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**.

Compound	**1a**	**2**	**3a**	**3b**	**4**
formula	$C_{32}H_{27}BrP_2$	$C_{64}H_{54}MgP_4$	$C_{48}H_{68}Br_2Ca_2O_{10}P_2$	$C_{56}H_{88}Ca_2I_2O_{12}P_2$	$C_{12}H_{28}Br_2CaO_5$
fw (g·mol^{-1})	553.39	971.26	1106.94	1349.16	452.24
T/°C	−140(2)	−140(2)	−140(2)	−140(2)	−140(2)
crystal system	triclinic	monoclinic	monoclinic	monoclinic	orthorhombic
space group	$P\,\bar{1}$	$P\,2_1/c$	$P\,2_1/n$	$P\,2_1/n$	P bcn
a/Å	9.3025(3)	12.4695(2)	11.3347(4)	12.3778(3)	11.4609(3)
b/Å	10.1879(4)	20.0948(3)	19.4430(8)	17.8753(4)	11.5457(3)
c/Å	15.2499(6)	20.8722(3)	12.3105(4)	14.3016(3)	14.2003(3)
α/°	104.318(2)	90	90	90	90
β/°	106.891(2)	90.828(1)	101.618(2)	103.851(1)	90
γ/°	95.661(2)	90	90	90	90
V/Å^3	1317.12(8)	5229.44(14)	2657.41(17)	3072.31(12)	1879.04(8)
Z	2	4	2	2	4
ρ (g·cm^{-3})	1.395	1.234	1.383	1.458	1.599
μ (cm^{-1})	17.01	1.97	18.3	12.99	46
measured data	14,817	34,467	15,087	17,438	8358
data with $I > 2\sigma(I)$	5142	10,279	4113	6320	1974
unique data (R_{int})	5981/0.0318	11,953/0.0528	5811/0.0421	6997/0.0214	2138/0.0234
wR_2 (all data, on F^2) [a]	0.0863	0.1342	0.3082	0.1914	0.0452
R_1 ($I > 2\sigma(I)$) [a]	0.0380	0.0576	0.1127	0.0701	0.0185
s [b]	1.064	1.128	1.091	1.062	1.099
Res. dens./e·Å^{-3}	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 $T_{min/max}$	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

[a] Definition of the R indices: $R_1 = (\Sigma||F_o| - |F_c||)/\Sigma|F_o|$; w$R_2 = \{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$ with $w^{-1} = \sigma^2(F_o^2) + (aP)^2$+bP; P = $[2F_c^2 + \mathrm{Max}(F_o^2]/3$; [b] $s = \{\Sigma[w(F_o^2 - F_c^2)^2]/(N_o - N_p)\}^{1/2}$.

Cartesian coordinates of calculated molecules

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

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

$[(thf)_2Mg]^{2+}$

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

$[(thf)_3Mg]^{2+}$

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

$[(thf)_4Mg]^{2+}$

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

$[(thf)_5Mg]^{2+}$

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

$[(thf)_6Mg]^{2+}$

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

$[(PMe_3)Mg]^{2+}$

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

$[(PMe_3)_2Mg]^{2+}$

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

$[(PMe_3)_3Mg]^{2+}$

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

$[(PMe_3)_4Mg]^{2+}$

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

$[(thf)Ca]^{2+}$

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

$[(thf)_2Ca]^{2+}$

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

$[(thf)_3Ca]^{2+}$

Ca	0.304304	−1.299088	0.393399
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

$[(thf)_4Ca]^{2+}$

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

$[(thf)_5Ca]^{2+}$

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

$[(thf)_6Ca]^{2+}$

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

$[(PMe_3)Ca]^{2+}$

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

$[(PMe_3)_2Ca]^{2+}$

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

$[(PMe_3)_3Ca]^{2+}$

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

$[(PMe_3)_4Ca]^{2+}$

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

$[(PMe_3)_5Ca]^{2+}$

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

$[(PMe_3)_6Ca]^{2+}$

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