.1342	0.3082	0.1914	0.0452
<i>R</i> <sub>1</sub> ( <i>I</i> > 2σ( <i>I</i> )) <sup>a)</sup>	0.0380	0.0576	0.1127	0.0701	0.0185
<i>s</i> <sup>b)</sup>	1.064	1.128	1.091	1.062	1.099
Res. dens./e·Å <sup>-3</sup>	0.408/-0.411	0.691/-0.363	1.342/-0.648	2.123/-1.078	0.319/-0.281
absorpt method	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan
absorpt corr <i>T</i> <sub>min</sub> / <sub>max</sub>	0.6317/0.7456	0.6382/0.7456	0.5212/0.7456	0.6755/0.7456	0.5713/0.7456
CCDC No.	1509090	1509091	motif	1509092	1509093

<sup>a)</sup> Definition of the *R* indices:  $R_1 = (\sum ||F_o| - |F_c||) / \sum |F_o|$ ;

$wR_2 = \{\sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2]\}^{1/2}$  with  $w^{-1} = \sigma^2(F_o^2) + (aP)^2 + bP$ ;  $P = [2F_c^2 + \text{Max}(F_o^2)]/3$ ;

<sup>b)</sup>  $s = \{\sum [w(F_o^2 - F_c^2)^2] / (N_o - N_p)\}^{1/2}$ .

## Cartesian coordinates of calculated molecules:

$[(\text{thf})\text{Mg}]^{2+}$

Mg	0.597752	-0.852137	-0.142065
O	-1.371456	-0.887275	0.009491
C	-2.224413	-2.096137	-0.170780
C	-2.228261	0.308621	0.223439
C	-3.625922	-1.626835	0.189477
H	-2.137542	-2.395780	-1.215744
H	-1.830202	-2.872443	0.482646
C	-3.612031	-0.143075	-0.207502
H	-2.178467	0.554874	1.284795
H	-1.811432	1.118717	-0.373103
H	-3.804991	-1.737025	1.261147
H	-4.384252	-2.197729	-0.346310
H	-4.391076	0.433386	0.291452
H	-3.734569	-0.028497	-1.286964

$[(\text{thf})_2\text{Mg}]^{2+}$

Mg	0.534284	-0.518781	0.485893
O	-1.426737	-0.714141	0.197173
C	-2.149938	-2.006747	0.093818
C	-2.381471	0.412049	0.046067
C	-3.524381	-1.631517	-0.435163
H	-1.576880	-2.652478	-0.569044
H	-2.192260	-2.433948	1.096294
C	-3.752681	-0.234245	0.160413
H	-2.160338	1.134387	0.830424
H	-2.208883	0.853361	-0.936349
H	-4.280531	-2.351137	-0.121450
H	-3.518421	-1.589877	-1.526589
H	-4.058034	-0.304621	1.206849
H	-4.507004	0.336573	-0.381124
O	2.490445	-0.723179	0.184285
C	3.521454	-0.588835	1.245953
C	3.130602	-1.124876	-1.092919
C	4.777766	-1.190431	0.635610
H	3.627569	0.475870	1.456402
H	3.157187	-1.114587	2.127252
C	4.613443	-0.889982	-0.862058
H	2.899438	-2.178006	-1.257222
H	2.695357	-0.513554	-1.881520
H	4.812719	-2.267998	0.811173
H	5.677525	-0.743748	1.058644
H	5.220375	-1.541482	-1.490846
H	4.877886	0.146885	-1.081562

$[(\text{thf})_3\text{Mg}]^{2+}$

Mg	0.539190	-1.087197	0.172964
O	-1.403290	-1.401962	-0.226884
C	-2.014955	-2.741177	-0.394345
C	-2.438328	-0.355231	-0.379782
C	-3.394104	-2.463851	-0.971772
H	-1.361796	-3.321137	-1.044704
H	-2.065664	-3.201520	0.593386
C	-3.758005	-1.109575	-0.345678
H	-2.312546	0.358582	0.433198
H	-2.266342	0.135228	-1.339125
H	-4.100732	-3.252258	-0.712594
H	-3.347612	-2.386448	-2.060417
H	-4.099935	-1.239600	0.683770
H	-4.532723	-0.580915	-0.901292
O	1.927201	-1.978904	-0.986477
C	3.291501	-2.356314	-0.551410
C	1.783935	-2.199430	-2.443888
C	3.915234	-3.026903	-1.768209
H	3.809492	-1.438336	-0.271762
H	3.192163	-3.010208	0.313941

C	3.211225	-2.335080	-2.945444
H	1.208099	-3.116104	-2.581892
H	1.237740	-1.351097	-2.852450
H	3.699820	-4.097798	-1.768739
H	4.996969	-2.894408	-1.785239
H	3.257766	-2.917188	-3.865934
H	3.647251	-1.351424	-3.135452
O	1.025025	0.396292	1.437684
C	0.355922	0.686327	2.727241
C	2.143484	1.345173	1.229451
C	1.311879	1.619645	3.452798
H	-0.597649	1.164747	2.498736
H	0.187339	-0.264385	3.231205
C	1.954856	2.407041	2.301979
H	3.072215	0.787609	1.356917
H	2.070097	1.722818	0.210646
H	2.066169	1.048880	3.999455
H	0.784324	2.259365	4.160425
H	2.904540	2.864018	2.580357
H	1.283423	3.193642	1.949996

[ (thf)<sub>4</sub>Mg ]<sup>2+</sup>

Mg	-0.115398	-0.712195	0.105198
O	-2.126624	-0.536974	0.353717
C	-2.794989	0.607205	1.002194
C	-3.144379	-1.459732	-0.197302
C	-4.209153	0.587906	0.446544
H	-2.773173	0.439131	2.080787
H	-2.226279	1.504565	0.758793
C	-4.482212	-0.914757	0.287098
H	-3.050229	-1.434039	-1.284489
H	-2.917716	-2.460431	0.168960
H	-4.249093	1.095519	-0.520414
H	-4.912794	1.076215	1.121032
H	-5.280546	-1.127877	-0.423892
H	-4.750984	-1.358379	1.248249
O	0.577608	0.131831	1.821949
C	1.284613	1.426416	1.927630
C	0.353504	-0.419955	3.171371
C	1.602877	1.589566	3.409604
H	2.168306	1.377130	1.292936
H	0.603515	2.194806	1.558649
C	0.497345	0.775460	4.097020
H	-0.634056	-0.880642	3.180127
H	1.118152	-1.177463	3.354219
H	1.602651	2.639218	3.703620
H	2.584460	1.169033	3.639557
H	-0.436598	1.341355	4.138926
H	0.763329	0.471822	5.109742
O	0.333472	0.535002	-1.440135
C	1.696601	0.946852	-1.835238
C	-0.645871	1.057856	-2.414893
C	1.554986	1.435776	-3.267938
H	2.007852	1.745067	-1.159210
H	2.351472	0.083948	-1.718890
C	0.140761	2.033377	-3.279238
H	-1.022580	0.209502	-2.989403
H	-1.459462	1.515489	-1.853993
H	1.629505	0.601336	-3.968984
H	2.325414	2.164953	-3.519300
H	-0.280195	2.107025	-4.282028
H	0.140712	3.030154	-2.831843
O	0.657839	-2.519699	-0.411597
C	0.454968	-3.124903	-1.742393
C	1.445943	-3.433395	0.441365
C	1.459194	-4.265321	-1.802604
H	-0.575798	-3.481008	-1.792036
H	0.617057	-2.344214	-2.484624
C	1.519338	-4.736885	-0.342133

H	2.427004	-2.977284	0.583980
H	0.934488	-3.523408	1.398216
H	2.435137	-3.901038	-2.131778
H	1.135148	-5.049418	-2.487111
H	2.430737	-5.289193	-0.112363
H	0.663274	-5.374253	-0.108243

[(thf)<sub>5</sub>Mg]<sup>2+</sup>

Mg	-2.067288	0.545615	-0.274471
O	-2.894577	2.372993	-0.879883
C	-4.125243	3.002151	-0.416590
C	-2.126343	3.442298	-1.506094
C	-4.513044	3.957238	-1.544967
H	-4.844770	2.212360	-0.220583
H	-3.909543	3.538873	0.512461
C	-3.163256	4.316942	-2.223967
H	-1.609552	3.996294	-0.717101
H	-1.390960	2.977180	-2.159521
H	-5.030189	4.834142	-1.155183
H	-5.179598	3.461721	-2.251889
H	-2.914882	5.372455	-2.112073
H	-3.195089	4.093691	-3.290478
O	-1.222161	0.240667	-2.160156
C	0.193673	-0.090512	-2.383037
C	-1.920052	0.323781	-3.455524
C	0.429713	0.179686	-3.860815
H	0.791624	0.533113	-1.720044
H	0.339420	-1.141811	-2.126881
C	-0.922270	-0.193706	-4.483989
H	-2.829723	-0.271519	-3.384917
H	-2.182165	1.369155	-3.625720
H	1.258195	-0.411041	-4.252082
H	0.652348	1.237129	-4.024586
H	-1.008076	-1.277492	-4.592946
H	-1.081791	0.262706	-5.461052
O	-4.002249	-0.209309	0.030170
C	-4.529057	-0.534067	1.363725
C	-4.954341	-0.651026	-1.001597
C	-5.989076	-0.901227	1.135802
H	-3.948177	-1.370385	1.759225
H	-4.386964	0.341211	1.997450
C	-5.963033	-1.523877	-0.267208
H	-5.416178	0.238530	-1.435163
H	-4.392544	-1.180734	-1.771442
H	-6.616366	-0.006608	1.148664
H	-6.355382	-1.587994	1.899021
H	-6.936715	-1.510391	-0.757352
H	-5.615956	-2.559014	-0.222935
O	-1.307424	-1.276175	0.396318
C	-0.272453	-1.549797	1.403135
C	-1.723563	-2.533799	-0.237243
C	-0.285393	-3.061415	1.587599
H	0.682265	-1.199598	1.005719
H	-0.520100	-0.990920	2.303558
C	-0.688804	-3.564206	0.194987
H	-2.721617	-2.781061	0.130224
H	-1.762649	-2.366485	-1.313921
H	-1.029511	-3.352658	2.333098
H	0.686685	-3.435020	1.910569
H	-1.104333	-4.572057	0.207509
H	0.170727	-3.556279	-0.479943
O	-0.920629	1.536880	1.172604
C	-1.514274	1.964099	2.447808
C	0.449099	2.057481	1.065180
C	-0.527396	2.962207	3.040836
H	-2.494030	2.393240	2.235817
H	-1.630114	1.076403	3.073790
C	0.817603	2.480264	2.479379
H	1.075945	1.262550	0.661870

H	0.438876	2.903346	0.374155
H	-0.560142	2.960512	4.130436
H	-0.748949	3.973620	2.691889
H	1.189493	1.625220	3.049109
H	1.582726	3.256864	2.482999

[ (thf)<sub>6</sub>Mg]<sup>2+</sup>

Mg	-0.358043	0.564146	0.000120
O	-0.356680	0.026297	-2.098831
C	-0.194400	-1.328711	-2.642399
C	-0.511143	0.973996	-3.211970
C	-0.009870	-1.154993	-4.145010
H	0.655210	-1.796669	-2.150664
H	-1.096708	-1.898313	-2.410142
C	-0.813237	0.118639	-4.433444
H	-1.305523	1.670601	-2.955047
H	0.427633	1.520602	-3.324612
H	-0.369984	-2.024031	-4.696272
H	1.044956	-1.006912	-4.389848
H	-1.882007	-0.102499	-4.492717
H	-0.513250	0.614445	-5.357022
O	-0.071640	-1.514428	0.509535
C	-1.151838	-2.484794	0.737768
C	1.223076	-2.185643	0.687628
C	-0.478379	-3.849837	0.746886
H	-1.614457	-2.253860	1.699618
H	-1.886661	-2.365595	-0.054512
C	0.904270	-3.530496	1.326843
H	1.682992	-2.305548	-0.295851
H	1.857353	-1.547250	1.298281
H	-0.388692	-4.238862	-0.270517
H	-1.037611	-4.571498	1.342903
H	1.656585	-4.280663	1.082269
H	0.853377	-3.437422	2.414691
O	-2.505998	0.297827	0.050792
C	-3.357639	0.506858	1.229975
C	-3.345746	-0.132153	-1.076185
C	-4.782328	0.553677	0.697972
H	-3.209516	-0.336373	1.908300
H	-3.039293	1.424552	1.718685
C	-4.718857	-0.421723	-0.483104
H	-3.383129	0.682570	-1.802173
H	-2.879708	-0.998137	-1.541468
H	-5.032036	1.561049	0.354694
H	-5.506626	0.260284	1.458310
H	-5.512611	-0.264284	-1.213793
H	-4.777663	-1.454429	-0.130471
O	-0.644352	2.642255	-0.510529
C	0.435605	3.612811	-0.738808
C	-1.939269	3.313136	-0.688744
C	-0.237908	4.977806	-0.745504
H	1.171272	3.492570	0.052505
H	0.897144	3.383072	-1.701470
C	-1.620672	4.659220	-1.325566
H	-2.572638	2.675584	-1.301258
H	-2.400219	3.430935	0.294459
H	0.321047	5.700430	-1.340617
H	-0.327233	5.365216	0.272547
H	-1.570011	4.568093	-2.413580
H	-2.373040	5.408841	-1.079493
O	1.789758	0.830110	-0.050794
C	2.629479	1.260543	1.076073
C	2.641374	0.621277	-1.230071
C	4.002449	1.550539	0.482863
H	2.163117	2.126396	1.541249
H	2.667226	0.445868	1.802084
C	4.066153	0.575148	-0.698194
H	2.323397	-0.296664	-1.718533
H	2.492770	1.464326	-1.908500

H	4.796305	1.393351	1.213500
H	4.060977	2.583258	0.130228
H	4.316338	-0.432116	-0.354931
H	4.790225	0.868800	-1.458643
O	-0.359618	1.101485	2.099064
C	-0.522043	2.456504	2.642680
C	-0.205879	0.153650	3.212158
C	-0.706825	2.282690	4.145249
H	0.380283	3.026122	2.410527
H	-1.371638	2.924477	2.150911
C	0.096081	1.008791	4.433809
H	-1.144915	-0.392592	3.324459
H	0.588292	-0.543248	2.955381
H	-1.761753	2.134820	4.389792
H	-0.346701	3.151608	4.696662
H	-0.204446	0.513003	5.357226
H	1.164893	1.229519	4.493586

[ (PMe<sub>3</sub>)Mg]<sup>2+</sup>

Mg	3.551874	0.345375	0.082439
P	0.998650	0.246089	-0.012338
C	0.276485	1.150940	-1.434796
H	-0.810696	1.185470	-1.336780
H	0.666125	2.169735	-1.464641
H	0.535845	0.644472	-2.365156
C	0.290805	1.041786	1.483316
H	-0.799904	1.022735	1.438940
H	0.623139	0.510402	2.376674
H	0.628241	2.077848	1.541626
C	0.277138	-1.436947	-0.069387
H	0.603100	-1.950597	-0.974500
H	0.603833	-2.008119	0.800257
H	-0.813115	-1.373691	-0.065654

[ (PMe<sub>3</sub>)<sub>2</sub>Mg]<sup>2+</sup>

Mg	3.194039	0.717791	0.394266
P	0.639947	0.396840	0.035556
C	-0.101735	1.648476	-1.084919
H	-1.172072	1.463282	-1.196815
H	0.046410	2.648243	-0.674125
H	0.372481	1.593982	-2.065707
C	-0.361108	0.493492	1.570895
H	-1.417711	0.347198	1.337917
H	-0.040612	-0.277833	2.272823
H	-0.230421	1.471659	2.035752
C	0.190153	-1.218015	-0.713192
H	0.672611	-1.323174	-1.686255
H	0.516758	-2.033037	-0.065529
H	-0.892558	-1.279008	-0.843670
P	5.739897	0.307384	0.132860
C	6.666532	1.766622	-0.486112
H	7.727023	1.524685	-0.582931
H	6.278480	2.066141	-1.460841
H	6.553345	2.598427	0.210294
C	6.147068	-1.046241	-1.039220
H	7.229794	-1.176643	-1.097089
H	5.694395	-1.979267	-0.700257
H	5.763778	-0.807738	-2.032233
C	6.582880	-0.157133	1.696456
H	6.453598	0.634040	2.436595
H	6.153470	-1.080069	2.089042
H	7.649339	-0.308070	1.516435

[ (PMe<sub>3</sub>)<sub>3</sub>Mg]<sup>2+</sup>

Mg	3.345011	0.562009	0.178255
P	1.080694	-0.412313	-0.704910
C	0.792675	-0.182825	-2.507298
H	-0.170361	-0.611843	-2.793346
H	0.794044	0.881287	-2.750009

H	1.583701	-0.672905	-3.076895
C	-0.425862	0.296589	0.075234
H	-1.322000	-0.176472	-0.332603
H	-0.398501	0.136879	1.154209
H	-0.471854	1.369427	-0.118759
C	0.907310	-2.225877	-0.448779
H	1.717791	-2.752351	-0.955553
H	0.953867	-2.456020	0.617028
H	-0.047339	-2.575742	-0.846874
P	5.612767	-0.303878	-0.821169
C	6.861911	1.016622	-1.105805
H	7.780563	0.590546	-1.514602
H	6.467292	1.751693	-1.809494
H	7.088698	1.521707	-0.165414
C	5.468277	-1.144813	-2.450548
H	6.452476	-1.466522	-2.798517
H	4.820240	-2.018285	-2.360217
H	5.036803	-0.461734	-3.184090
C	6.481210	-1.531003	0.238673
H	6.708758	-1.088391	1.209456
H	5.844838	-2.403991	0.393010
H	7.412712	-1.849304	-0.234323
P	3.354313	2.238725	2.200642
C	5.025715	2.599878	2.877236
H	5.466347	1.685130	3.276654
H	5.673629	2.986769	2.089007
H	4.958314	3.338936	3.678457
C	2.381287	1.717102	3.670300
H	1.337628	1.567194	3.389871
H	2.777481	0.779300	4.063271
H	2.435169	2.481328	4.448936
C	2.670351	3.891903	1.772448
H	3.230909	4.321845	0.940663
H	1.624490	3.793852	1.476116
H	2.734721	4.564608	2.630238

[ (PMe<sub>3</sub>)<sub>4</sub>Mg ]<sup>2+</sup>

Mg	3.195903	0.943726	-0.386288
P	1.039676	-0.585128	-0.488844
C	0.394140	-0.828330	-2.194990
H	-0.463900	-1.504038	-2.186858
H	0.086247	0.130889	-2.614366
H	1.175495	-1.251576	-2.828437
C	-0.422903	0.015000	0.451781
H	-1.251934	-0.690088	0.360513
H	-0.163632	0.125705	1.505998
H	-0.738191	0.985652	0.065402
C	1.291738	-2.298177	0.132675
H	2.118364	-2.767079	-0.403869
H	1.536006	-2.273240	1.195640
H	0.387818	-2.894825	-0.009658
P	5.371391	-0.553097	-0.621081
C	6.945059	0.397420	-0.725822
H	7.798025	-0.282141	-0.783298
H	6.935815	1.029941	-1.614650
H	7.056183	1.032134	0.154266
C	5.471253	-1.696224	-2.060397
H	6.394807	-2.278012	-2.019675
H	4.620493	-2.378943	-2.056087
H	5.453646	-1.121150	-2.988096
C	5.624452	-1.650528	0.835749
H	5.688612	-1.043172	1.740821
H	4.779729	-2.334293	0.932967
H	6.542930	-2.231970	0.729822
P	3.445838	2.123333	2.002753
C	5.130528	2.767163	2.366968
H	5.848542	1.946203	2.336110
H	5.415085	3.508221	1.618081
H	5.161039	3.230550	3.355704

C	3.079280	1.021467	3.432567
H	2.044402	0.679648	3.376521
H	3.735824	0.149897	3.414946
H	3.224684	1.555442	4.374206
C	2.347877	3.572631	2.295225
H	2.558604	4.353265	1.563016
H	1.303430	3.271973	2.195180
H	2.506077	3.976089	3.297980
C	3.249958	1.632616	-4.059472
H	3.253947	2.310888	-4.915116
H	4.151207	1.017399	-4.089451
H	2.379449	0.977691	-4.125171
C	1.736612	3.675433	-2.659185
H	1.672806	4.349756	-1.803516
H	1.816526	4.267788	-3.573413
H	0.825661	3.076168	-2.701045
C	4.629070	3.728388	-2.611002
H	4.651767	4.394808	-1.747167
H	5.562615	3.163811	-2.640686
H	4.547816	4.328319	-3.520220
P	3.199874	2.574159	-2.476674

[ (thf)Ca]<sup>2+</sup>

Ca	0.946702	-0.885335	-0.002643
O	-1.397800	-0.886944	-0.002131
C	-2.246960	-2.076354	-0.197318
C	-2.246947	0.301251	0.198309
C	-3.648576	-1.629034	0.196301
H	-2.185455	-2.360117	-1.250116
H	-1.848318	-2.876591	0.425915
C	-3.648220	-0.145124	-0.196958
H	-2.185945	0.580820	1.252327
H	-1.848235	1.104141	-0.421486
H	-3.799020	-1.741836	1.272760
H	-4.415355	-2.206643	-0.320282
H	-4.415415	0.432578	0.318898
H	-3.797318	-0.032148	-1.273598

[ (thf)<sub>2</sub>Ca]<sup>2+</sup>

Ca	0.525483	-0.601045	0.648714
O	-1.769946	-0.777984	0.218078
C	-2.566821	-2.015011	0.222072
C	-2.639930	0.368208	-0.093640
C	-3.915548	-1.626359	-0.370319
H	-2.028517	-2.763022	-0.360658
H	-2.656422	-2.348951	1.257923
C	-4.059806	-0.159018	0.059464
H	-2.387145	1.174030	0.595990
H	-2.429086	0.679387	-1.119412
H	-4.717917	-2.261476	0.005597
H	-3.894580	-1.707857	-1.459738
H	-4.384806	-0.092402	1.100743
H	-4.765637	0.397449	-0.557522
O	2.829556	-0.836581	0.234457
C	3.871367	-0.770031	1.277230
C	3.456012	-1.085680	-1.069476
C	5.168850	-1.166795	0.580433
H	3.900239	0.257207	1.646143
H	3.582771	-1.443854	2.084452
C	4.922685	-0.733372	-0.871931
H	3.319888	-2.141550	-1.316085
H	2.944494	-0.467392	-1.807914
H	5.320603	-2.247315	0.636362
H	6.031911	-0.676409	1.031107
H	5.564312	-1.251765	-1.584755
H	5.076479	0.342543	-0.986914

[ (thf)<sub>3</sub>Ca]<sup>2+</sup>

Ca	0.304304	-1.299088	0.393399
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O	-1.979082	-1.597494	-0.113290
C	-2.639095	-2.909589	-0.171242
C	-2.906063	-0.561002	-0.593028
C	-3.818132	-2.712494	-1.111606
H	-1.902073	-3.635460	-0.517637
H	-2.964116	-3.170806	0.838945
C	-4.241562	-1.269516	-0.799567
H	-2.942901	0.230990	0.154980
H	-2.504333	-0.164735	-1.528068
H	-4.610971	-3.437451	-0.926197
H	-3.500128	-2.807721	-2.152953
H	-4.838558	-1.236600	0.114779
H	-4.819347	-0.811519	-1.602562
O	2.054213	-1.944007	-1.033562
C	3.427820	-2.230457	-0.591886
C	1.967639	-2.079218	-2.494896
C	4.111601	-2.858552	-1.798707
H	3.893109	-1.283745	-0.308169
H	3.366986	-2.885412	0.277616
C	3.411477	-2.161088	-2.973947
H	1.413699	-2.994683	-2.714647
H	1.422399	-1.217867	-2.881622
H	3.930467	-3.935871	-1.826541
H	5.188844	-2.691459	-1.784187
H	3.495580	-2.714001	-3.909739
H	3.822491	-1.160223	-3.127467
O	1.240321	0.409196	1.723541
C	0.722449	0.812055	3.039968
C	2.379189	1.262480	1.360391
C	1.739923	1.804433	3.590782
H	-0.256823	1.270812	2.885476
H	0.614855	-0.085543	3.649197
C	2.310580	2.444431	2.317136
H	3.293128	0.680059	1.498700
H	2.272426	1.533375	0.309936
H	2.525049	1.282342	4.143017
H	1.274280	2.528094	4.260162
H	3.290366	2.897121	2.471331
H	1.633168	3.211135	1.932827

[(thf)<sub>4</sub>Ca]<sup>2+</sup>

Ca	-0.079539	-0.410290	-0.006415
O	-2.416154	-0.449449	0.210164
C	-3.217874	0.595149	0.856259
C	-3.289850	-1.541393	-0.237081
C	-4.666375	0.247937	0.532381
H	-3.020466	0.556248	1.930351
H	-2.893578	1.558748	0.460363
C	-4.628675	-1.284662	0.442631
H	-3.368479	-1.484813	-1.325487
H	-2.822343	-2.483499	0.047248
H	-4.960759	0.682058	-0.426237
H	-5.350466	0.613443	1.298563
H	-5.458767	-1.698814	-0.130200
H	-4.643735	-1.729724	1.440720
O	0.703148	0.300822	2.083680
C	1.652260	1.393720	2.343585
C	0.239753	-0.258524	3.356025
C	1.856085	1.410018	3.856916
H	2.565120	1.191300	1.782993
H	1.196891	2.317554	1.980465
C	0.542194	0.817239	4.387673
H	-0.819828	-0.491836	3.247083
H	0.799269	-1.177522	3.551706
H	2.049005	2.417664	4.225286
H	2.700063	0.775522	4.137174
H	-0.249291	1.571070	4.398220
H	0.638111	0.403119	5.391636
O	0.487534	0.780186	-1.941142

C	1.823723	0.911737	-2.539317
C	-0.478547	1.561913	-2.721144
C	1.612451	1.664483	-3.849665
H	2.445461	1.475536	-1.840353
H	2.233968	-0.089678	-2.670041
C	0.366432	2.512239	-3.556118
H	-1.048714	0.870544	-3.347030
H	-1.151674	2.058558	-2.021607
H	1.415356	0.965627	-4.665974
H	2.483741	2.263664	-4.114791
H	-0.154313	2.830773	-4.459488
H	0.629285	3.401801	-2.977857
O	0.636629	-2.626585	-0.383542
C	0.425195	-3.357414	-1.638804
C	1.476238	-3.421588	0.521318
C	1.449219	-4.484452	-1.618797
H	-0.599510	-3.737392	-1.638480
H	0.554279	-2.648941	-2.457987
C	1.560050	-4.802587	-0.120148
H	2.455278	-2.940512	0.580514
H	1.008605	-3.419680	1.506571
H	2.408882	-4.139744	-2.012061
H	1.122813	-5.338745	-2.212370
H	2.487870	-5.312967	0.139416
H	0.723164	-5.426803	0.202603

[(thf)<sub>5</sub>Ca]<sup>2+</sup>

Ca	-1.900671	0.569111	-0.298012
O	-2.763280	2.660041	-1.081295
C	-4.138137	3.145490	-0.945629
C	-1.948963	3.671038	-1.757991
C	-4.232497	4.349481	-1.873806
H	-4.808258	2.327293	-1.207365
H	-4.298202	3.428299	0.098343
C	-2.812033	4.927806	-1.803349
H	-1.024375	3.796924	-1.193014
H	-1.714406	3.299323	-2.758948
H	-4.997699	5.054700	-1.548122
H	-4.468534	4.032030	-2.892744
H	-2.681940	5.514469	-0.890390
H	-2.563576	5.560468	-2.655878
O	-1.304216	-0.028603	-2.523813
C	0.054078	-0.253223	-3.024928
C	-2.266136	-0.165914	-3.619472
C	-0.121367	-0.828029	-4.425879
H	0.571239	0.709607	-3.043904
H	0.560871	-0.923375	-2.330141
C	-1.428000	-0.170772	-4.892661
H	-2.803476	-1.107813	-3.481352
H	-2.967013	0.667066	-3.556833
H	-0.230126	-1.914601	-4.383843
H	0.727806	-0.593642	-5.068475
H	-1.916939	-0.717792	-5.699255
H	-1.243479	0.851155	-5.233553
O	-4.119342	-0.224559	0.125920
C	-4.935736	0.105721	1.295498
C	-4.881201	-1.091287	-0.781587
C	-6.363625	-0.226902	0.885900
H	-4.600444	-0.511892	2.133191
H	-4.764041	1.157398	1.528907
C	-6.162210	-1.443719	-0.029963
H	-5.088220	-0.521966	-1.690678
H	-4.260315	-1.954770	-1.025113
H	-6.808332	0.604150	0.332474
H	-6.995123	-0.443214	1.747972
H	-6.997303	-1.606597	-0.711773
H	-6.023599	-2.350393	0.563720
O	-0.732052	-1.441018	0.312387
C	0.273289	-1.613126	1.364642

C	-1.048026	-2.741895	-0.280052
C	0.412299	-3.120355	1.558191
H	1.204871	-1.161264	1.014589
H	-0.071836	-1.084368	2.252752
C	0.075933	-3.667894	0.164108
H	-2.017361	-3.067848	0.107766
H	-1.117621	-2.605502	-1.359248
H	-0.309418	-3.481862	2.295247
H	1.412030	-3.394729	1.896157
H	-0.238203	-4.712033	0.178724
H	0.935569	-3.575779	-0.504764
O	-0.994840	1.618783	1.626436
C	-1.650486	1.591642	2.936627
C	0.239869	2.404392	1.708742
C	-0.629850	2.164913	3.913558
H	-2.549980	2.210355	2.877236
H	-1.935125	0.561068	3.153199
C	0.152380	3.150610	3.033975
H	1.085398	1.712197	1.687979
H	0.279911	3.054680	0.833715
H	0.027849	1.375593	4.286269
H	-1.110636	2.642221	4.767831
H	1.139282	3.387574	3.432277
H	-0.404034	4.083571	2.913252

[ (thf)<sub>6</sub>Ca]<sup>2+</sup>

Ca	-0.379073	0.576811	0.006152
O	-0.406586	-0.016479	-2.348881
C	-0.260646	-1.355560	-2.919797
C	-0.590683	0.955826	-3.429037
C	-0.041190	-1.143059	-4.413134
H	0.571234	-1.852127	-2.420521
H	-1.180432	-1.913428	-2.722639
C	-0.851584	0.131315	-4.684460
H	-1.415977	1.613405	-3.157424
H	0.326096	1.544860	-3.514331
H	-0.378236	-1.998667	-4.999178
H	1.018009	-0.976709	-4.625451
H	-1.915482	-0.101888	-4.777392
H	-0.536462	0.656024	-5.586918
O	-0.110541	-1.742037	0.626698
C	-1.176994	-2.708835	0.887359
C	1.190624	-2.392923	0.800350
C	-0.503272	-4.073772	0.836043
H	-1.592185	-2.501701	1.877516
H	-1.951430	-2.565858	0.135935
C	0.892893	-3.766527	1.394098
H	1.662423	-2.466329	-0.182856
H	1.803975	-1.760439	1.443331
H	-0.437364	-4.429927	-0.195369
H	-1.044197	-4.817391	1.422237
H	1.642607	-4.503778	1.105650
H	0.865059	-3.715251	2.485376
O	-2.753577	0.161251	0.038827
C	-3.602401	0.329188	1.222158
C	-3.583430	-0.207101	-1.106614
C	-5.040192	0.257899	0.715942
H	-3.372780	-0.484356	1.914098
H	-3.349620	1.281005	1.688837
C	-4.916229	-0.648674	-0.516533
H	-3.699593	0.672761	-1.745661
H	-3.062487	-0.985659	-1.662628
H	-5.395625	1.250167	0.426623
H	-5.716515	-0.139019	1.473688
H	-5.736050	-0.522871	-1.224550
H	-4.876114	-1.700170	-0.220423
O	-0.575996	2.902134	-0.576978
C	0.521437	3.814897	-0.903473
C	-1.852280	3.606739	-0.705461

C	-0.105923	5.203514	-0.965968
H	1.288877	3.711327	-0.137561
H	0.934903	3.513232	-1.869286
C	-1.532769	4.901436	-1.443389
H	-2.546441	2.954190	-1.234909
H	-2.237252	3.798629	0.299737
H	0.439968	5.864988	-1.639529
H	-0.122449	5.663098	0.025671
H	-1.551960	4.742742	-2.524773
H	-2.242396	5.693006	-1.200820
O	2.009555	0.954060	-0.012839
C	2.832805	1.341049	1.132800
C	2.866582	0.728761	-1.178340
C	4.212833	1.643187	0.560151
H	2.360305	2.195524	1.617391
H	2.858747	0.503299	1.834887
C	4.289989	0.683342	-0.635441
H	2.543746	-0.194619	-1.659116
H	2.722838	1.563691	-1.868881
H	5.002332	1.478569	1.294048
H	4.268918	2.681223	0.222080
H	4.543060	-0.326640	-0.302408
H	5.020583	0.990034	-1.384585
O	-0.508625	1.178714	2.342276
C	-0.606572	2.533268	2.888652
C	-0.339231	0.226530	3.435358
C	-0.535971	2.381803	4.409585
H	0.228575	3.112510	2.490347
H	-1.542307	2.976495	2.546249
C	0.208987	1.051102	4.589966
H	-1.315329	-0.205651	3.676450
H	0.324458	-0.561759	3.085102
H	-1.540574	2.314237	4.833977
H	-0.025918	3.224777	4.876494
H	0.018237	0.583105	5.556360
H	1.287499	1.191535	4.480047

[ (PMe<sub>3</sub>) Ca ]<sup>2+</sup>

Ca	4.048106	0.384488	-0.002224
P	1.038630	0.236608	0.000137
C	0.261452	1.135074	-1.412862
H	-0.827499	1.135533	-1.324515
H	0.615472	2.167845	-1.435113
H	0.540060	0.653925	-2.352219
C	0.253059	1.026559	1.471439
H	-0.835997	0.986071	1.395221
H	0.564040	0.508441	2.380741
H	0.564308	2.070294	1.543281
C	0.224291	-1.416037	-0.057792
H	0.521183	-1.946433	-0.964038
H	0.527321	-2.009511	0.806634
H	-0.862908	-1.307361	-0.048689

[ (PMe<sub>3</sub>)<sub>2</sub>Ca ]<sup>2+</sup>

Ca	3.185789	1.739198	1.504760
P	0.675589	0.546345	0.279235
C	0.178292	1.296909	-1.332722
H	-0.741291	0.839176	-1.705074
H	0.015210	2.369054	-1.208920
H	0.968472	1.149370	-2.070459
C	-0.872700	0.671967	1.275085
H	-1.717023	0.237036	0.734989
H	-0.750065	0.143386	2.222225
H	-1.091602	1.719780	1.489558
C	0.756413	-1.253554	-0.119632
H	1.603532	-1.451173	-0.779444
H	0.890737	-1.829241	0.797987
H	-0.161448	-1.583466	-0.611969
P	5.697459	0.521294	0.301254

C	6.970632	1.730282	-0.267445
H	7.824838	1.216159	-0.714433
H	6.534583	2.403613	-1.007980
H	7.319166	2.325293	0.578658
C	5.433285	-0.523735	-1.196039
H	6.378871	-0.940055	-1.550998
H	4.751688	-1.343790	-0.962380
H	4.991114	0.077165	-1.992671
C	6.659737	-0.596620	1.411235
H	6.958232	-0.057290	2.312322
H	6.041095	-1.446772	1.705612
H	7.555172	-0.968296	0.907243

[ (PMe<sub>3</sub>)<sub>3</sub>Ca ]<sup>2+</sup>

Ca	3.105897	0.493844	0.249929
P	0.575599	-0.726217	-0.972598
C	0.390564	-0.516851	-2.798236
H	-0.540556	-0.966119	-3.151558
H	0.388719	0.545758	-3.049800
H	1.228593	-0.990905	-3.312928
C	-1.013516	-0.042177	-0.325504
H	-1.870684	-0.519507	-0.806775
H	-1.075733	-0.207748	0.751833
H	-1.057018	1.032614	-0.512420
C	0.350582	-2.545388	-0.748641
H	1.179084	-3.082496	-1.214287
H	0.337256	-2.788236	0.315795
H	-0.586373	-2.880707	-1.200006
P	5.857809	-0.342613	-0.800206
C	7.114389	0.998448	-0.978712
H	8.044262	0.608052	-1.399385
H	6.730019	1.782073	-1.634653
H	7.324388	1.437732	-0.001636
C	5.819585	-1.088568	-2.489359
H	6.822253	-1.381221	-2.810025
H	5.176246	-1.970758	-2.488596
H	5.415693	-0.367028	-3.202470
C	6.765644	-1.613717	0.183078
H	6.955734	-1.236322	1.189706
H	6.163640	-2.520973	0.261764
H	7.719799	-1.861236	-0.287996
P	3.475319	2.546714	2.505225
C	5.229448	2.862566	2.988134
H	5.688518	1.938371	3.344277
H	5.793957	3.219300	2.124669
H	5.285649	3.612812	3.780716
C	2.685582	2.141850	4.124468
H	1.605407	2.047190	3.998114
H	3.074690	1.191653	4.496293
H	2.888428	2.920904	4.863271
C	2.846797	4.247996	2.159591
H	3.331588	4.645679	1.265591
H	1.769906	4.216917	1.984651
H	3.048909	4.917373	2.999184

[ (PMe<sub>3</sub>)<sub>4</sub>Ca ]<sup>2+</sup>

Ca	3.173640	0.938509	-0.525996
P	0.639416	-0.869505	-0.534070
C	0.029599	-1.332087	-2.216594
H	-0.856674	-1.967803	-2.149946
H	-0.224864	-0.432181	-2.779573
H	0.809811	-1.869617	-2.759193
C	-0.877433	-0.168115	0.253584
H	-1.713757	-0.867253	0.177787
H	-0.684172	0.038635	1.308102
H	-1.153137	0.767336	-0.236856
C	0.783674	-2.514175	0.294080
H	1.574266	-3.099609	-0.178855
H	1.036571	-2.380483	1.347592

H	-0.155453	-3.068611	0.224881
P	5.716718	-0.853873	-0.531614
C	7.292116	0.108943	-0.616507
H	8.159207	-0.555545	-0.606673
H	7.312438	0.701774	-1.533303
H	7.357870	0.789221	0.234825
C	5.901655	-2.039197	-1.937169
H	6.842174	-2.590539	-1.862165
H	5.073584	-2.750739	-1.933712
H	5.885185	-1.495104	-2.883650
C	5.992990	-1.936508	0.939588
H	6.011801	-1.331288	1.847973
H	5.180637	-2.660738	1.024975
H	6.939456	-2.475873	0.853741
P	3.530328	2.276472	2.242052
C	5.178292	3.041953	2.578042
H	5.964722	2.290672	2.482328
H	5.371846	3.838704	1.857300
H	5.212615	3.461790	3.586361
C	3.343570	1.106702	3.661445
H	2.337239	0.683518	3.663466
H	4.061514	0.289545	3.562918
H	3.514751	1.614422	4.613690
C	2.363726	3.639023	2.683459
H	2.465565	4.458841	1.969715
H	1.335773	3.274120	2.646429
H	2.569055	4.017708	3.687586
C	3.183070	2.226128	-4.564643
H	3.165207	3.017126	-5.318485
H	4.084021	1.625701	-4.705309
H	2.312899	1.582482	-4.707908
C	1.706069	4.074335	-2.932886
H	1.649828	4.666514	-2.017787
H	1.779451	4.750663	-3.787908
H	0.787593	3.491219	-3.023652
C	4.584645	4.120802	-2.920454
H	4.620286	4.707430	-2.000808
H	5.521079	3.567238	-3.013283
H	4.491616	4.801170	-3.770335
P	3.163661	2.941708	-2.862228

[ (PMe<sub>3</sub>)<sub>5</sub>Ca]<sup>2+</sup>

Ca	-3.062731	0.692866	-0.048306
P	-5.299685	-1.408082	0.302309
P	-4.090341	3.623276	-0.791987
P	-2.725882	0.250502	-3.138322
P	-0.740576	-1.342906	0.399945
P	-3.124482	1.474086	3.051597
C	-5.720476	-2.457876	-1.159449
H	-6.516162	-3.166136	-0.915519
H	-6.053779	-1.824963	-1.984076
H	-4.840274	-3.014270	-1.487148
C	-6.956931	-0.744090	0.784626
H	-7.327687	-0.070256	0.010138
H	-7.676757	-1.555052	0.920447
H	-6.876351	-0.185184	1.719134
C	-5.006616	-2.674322	1.617408
H	-5.854887	-3.359012	1.692781
H	-4.109080	-3.251008	1.388295
H	-4.864337	-2.182956	2.581748
C	-5.060735	4.521198	0.500485
H	-4.460141	4.630665	1.404620
H	-5.346935	5.515502	0.148589
H	-5.964776	3.961248	0.747715
C	-5.165194	3.856770	-2.278864
H	-5.465080	4.903020	-2.377226
H	-4.624233	3.563572	-3.179254
H	-6.061831	3.239400	-2.194684
C	-2.720452	4.822792	-1.123392

H	-2.126450	4.483848	-1.974138
H	-3.111365	5.819959	-1.341476
H	-2.066493	4.883879	-0.251270
C	-4.270224	0.372987	-4.147855
H	-4.758247	1.333581	-3.979810
H	-4.047333	0.270310	-5.212850
H	-4.961161	-0.420559	-3.856350
C	-1.615630	1.478284	-3.963214
H	-1.548219	1.288185	-5.037125
H	-1.995111	2.489322	-3.806077
H	-0.614940	1.413462	-3.530099
C	-2.028583	-1.345671	-3.760952
H	-2.012311	-1.355297	-4.853701
H	-1.008675	-1.479550	-3.397017
H	-2.637225	-2.182103	-3.412647
C	0.811687	-0.848613	-0.476993
H	1.580218	-1.620437	-0.389348
H	0.602994	-0.672380	-1.533903
H	1.193771	0.079173	-0.045083
C	-1.002672	-3.068160	-0.211601
H	-1.243587	-3.061205	-1.275034
H	-0.105516	-3.672925	-0.057676
H	-1.832742	-3.528888	0.327258
C	-0.115334	-1.656559	2.110237
H	0.721996	-2.358509	2.092586
H	0.218327	-0.720619	2.562095
H	-0.913504	-2.074925	2.725784
C	-1.933490	2.824398	3.484682
H	-2.131386	3.706056	2.871292
H	-2.020516	3.102060	4.538249
H	-0.911067	2.493381	3.291560
C	-4.716368	2.155467	3.705151
H	-5.025011	3.023500	3.121542
H	-5.501436	1.399916	3.638308
H	-4.606698	2.455102	4.750410
C	-2.730806	0.202068	4.334818
H	-3.440999	-0.624566	4.270072
H	-1.727692	-0.193283	4.173253
H	-2.783337	0.634119	5.337386

[ (PMe<sub>3</sub>)<sub>6</sub>Ca ]<sup>2+</sup>

Ca	-2.654225	0.325257	0.057665
P	-2.396833	-0.321463	-3.145430
P	-3.170727	1.225046	3.061780
P	0.490610	0.489938	0.501583
C	-3.583735	0.586703	-4.238965
H	-3.383287	0.374216	-5.292177
H	-4.606484	0.282968	-4.011068
H	-3.500211	1.662602	-4.074049
C	-0.781287	0.046656	-3.972720
H	-0.000392	-0.590324	-3.554414
H	-0.845225	-0.136873	-5.048269
H	-0.499786	1.087794	-3.805869
C	-2.667546	-2.072212	-3.683763
H	-2.607286	-2.161473	-4.771351
H	-1.906336	-2.715445	-3.237967
H	-3.647852	-2.421376	-3.354892
C	1.564276	0.207348	-0.977263
H	1.409688	-0.802136	-1.361853
H	1.306117	0.918192	-1.764423
H	2.619645	0.328518	-0.720506
C	1.166778	2.096529	1.124876
H	2.243984	2.020184	1.292906
H	0.984225	2.887637	0.396233
H	0.681998	2.369683	2.062970
C	1.223635	-0.695661	1.718409
H	1.054962	-1.722911	1.393102
H	2.299689	-0.532091	1.816980
H	0.757186	-0.561866	2.695812

C	-3.865202	0.008612	4.270600
H	-4.789514	-0.423172	3.882679
H	-3.149162	-0.796871	4.438724
H	-4.074797	0.494746	5.226686
C	-4.363224	2.629504	3.242495
H	-4.496755	2.897162	4.293669
H	-3.993851	3.501516	2.701868
H	-5.333004	2.354665	2.824611
C	-1.708634	1.866767	3.995924
H	-0.940134	1.093987	4.061528
H	-1.288375	2.729026	3.475897
H	-1.992482	2.170323	5.006639
P	-5.813880	0.049682	-0.419266
C	-6.654060	1.446149	-1.296633
H	-7.723884	1.248299	-1.401494
H	-6.520629	2.372465	-0.735983
H	-6.221508	1.579124	-2.289904
C	-6.431376	-1.400028	-1.390829
H	-6.001515	-1.393790	-2.393557
H	-6.144090	-2.329363	-0.897939
H	-7.520490	-1.368182	-1.475496
C	-6.855377	-0.083560	1.105899
H	-6.714510	0.797725	1.733713
H	-7.914118	-0.165523	0.847279
H	-6.565301	-0.963488	1.682639
P	-2.557859	-2.791309	0.799523
C	-1.345417	-3.809091	-0.160463
H	-1.319221	-4.836562	0.211106
H	-1.627988	-3.824048	-1.214472
H	-0.344678	-3.380724	-0.078748
C	-4.078083	-3.836339	0.671411
H	-4.412397	-3.878411	-0.366172
H	-3.876972	-4.853437	1.017361
H	-4.878970	-3.409056	1.277553
C	-2.033823	-3.144188	2.539752
H	-2.792138	-2.775386	3.232295
H	-1.909712	-4.218297	2.698256
H	-1.090309	-2.641975	2.760680
P	-2.588156	3.443293	-0.740046
C	-4.100341	4.320810	-1.344817
H	-3.859873	5.346474	-1.636177
H	-4.518948	3.798706	-2.205820
H	-4.855287	4.348351	-0.556981
C	-1.406942	3.761861	-2.131358
H	-1.750385	3.256253	-3.035348
H	-1.325677	4.831501	-2.339703
H	-0.417236	3.375223	-1.879211
C	-1.974810	4.647947	0.525077
H	-2.677370	4.703956	1.357596
H	-1.006320	4.331577	0.914360
H	-1.871614	5.644099	0.087261