Supporting information to the manuscript:

Thermodynamics of the condensation of the $(Me_3Sn)_8Si_8O_{20}$ building block with M–X (M = B, Al, Si, P, Ti, V, Zn, Sn, Sb, X = Cl, Me, Et) precursors by DFT-D3 calculations

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Table S49 Equilibrium geometries of structures with B as the central atom.

py–BCl_3, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
B	-0.00361	0.00236	-0.08651
Cl	1.48913	0.97564	-0.57712
Cl	0.13323	-1.77516	-0.57504
Cl	-1.54995	0.76405	-0.72745
N	-0.01855	0.01003	1.53780
C	-1.03318	0.50826	2.25657
C	1.05065	-0.51583	2.16490
C	1.13148	-0.55682	3.53926
C	0.08375	-0.04272	4.29483
C	-1.01173	0.49641	3.63984
H	1.82797	-0.89737	1.52340
H	2.00515	-0.98675	4.00525
H	0.12415	-0.06358	5.37500
H	-1.84925	0.90712	4.18319
H	-1.85394	0.91143	1.68636
py–BCl_3, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
B	-0.00319	0.00210	-0.08428
Cl	1.48062	0.96704	-0.57037
Cl	0.13431	-1.76326	-0.56798
Cl	-1.54041	0.75975	-0.71741
N	-0.02036	0.01110	1.53259
C	-1.03147	0.50662	2.24749
C	1.04580	-0.51251	2.15409
C	1.12932	-0.55496	3.52579
C	0.08375	-0.04292	4.28025
C	-1.01055	0.49484	3.62821
H	1.82232	-0.89293	1.50634
H	2.00518	-0.98538	3.99056
H	0.12490	-0.06427	5.36202
H	-1.84946	0.90541	4.17239
H	-1.85261	0.90924	1.67210
py–BCl_2OSiH_3, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
B	-0.05531	0.01126	-0.04837
Cl	1.45777	0.98385	-0.58982
Cl	0.10625	-1.78598	-0.56560
O	-1.26398	0.59772	-0.41586
N	0.00178	-0.00437	1.57510
C	-1.02271	0.48241	2.28565
C	1.07736	-0.51148	2.19813
C	1.15799	-0.54491	3.57390
C	0.10124	-0.04274	4.32508
C	-1.00376	0.47769	3.66886
H	1.85773	-0.88313	1.55364
H	2.03670	-0.95914	4.04463
H	0.14156	-0.05808	5.40540
H	-1.84642	0.87733	4.21265
H	-1.84331	0.86769	1.70262
Si	-1.93736	1.00941	-1.85638
H	-3.26125	1.58897	-1.53640
H	-2.11677	-0.17464	-2.72415
H	-1.11871	2.01782	-2.56288
py–BCl_2OSiH_3, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
B	-0.05662	0.01434	-0.04461
Cl	1.44526	0.97612	-0.58136
Cl	0.10083	-1.76739	-0.56052
O	-1.26610	0.60468	-0.40446
N	-0.00060	-0.00310	1.57153

C	-1.02026	0.47933	2.28170
C	1.07372	-0.50813	2.18650
C	1.16007	-0.54480	3.55931
C	0.10692	-0.04635	4.31246
C	-0.99860	0.47276	3.66229
H	1.85244	-0.87695	1.53400
H	2.04230	-0.95950	4.02632
H	0.15048	-0.06350	5.39426
H	-1.84166	0.87108	4.20927
H	-1.84290	0.86532	1.69753
Si	-1.91991	0.99580	-1.85567
H	-3.24748	1.59073	-1.55823
H	-2.09915	-0.20497	-2.70917
H	-1.08533	1.99090	-2.57331

py–BCl(OSiH$_3$)$_2$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
B	-0.02042	0.15708	-0.02787
O	1.13019	0.87033	-0.42814
Cl	0.10600	-1.70537	-0.53178
O	-1.27656	0.69161	-0.37503
N	0.00179	0.08683	1.60546
C	-1.14607	-0.06780	2.27800
C	1.16971	0.11230	2.25838
C	1.22710	-0.01828	3.63257
C	0.04530	-0.18134	4.34299
C	-1.15926	-0.20554	3.65253
H	2.04190	0.24272	1.63839
H	2.18487	0.00739	4.13003
H	0.06280	-0.28807	5.41884
H	-2.10055	-0.32963	4.16650
H	-2.03688	-0.07359	1.67062
Si	-1.94650	1.14403	-1.79697
H	-3.30123	1.65602	-1.48954
H	-2.05576	0.00931	-2.74088
H	-1.16073	2.22313	-2.44203
Si	2.06445	0.70927	-1.76797
H	2.78665	1.99072	-1.93754
H	1.25010	0.44664	-2.97528
H	3.05951	-0.37523	-1.60467

py–BCl(OSiH$_3$)$_2$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
B	-0.02125	0.14875	-0.02581
O	1.12513	0.87248	-0.41603
Cl	0.11040	-1.68342	-0.54564
O	-1.27745	0.68850	-0.36166
N	0.00138	0.07612	1.60058
C	-1.14214	-0.07268	2.27129
C	1.16534	0.10667	2.24962
C	1.22488	-0.01254	3.62216
C	0.04568	-0.16860	4.33259
C	-1.15656	-0.19862	3.64444
H	2.03757	0.23492	1.62519
H	2.18456	0.01789	4.11878
H	0.06342	-0.26512	5.41102
H	-2.09959	-0.31756	4.15943
H	-2.03383	-0.08120	1.66112
Si	-1.93545	1.13519	-1.78684
H	-3.29747	1.64763	-1.48939
H	-2.03742	-0.00559	-2.73273
H	-1.14546	2.21823	-2.43208
Si	2.05159	0.69538	-1.75466
H	2.78672	1.97396	-1.93263

H	1.23108	0.43336	-2.96499
H	3.04265	-0.39980	-1.58971
py–B(OSiH$_3$)$_3$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
B	0.02132	-0.07434	-0.21468
O	1.34710	0.34560	-0.57317
O	-0.24327	-1.44625	-0.51671
O	-1.00483	0.83779	-0.62763
N	0.00986	-0.00615	1.47503
C	-0.76154	0.85564	2.14187
C	0.83893	-0.82091	2.13844
C	0.91888	-0.80248	3.51701
C	0.11720	0.08679	4.22360
C	-0.73449	0.92892	3.52435
H	1.43386	-1.48201	1.52693
H	1.59592	-1.47320	4.02444
H	0.15914	0.12219	5.30353
H	-1.37102	1.63559	4.03546
H	-1.39132	1.47920	1.52722
Si	-2.29366	0.55692	-1.59487
H	-2.87775	1.87481	-1.93342
H	-3.33085	-0.25118	-0.90608
H	-1.91070	-0.13960	-2.84488
Si	0.55482	-2.44497	-1.53333
H	-0.29306	-3.64269	-1.73004
H	1.84982	-2.88550	-0.95120
H	0.82392	-1.82400	-2.85111
Si	1.75399	1.79460	-1.21609
H	3.22452	1.79731	-1.39141
H	1.38904	2.91798	-0.31441
H	1.11600	2.02857	-2.53265
py–B(OSiH$_3$)$_3$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
B	0.01624	-0.06001	-0.20475
O	1.34582	0.33426	-0.56652
O	-0.27515	-1.42278	-0.51462
O	-0.99426	0.86773	-0.61490
N	0.01024	0.00060	1.46820
C	-0.76600	0.84638	2.13993
C	0.84535	-0.80937	2.12016
C	0.92758	-0.80371	3.49588
C	0.11993	0.07010	4.20919
C	-0.73859	0.90865	3.52017
H	1.44682	-1.45905	1.49862
H	1.61312	-1.47344	3.99614
H	0.16276	0.09640	5.29094
H	-1.38214	1.60614	4.03806
H	-1.40212	1.46948	1.52718
Si	-2.25860	0.53558	-1.59730
H	-2.89261	1.83539	-1.93714
H	-3.27351	-0.31964	-0.92314
H	-1.83135	-0.13792	-2.85166
Si	0.54434	-2.42088	-1.51007
H	-0.31288	-3.61113	-1.74256
H	1.81759	-2.88153	-0.88347
H	0.87078	-1.79752	-2.81945
Si	1.73756	1.77895	-1.22242
H	3.21189	1.78826	-1.40565
H	1.37051	2.91158	-0.32557
H	1.09100	1.99817	-2.54293
py–BCl$_2$OSi(OSiH$_3$)$_3$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
B	-0.26239	-0.15754	0.25029

Cl	-1.08559	1.51092	0.04090
Cl	1.38333	-0.19335	-0.61074
O	-1.08170	-1.22330	-0.13546
N	0.09038	-0.35679	1.84736
C	0.60794	-1.55019	2.18888
C	0.90167	-1.86038	3.49898
C	0.65759	-0.91401	4.48696
C	0.13036	0.31529	4.12346
C	-0.14361	0.56373	2.79069
H	0.76797	-2.24068	1.37724
H	1.30804	-2.83161	3.73611
H	-0.07553	1.08023	4.85669
H	0.87512	-1.13430	5.52279
H	-0.56035	1.49383	2.44069
Si	-2.45980	-1.89770	0.33668
O	-3.62836	-0.83318	0.69086
O	-2.15574	-2.77117	1.68670
O	-2.97643	-2.87709	-0.83403
Si	-4.14625	0.48562	1.51318
Si	-4.30869	-3.65080	-1.39254
Si	-2.81878	-3.16791	3.12790
H	-4.37992	1.61622	0.59695
H	-5.41491	0.12271	2.18470
H	-3.16297	0.86388	2.55275
H	-1.78540	-3.86663	3.92292
H	-3.99166	-4.05096	2.95048
H	-3.23529	-1.94511	3.85434
H	-3.86699	-4.74735	-2.27787
H	-5.16986	-2.71609	-2.14860
H	-5.08288	-4.21372	-0.26096

py–$BCl_2OSi(OSiH_3)_3$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
B	-0.26813	-0.16503	0.26542
Cl	-1.09936	1.48257	0.05696
Cl	1.36090	-0.19193	-0.60069
O	-1.07606	-1.24171	-0.11102
N	0.09726	-0.34961	1.85115
C	0.61794	-1.53560	2.19227
C	0.93368	-1.83462	3.49753
C	0.70790	-0.88005	4.47795
C	0.17708	0.34404	4.11272
C	-0.11881	0.57778	2.78453
H	0.76512	-2.23177	1.37938
H	1.34532	-2.80502	3.73614
H	-0.01526	1.11812	4.84222
H	0.94323	-1.09075	5.51363
H	-0.54094	1.50625	2.42770
Si	-2.46260	-1.90347	0.34411
O	-3.62846	-0.83659	0.68229
O	-2.17600	-2.78199	1.68881
O	-2.96655	-2.87361	-0.83561
Si	-4.13784	0.48608	1.49662
Si	-4.30115	-3.62882	-1.40245
Si	-2.85832	-3.19011	3.11377
H	-4.34698	1.62412	0.57526
H	-5.42442	0.13798	2.15260
H	-3.16123	0.85369	2.55470
H	-1.82335	-3.86930	3.93299
H	-4.01078	-4.10286	2.91168
H	-3.31835	-1.97254	3.83360
H	-3.86437	-4.72308	-2.30096

H	-5.15555	-2.67644	-2.15366
H	-5.08582	-4.19925	-0.27543

Table S50 Equilibrium geometries of structures with Al as the central atom.

py–$AlCl_3$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Al	0.01009	-0.00131	-0.15461
Cl	1.96452	0.63148	-0.70127
Cl	-1.55411	1.37148	-0.58026
Cl	-0.46511	-2.02263	-0.60728
N	0.03744	-0.00424	1.82965
C	-1.06130	-0.43948	2.47076
C	-1.14408	-0.45035	3.84900
C	-0.05942	0.00217	4.59016
C	1.07275	0.45015	3.92459
C	1.08772	0.43340	2.54153
H	-1.87477	-0.77979	1.84649
H	-2.04369	-0.80778	4.32711
H	1.93745	0.80924	4.46227
H	-0.09787	0.00515	5.67074
H	1.93936	0.76682	1.96701
py–$AlCl_3$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Al	0.00956	-0.00081	-0.15336
Cl	1.95737	0.63021	-0.69266
Cl	-1.54931	1.36502	-0.57749
Cl	-0.46566	-2.01431	-0.59876
N	0.03980	-0.00286	1.82526
C	-1.05550	-0.43695	2.46136
C	-1.14102	-0.45053	3.83690
C	-0.05885	-0.00031	4.57732
C	1.07163	0.44761	3.91500
C	1.08585	0.43217	2.53455
H	-1.86937	-0.77670	1.83297
H	-2.04268	-0.80913	4.31350
H	1.93765	0.80637	4.45368
H	-0.09797	0.00108	5.65953
H	1.93860	0.76620	1.95733
py–$AlCl_3$(THF), B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Al	-0.08920	-0.10506	0.05899
Cl	-0.74581	1.94885	-0.18596
Cl	2.02771	-0.60188	0.05025
Cl	-1.59601	-1.69259	0.20301
N	-0.02201	0.01066	2.16108
C	0.25684	-1.12284	2.82446
C	0.37293	-1.16754	4.20053
C	0.19487	0.00171	4.92909
C	-0.09415	1.17220	4.24581
C	-0.19429	1.13654	2.86405
H	0.38439	-2.00917	2.22223
H	0.59978	-2.10499	4.68646
H	-0.24150	2.10756	4.76532
H	0.27992	-0.00218	6.00726
H	-0.41798	2.01903	2.28581
H	-0.35400	-0.13331	-4.74471
H	1.38900	-1.39876	-2.89635
H	-1.07291	1.22827	-2.86945
C	-1.08960	-0.60674	-4.09248
C	0.38842	-1.60803	-2.52289
H	-0.11666	-2.55576	-4.41148
C	-1.21268	0.15664	-2.78623
O	-0.12504	-0.35848	-1.95354
C	-0.59154	-1.97477	-3.62299
H	-2.03889	-0.65262	-4.62347

H	0.44563	-2.34371	-1.72784
H	-2.15320	-0.05269	-2.27752
H	-1.41585	-2.55721	-3.21059

py–$AlCl_3$(THF), PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Al	-0.06669	-0.10209	0.05755
Cl	-0.66786	1.95837	-0.19332
Cl	2.03210	-0.63615	0.01618
Cl	-1.57941	-1.66338	0.23519
N	0.00683	0.02328	2.14551
C	0.40144	-1.07530	2.79822
C	0.46686	-1.13686	4.17423
C	0.10946	-0.01905	4.91176
C	-0.29970	1.11709	4.23790
C	-0.33773	1.09813	2.85537
H	0.67105	-1.92354	2.18348
H	0.79380	-2.04958	4.65322
H	-0.58902	2.01522	4.76636
H	0.14985	-0.03603	5.99397
H	-0.64898	1.95878	2.27955
H	-0.38002	-0.13030	-4.70942
H	1.35611	-1.41834	-2.89095
H	-1.10382	1.22458	-2.82771
C	-1.11947	-0.60153	-4.05789
C	0.35305	-1.60697	-2.50740
H	-0.17234	-2.55758	-4.38477
C	-1.22818	0.14840	-2.75048
O	-0.13274	-0.35761	-1.94842
C	-0.63515	-1.96770	-3.59439
H	-2.07160	-0.63532	-4.58674
H	0.40658	-2.34228	-1.70776
H	-2.16192	-0.07592	-2.23006
H	-1.46364	-2.53974	-3.17219

py–$AlCl_2OSiH_3$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Al	-0.11647	-0.03912	0.01227
Cl	-0.45556	1.98379	-0.56393
Cl	1.78250	-0.79754	-0.57843
O	-1.42586	-1.11230	-0.13454
N	0.04896	0.08021	1.98368
C	-0.51673	-0.85732	2.76019
C	-0.38278	-0.83933	4.13650
C	0.35722	0.17727	4.72516
C	0.93990	1.14487	3.91695
C	0.76475	1.06545	2.54872
H	-1.08219	-1.61590	2.23958
H	-0.85277	-1.60944	4.72962
H	1.52138	1.95237	4.33583
H	0.47749	0.21603	5.79905
H	1.18631	1.79398	1.87140
Si	-2.52692	-2.05089	-0.86478
H	-3.13898	-2.94967	0.14823
H	-1.91457	-2.89211	-1.92122
H	-3.60701	-1.23855	-1.47463

py–$AlCl_2OSiH_3$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Al	-0.11642	-0.04053	0.01479
Cl	-0.45163	1.97552	-0.55500
Cl	1.77427	-0.79357	-0.57580
O	-1.42423	-1.11227	-0.12780
N	0.04757	0.07841	1.98083
C	-0.51576	-0.85430	2.75547
C	-0.38237	-0.83547	4.12918

C	0.35649	0.18001	4.71412
C	0.93758	1.14428	3.90594
C	0.76094	1.06106	2.54077
H	-1.08263	-1.61451	2.23381
H	-0.85325	-1.60597	4.72372
H	1.52017	1.95406	4.32258
H	0.47748	0.22072	5.78949
H	1.18200	1.78920	1.85887
Si	-2.51994	-2.04595	-0.86403
H	-3.13699	-2.95280	0.14569
H	-1.90281	-2.88552	-1.92576
H	-3.60207	-1.22935	-1.47613

py–$AlCl_2OSiH_3$(THF), B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Al	-0.04636	-0.05452	0.00257
Cl	-0.61669	2.03719	-0.17041
O	1.60054	-0.58017	0.07698
Cl	-1.62891	-1.56528	0.03671
N	-0.03096	0.00097	2.13031
C	0.21197	-1.16987	2.73825
C	0.36728	-1.27956	4.10712
C	0.26747	-0.13469	4.88712
C	0.01482	1.07585	4.26118
C	-0.12799	1.10299	2.88215
H	0.27792	-2.03350	2.09421
H	0.56339	-2.24616	4.54723
H	-0.07228	1.99374	4.82386
H	0.38487	-0.18773	5.96094
H	-0.32442	2.01885	2.34593
Si	3.14296	-0.44241	0.52049
H	3.28631	-0.38871	2.00162
H	3.77570	0.78005	-0.03680
H	3.91622	-1.61778	0.04146
H	-1.73484	-1.01728	-4.58088
H	1.38913	-0.71758	-3.47052
H	-0.78160	0.89233	-3.57175
C	-1.50796	-1.17826	-3.52827
C	0.77692	-1.21048	-2.71216
H	0.05857	-2.55044	-4.26335
C	-1.10828	0.13870	-2.85441
O	0.03531	-0.17671	-2.01783
C	-0.28855	-2.11050	-3.32997
H	-2.38849	-1.59742	-3.04915
H	1.41676	-1.68714	-1.98040
H	-1.87137	0.56368	-2.21357
H	-0.54081	-2.91547	-2.64377

py–$AlCl_2OSiH_3$(THF), PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Al	-0.04711	-0.05795	0.00843
Cl	-0.61496	2.02376	-0.16962
O	1.59769	-0.58476	0.07621
Cl	-1.62564	-1.55797	0.03742
N	-0.03468	0.00146	2.11848
C	0.19236	-1.16866	2.72286
C	0.34992	-1.28229	4.08856
C	0.26965	-0.13835	4.86671
C	0.03299	1.07334	4.24305
C	-0.11323	1.10110	2.86726
H	0.24243	-2.03381	2.07509
H	0.53302	-2.25350	4.52751
H	-0.03885	1.99409	4.80589
H	0.38984	-0.19285	5.94174

H	-0.29907	2.02023	2.32759
Si	3.13464	-0.43225	0.52295
H	3.27864	-0.41512	2.01019
H	3.74950	0.81904	-0.00217
H	3.93050	-1.58456	0.01179
H	-1.72694	-1.01644	-4.56124
H	1.37082	-0.69918	-3.47798
H	-0.78051	0.88784	-3.55607
C	-1.49998	-1.17890	-3.50771
C	0.77294	-1.19577	-2.70770
H	0.05822	-2.55506	-4.23859
C	-1.10026	0.13176	-2.83511
O	0.03658	-0.17912	-2.01057
C	-0.28604	-2.10339	-3.30854
H	-2.38261	-1.59891	-3.02961
H	1.43147	-1.66674	-1.98511
H	-1.86456	0.55742	-2.19162
H	-0.53356	-2.90200	-2.61059

py–AlCl(OSiH$_3$)$_2$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Al	0.04431	0.00268	-0.28221
Cl	0.10219	2.09461	-0.72641
O	1.47239	-0.86771	-0.61023
O	-1.43606	-0.73797	-0.66982
N	0.03598	-0.02625	1.70090
C	0.84235	-0.86238	2.37210
C	0.82553	-0.93717	3.75337
C	-0.05048	-0.12315	4.45825
C	-0.88299	0.74110	3.75836
C	-0.81189	0.76323	2.37854
H	1.50134	-1.46279	1.76233
H	1.48968	-1.62048	4.26106
H	-1.57603	1.39170	4.27026
H	-0.08344	-0.15972	5.53847
H	-1.42547	1.42297	1.78188
Si	-2.84721	-1.02407	-1.40383
Si	2.71461	-1.45475	-1.46513
H	3.52613	-2.34831	-0.59698
H	3.59695	-0.36977	-1.95946
H	2.24867	-2.24619	-2.63054
H	-3.45622	-2.26559	-0.86289
H	-2.67672	-1.19199	-2.86843
H	-3.80559	0.08830	-1.17539

py–AlCl(OSiH$_3$)$_2$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Al	0.04017	-0.00649	-0.27568
Cl	0.08571	2.07655	-0.71751
O	1.46943	-0.87196	-0.59724
O	-1.43477	-0.75412	-0.65949
N	0.03707	-0.03116	1.70190
C	0.84546	-0.85794	2.37150
C	0.83615	-0.92506	3.75055
C	-0.03700	-0.11036	4.45226
C	-0.87302	0.74560	3.75238
C	-0.80663	0.75781	2.37484
H	1.50449	-1.46072	1.75994
H	1.50563	-1.60461	4.25934
H	-1.56665	1.39913	4.26275
H	-0.06509	-0.14010	5.53445
H	-1.42462	1.41340	1.77391
Si	-2.83253	-1.00202	-1.42488
Si	2.70438	-1.44917	-1.46247

H	3.53315	-2.33904	-0.59896
H	3.57736	-0.35525	-1.96786
H	2.23229	-2.24734	-2.62683
H	-3.47948	-2.24111	-0.91071
H	-2.63482	-1.15705	-2.89233
H	-3.77719	0.12961	-1.20304

py–AlCl(OSiH$_3$)$_2$(THF), B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Al	-0.04193	-0.06421	0.05321
O	-0.39844	1.62904	0.00255
Cl	2.03094	-0.72053	0.00307
O	-1.27040	-1.26666	-0.07338
N	-0.06934	-0.05966	2.13573
C	0.30552	-1.15520	2.81005
C	0.33575	-1.19913	4.19195
C	-0.03568	-0.06764	4.90687
C	-0.43292	1.06308	4.20881
C	-0.43784	1.02861	2.82383
H	0.60076	-2.00406	2.21103
H	0.65072	-2.10283	4.69251
H	-0.73242	1.96523	4.72182
H	-0.01553	-0.06924	5.98820
H	-0.72764	1.87810	2.22518
Si	-2.55839	-2.18151	0.21454
Si	0.04195	2.99551	-0.74265
H	-2.68397	-2.52902	1.65630
H	-2.47638	-3.45362	-0.54975
H	-3.81127	-1.49289	-0.19507
H	-0.16936	4.14520	0.17678
H	-0.77868	3.24413	-1.95765
H	1.46854	2.99104	-1.15053
H	-2.11730	-0.99949	-4.34037
H	0.88421	-0.48948	-3.88338
H	-1.35628	1.00165	-3.40289
C	-1.80664	-1.14601	-3.30675
C	0.56145	-0.97965	-2.96027
H	-0.34571	-2.58392	-4.12095
C	-1.40939	0.19741	-2.66901
O	-0.07425	0.01431	-2.12457
C	-0.52962	-2.00618	-3.21655
H	-2.63506	-1.60851	-2.77547
H	1.42633	-1.34916	-2.42296
H	-2.05522	0.50089	-1.85296
H	-0.59411	-2.69194	-2.37460

py–AlCl(OSiH$_3$)$_2$(THF), PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Al	-0.04341	-0.06679	0.05412
O	-0.40293	1.62460	0.00722
Cl	2.01706	-0.73201	-0.00632
O	-1.27541	-1.26220	-0.06772
N	-0.06016	-0.05579	2.12589
C	0.34128	-1.13651	2.79909
C	0.36223	-1.18306	4.17853
C	-0.04724	-0.06654	4.89010
C	-0.47079	1.05078	4.19187
C	-0.46397	1.01649	2.80969
H	0.66860	-1.97554	2.19851
H	0.70045	-2.07957	4.67988
H	-0.80066	1.94499	4.70310
H	-0.03584	-0.06915	5.97314
H	-0.77402	1.85891	2.20677
Si	-2.55811	-2.17824	0.22121

Si	0.05346	2.97923	-0.74355
H	-2.68246	-2.52889	1.66738
H	-2.47461	-3.45423	-0.54679
H	-3.81805	-1.49083	-0.18734
H	-0.14689	4.14043	0.17134
H	-0.76563	3.23197	-1.96502
H	1.48525	2.95736	-1.15139
H	-2.11289	-0.98905	-4.31989
H	0.86915	-0.46003	-3.87468
H	-1.34645	1.00317	-3.38680
C	-1.79571	-1.13821	-3.28741
C	0.55734	-0.95874	-2.95029
H	-0.33675	-2.56505	-4.11134
C	-1.39772	0.19794	-2.65060
O	-0.07531	0.01513	-2.11001
C	-0.52199	-1.98872	-3.20514
H	-2.62231	-1.60475	-2.75297
H	1.43238	-1.32586	-2.42292
H	-2.04710	0.50457	-1.83484
H	-0.57883	-2.67708	-2.36235

py–Al(OSiH$_3$)$_3$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Al	0.03737	-0.08348	-0.37309
O	0.12008	1.58408	-0.75731
O	1.45920	-0.97695	-0.67424
O	-1.42873	-0.89459	-0.70984
N	-0.00661	-0.01674	1.60877
C	-0.50746	-1.05000	2.30161
C	-0.48661	-1.07828	3.68412
C	0.06660	-0.00318	4.36796
C	0.57798	1.06686	3.64597
C	0.52411	1.02561	2.26450
H	-0.93405	-1.84915	1.71208
H	-0.89888	-1.92705	4.20911
H	1.01162	1.92360	4.13991
H	0.09579	0.00145	5.44890
H	0.89554	1.82801	1.64394
Si	-2.70120	-1.48627	-1.50713
Si	-0.40439	2.91080	-1.51873
Si	2.93565	-1.27309	-1.25555
H	3.04440	-2.67712	-1.72514
H	3.96563	-1.06821	-0.20192
H	3.26757	-0.37706	-2.39289
H	-3.44613	-2.43431	-0.63678
H	-2.29160	-2.21824	-2.73218
H	-3.63770	-0.40553	-1.90741
H	0.72346	3.84647	-1.75640
H	-1.41576	3.62662	-0.69597
H	-1.02633	2.59304	-2.82922

py–Al(OSiH$_3$)$_3$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Al	0.03882	-0.08396	-0.36725
O	0.13239	1.58219	-0.74343
O	1.45004	-0.98774	-0.67104
O	-1.42879	-0.88515	-0.70182
N	-0.00594	-0.02344	1.60850
C	-0.48592	-1.06592	2.29223
C	-0.46760	-1.10189	3.67180
C	0.06250	-0.02159	4.35969
C	0.55272	1.05958	3.64548
C	0.50116	1.02245	2.26641
H	-0.89633	-1.87166	1.69609

H	-0.86491	-1.96250	4.19193
H	0.96924	1.92391	4.14398
H	0.09012	-0.02160	5.44230
H	0.85693	1.83576	1.64679
Si	-2.70783	-1.45526	-1.49688
Si	-0.39730	2.87537	-1.55127
Si	2.93716	-1.23566	-1.23778
H	3.08712	-2.63417	-1.72636
H	3.95413	-1.01893	-0.16735
H	3.26107	-0.31384	-2.36291
H	-3.44648	-2.42561	-0.63785
H	-2.31151	-2.16203	-2.74654
H	-3.65103	-0.36210	-1.86326
H	0.70670	3.50232	-2.32869
H	-0.91863	3.89867	-0.59901
H	-1.49433	2.53003	-2.49870

py–Al(OSiH$_3$)$_3$(THF), B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Al	0.01206	0.35729	-1.17617
O	-0.36855	2.02834	-0.93826
O	1.63830	-0.22045	-1.37005
O	-1.26388	-0.80635	-1.36753
N	0.05570	-0.00236	0.89222
C	0.37051	-1.24028	1.29571
C	0.36140	-1.60965	2.62827
C	0.01230	-0.66119	3.58112
C	-0.31366	0.62076	3.16259
C	-0.28156	0.91182	1.80752
H	0.63472	-1.93798	0.51451
H	0.62165	-2.61963	2.90900
H	-0.59071	1.38890	3.86975
H	-0.00550	-0.91838	4.63144
H	-0.52850	1.88829	1.41822
Si	-2.59183	-1.66370	-1.10157
Si	-0.05644	3.52709	-1.44878
Si	3.17961	-0.07848	-0.92635
H	3.58007	-1.19812	-0.02959
H	3.44284	1.18731	-0.19086
H	4.07485	-0.11405	-2.11211
H	-2.73091	-2.04836	0.33044
H	-2.57335	-2.91881	-1.89996
H	-3.81722	-0.91214	-1.48617
H	-0.17276	4.48124	-0.31426
H	-1.02035	3.96009	-2.49613
H	1.31023	3.65875	-2.01714
H	-2.07131	-0.18596	-5.57784
H	0.95787	0.26366	-5.05009
H	-1.26212	1.73108	-4.51810
C	-1.75778	-0.40591	-4.55821
C	0.61324	-0.29466	-4.17527
H	-0.29901	-1.77983	-5.48199
C	-1.34467	0.88675	-3.83213
O	-0.02891	0.63898	-3.27743
C	-0.48778	-1.28329	-4.53158
H	-2.58806	-0.89427	-4.05449
H	1.46029	-0.71711	-3.64947
H	-1.99728	1.15693	-3.00939
H	-0.56523	-2.03953	-3.75372

py–Al(OSiH$_3$)$_3$(THF), PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Al	0.00838	0.35109	-1.17417
O	-0.37166	2.02058	-0.93834

O	1.63099	-0.23155	-1.36794
O	-1.26575	-0.81004	-1.36527
N	0.05341	0.00022	0.88309
C	0.36217	-1.23544	1.28263
C	0.35764	-1.60670	2.61197
C	0.01913	-0.65897	3.56485
C	-0.30054	0.62246	3.14991
C	-0.27282	0.91238	1.79736
H	0.62037	-1.93418	0.49704
H	0.61397	-2.61995	2.88985
H	-0.57047	1.39333	3.85897
H	0.00442	-0.91722	4.61660
H	-0.51699	1.89194	1.40764
Si	-2.59181	-1.66519	-1.10162
Si	-0.04514	3.51058	-1.45567
Si	3.16476	-0.06112	-0.91766
H	3.57574	-1.16063	0.00693
H	3.40977	1.22711	-0.20511
H	4.07115	-0.11023	-2.10046
H	-2.72751	-2.06511	0.33175
H	-2.57902	-2.91719	-1.91450
H	-3.82207	-0.90623	-1.47526
H	-0.14713	4.47394	-0.32126
H	-1.01154	3.95237	-2.50417
H	1.32516	3.62723	-2.03160
H	-2.07203	-0.17503	-5.55970
H	0.94708	0.28507	-5.03759
H	-1.24688	1.72944	-4.50480
C	-1.74993	-0.39946	-4.54251
C	0.60710	-0.28217	-4.16441
H	-0.29428	-1.75836	-5.48190
C	-1.33232	0.88407	-3.81708
O	-0.03098	0.63192	-3.26415
C	-0.48481	-1.26933	-4.52680
H	-2.57819	-0.89141	-4.03490
H	1.46114	-0.70694	-3.64679
H	-1.98896	1.16000	-2.99583
H	-0.55734	-2.03402	-3.75406

py–AlMe(OSiH$_3$)$_2$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Al	0.14172	0.38675	-0.27152
C	0.45254	2.30731	-0.45964
O	1.44636	-0.66978	-0.66973
O	-1.42516	-0.19970	-0.69665
N	0.05145	0.06199	1.72113
C	1.15463	-0.29227	2.39448
C	1.14147	-0.49801	3.76291
C	-0.05269	-0.33456	4.45219
C	-1.19465	0.02746	3.74936
C	-1.10400	0.21645	2.38192
H	2.04542	-0.42081	1.79640
H	2.04971	-0.78592	4.27128
H	-2.14430	0.15693	4.24690
H	-0.09468	-0.49172	5.52127
H	-1.95900	0.48184	1.77665
Si	-2.40498	-1.26623	-1.41090
Si	2.09662	-1.89164	-1.50158
H	2.65688	-2.90660	-0.56891
H	3.20558	-1.41957	-2.36954
H	1.09986	-2.57481	-2.36707
H	-3.80922	-1.02693	-0.98459

H	-2.06088	-2.66545	-1.04098
H	-2.35380	-1.16404	-2.89165
H	0.54478	2.60215	-1.50839
H	1.37358	2.62331	0.03854
H	-0.36542	2.89730	-0.03642

py–AlMe(OSiH$_3$)$_2$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Al	0.14284	0.38244	-0.26749
C	0.44974	2.29983	-0.45648
O	1.45051	-0.66799	-0.65975
O	-1.42157	-0.20284	-0.69023
N	0.05244	0.05702	1.71876
C	1.15098	-0.29394	2.39108
C	1.13826	-0.49521	3.75750
C	-0.05390	-0.32922	4.44351
C	-1.19279	0.03003	3.74030
C	-1.09925	0.21370	2.37507
H	2.04331	-0.42437	1.79152
H	2.04768	-0.78215	4.26733
H	-2.14450	0.16204	4.23633
H	-0.09681	-0.48296	5.51467
H	-1.95452	0.47815	1.76573
Si	-2.39814	-1.26409	-1.40836
Si	2.08684	-1.88599	-1.50147
H	2.64175	-2.91757	-0.57641
H	3.20237	-1.41535	-2.36985
H	1.08008	-2.55572	-2.37465
H	-3.80542	-1.03593	-0.96943
H	-2.04519	-2.67095	-1.05658
H	-2.35770	-1.14486	-2.89300
H	0.54203	2.59088	-1.50694
H	1.37087	2.61812	0.04115
H	-0.36995	2.88992	-0.03547

py–AlMe(OSiH$_3$)$_2$(THF), B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Al	0.21549	-0.18554	0.09071
O	-0.07951	1.52788	0.02095
C	2.04105	-0.94380	0.08213
O	-1.20616	-1.21344	0.07227
N	0.15043	-0.13591	2.23452
C	0.14270	-1.30449	2.88494
C	0.15227	-1.38589	4.26644
C	0.16811	-0.20893	5.00423
C	0.17364	1.00330	4.32982
C	0.16496	0.99672	2.94312
H	0.12470	-2.19002	2.26487
H	0.14295	-2.35239	4.74870
H	0.18335	1.94355	4.86160
H	0.17408	-0.23786	6.08541
H	0.16767	1.90735	2.36323
Si	-2.73449	-1.47983	0.48876
H	-2.93365	-1.43780	1.96441
H	-3.17103	-2.82242	0.02012
H	-3.65904	-0.47932	-0.11163
H	-2.02705	-1.05221	-4.22625
H	1.01407	-1.14127	-3.74787
H	-0.87705	0.85349	-3.51632
C	-1.75818	-1.12900	-3.17352
C	0.58768	-1.42037	-2.77929
H	-0.63267	-2.93726	-3.75591
C	-1.08420	0.16932	-2.69180
O	0.18080	-0.21411	-2.09907

C	-0.69551	-2.22104	-2.93805
H	-2.66617	-1.33206	-2.61157
H	1.35177	-1.90003	-2.17878
H	-1.65366	0.69020	-1.93050
H	-0.90660	-2.75438	-2.01494
H	2.59395	-0.62928	0.97149
H	2.62961	-0.61994	-0.77954
H	2.05512	-2.03903	0.08470
Si	-0.67260	2.96162	-0.38441
H	0.02748	3.55363	-1.55496
H	-2.11958	2.89098	-0.72933
H	-0.53835	3.91789	0.75005

py–AlMe(OSiH$_3$)$_2$(THF), PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Al	0.21179	-0.18857	0.09358
O	-0.08079	1.52288	0.01988
C	2.03247	-0.95271	0.08529
O	-1.20721	-1.21633	0.07576
N	0.14768	-0.13092	2.22207
C	0.13793	-1.29691	2.86772
C	0.15135	-1.38311	4.24611
C	0.17387	-0.21039	4.98473
C	0.18164	1.00075	4.31463
C	0.16825	0.99592	2.93067
H	0.11566	-2.18189	2.24303
H	0.14049	-2.35247	4.72573
H	0.19660	1.94147	4.84829
H	0.18344	-0.24173	6.06740
H	0.17168	1.90904	2.34992
Si	-2.73503	-1.47213	0.48895
H	-2.93587	-1.44801	1.97005
H	-3.18578	-2.80904	0.00166
H	-3.65455	-0.45235	-0.09988
H	-2.01062	-1.04117	-4.21530
H	1.01353	-1.12553	-3.73136
H	-0.85872	0.85199	-3.50009
C	-1.74384	-1.12253	-3.16118
C	0.58657	-1.40896	-2.76220
H	-0.62146	-2.92621	-3.74516
C	-1.06978	0.16623	-2.67524
O	0.17969	-0.21814	-2.08160
C	-0.68828	-2.20977	-2.92654
H	-2.65581	-1.32602	-2.60228
H	1.35421	-1.89125	-2.16374
H	-1.64464	0.69143	-1.91642
H	-0.90150	-2.74512	-2.00289
H	2.58561	-0.64285	0.97713
H	2.62320	-0.62495	-0.77472
H	2.04511	-2.04870	0.08294
Si	-0.68172	2.95006	-0.38324
H	0.01528	3.54982	-1.55780
H	-2.13416	2.87329	-0.72619
H	-0.55016	3.90973	0.75531

py–AlMe$_2$OSiH$_3$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Al	-0.04286	-0.02425	-0.04548
C	-0.47237	1.83409	-0.54759
C	1.74012	-0.74662	-0.47720
O	-1.35048	-1.16046	-0.18508
N	0.01215	0.04081	1.99521
C	-0.53232	-0.94746	2.71802
C	-0.45805	-0.97082	4.10049

C	0.19816	0.06275	4.75460
C	0.75755	1.08777	4.00248
C	0.64313	1.04084	2.62492
H	-1.03611	-1.71427	2.14758
H	-0.90958	-1.78544	4.64724
H	1.27332	1.91285	4.47104
H	0.27096	0.07156	5.83346
H	1.05393	1.81623	1.99366
Si	-2.45844	-2.08085	-0.90400
H	-3.09800	-2.97739	0.09831
H	-1.87143	-2.94359	-1.96325
H	-3.53656	-1.27155	-1.53079
H	-0.63996	1.91149	-1.62637
H	0.32829	2.54370	-0.31494
H	-1.38335	2.19973	-0.06450
H	1.85444	-0.93071	-1.54949
H	1.92673	-1.69926	0.02769
H	2.54751	-0.06535	-0.18977

py–AlMe$_2$OSiH$_3$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Al	-0.04425	-0.02466	-0.03987
C	-0.47452	1.83050	-0.54006
C	1.73453	-0.74742	-0.47163
O	-1.34924	-1.16061	-0.17560
N	0.00924	0.03818	1.99302
C	-0.53367	-0.94473	2.71448
C	-0.45862	-0.96774	4.09433
C	0.19895	0.06344	4.74450
C	0.75770	1.08453	3.99209
C	0.64022	1.03451	2.61759
H	-1.04017	-1.71222	2.14272
H	-0.91177	-1.78235	4.64263
H	1.27630	1.91096	4.45850
H	0.27340	0.07354	5.82489
H	1.05115	1.80926	1.98170
Si	-2.45100	-2.07567	-0.90249
H	-3.09529	-2.98174	0.09505
H	-1.85856	-2.93509	-1.96800
H	-3.53213	-1.26288	-1.53074
H	-0.64252	1.90329	-1.61987
H	0.32578	2.54280	-0.31179
H	-1.38677	2.19633	-0.05821
H	1.84606	-0.93101	-1.54499
H	1.92066	-1.70118	0.03254
H	2.54393	-0.06685	-0.18599

py–AlMe$_2$OSiH$_3$(THF), B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Al	0.04128	0.43019	-1.16409
C	-0.49400	2.33311	-1.00013
C	1.95055	-0.11101	-1.29433
O	-1.21621	-0.78685	-1.37883
N	-0.00219	-0.01258	0.97096
C	0.23906	-1.28239	1.31626
C	0.25134	-1.70747	2.63316
C	0.00120	-0.77909	3.63555
C	-0.25293	0.53715	3.27886
C	-0.24581	0.87892	1.93438
H	0.42347	-1.96560	0.49945
H	0.44883	-2.74425	2.86375
H	-0.45517	1.29223	4.02465
H	0.00220	-1.07751	4.67507
H	-0.44049	1.89019	1.60807

Si	-2.55781	-1.61801	-1.11247
H	-2.69877	-2.02619	0.31444
H	-2.57936	-2.86572	-1.92532
H	-3.77852	-0.84369	-1.47183
H	-2.10648	-0.29866	-5.63473
H	0.91957	0.07836	-5.17713
H	-1.31878	1.66208	-4.64455
C	-1.80526	-0.47798	-4.60319
C	0.56533	-0.39561	-4.25519
H	-0.39610	-1.95131	-5.44422
C	-1.36331	0.83613	-3.93151
O	-0.03128	0.60992	-3.41913
C	-0.55922	-1.38341	-4.52935
H	-2.65045	-0.92419	-4.08468
H	1.41262	-0.81076	-3.72117
H	-1.98904	1.12095	-3.09249
H	-0.64685	-2.07851	-3.69746
H	2.47529	0.07454	-0.35269
H	2.48785	0.44729	-2.06574
H	2.09055	-1.17430	-1.51859
H	0.18115	2.88810	-0.33960
H	-1.50711	2.47521	-0.60930
H	-0.45123	2.84363	-1.96469

py–$AlMe_2OSiH_3$(THF), PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Al	0.04072	0.41773	-1.16337
C	-0.49031	2.32037	-0.99648
C	1.94683	-0.12683	-1.30345
O	-1.21486	-0.79764	-1.37759
N	0.00342	-0.01188	0.95449
C	0.26450	-1.27152	1.30401
C	0.27092	-1.69379	2.61914
C	-0.00760	-0.76993	3.61395
C	-0.28279	0.53746	3.25209
C	-0.26732	0.87391	1.90939
H	0.47086	-1.95318	0.48789
H	0.48685	-2.72740	2.85389
H	-0.50896	1.29168	3.99387
H	-0.01185	-1.06616	4.65574
H	-0.47867	1.88173	1.57541
Si	-2.56054	-1.61417	-1.10622
H	-2.69831	-2.02883	0.32453
H	-2.60141	-2.86272	-1.92661
H	-3.78083	-0.82460	-1.45519
H	-2.10342	-0.27956	-5.61140
H	0.90784	0.09246	-5.16165
H	-1.29902	1.66570	-4.62211
C	-1.79815	-0.46493	-4.58089
C	0.55818	-0.38753	-4.23899
H	-0.40084	-1.93637	-5.43183
C	-1.34732	0.83781	-3.90848
O	-0.02967	0.60323	-3.39920
C	-0.56188	-1.37013	-4.51442
H	-2.64549	-0.90998	-4.06091
H	1.41138	-0.80697	-3.71295
H	-1.97470	1.12900	-3.06932
H	-0.64878	-2.06853	-3.68281
H	2.47998	0.06311	-0.36642
H	2.47792	0.43092	-2.08095
H	2.08779	-1.19128	-1.52572
H	0.19017	2.87085	-0.33621

H	-1.50293	2.46735	-0.60409
H	-0.44617	2.83422	-1.96029
py–AlMe$_3$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Al	-0.00352	-0.00448	-0.15774
N	0.02194	-0.01096	1.90500
C	-1.08998	-0.37034	2.56080
C	-1.16388	-0.37582	3.94195
C	-0.04560	0.00507	4.67316
C	1.10628	0.37488	3.99349
C	1.10126	0.35355	2.60836
H	-1.93264	-0.65323	1.94574
H	-2.08073	-0.67223	4.42985
H	1.99848	0.67728	4.52187
H	-0.07316	0.01318	5.75416
H	1.96956	0.63071	2.02869
C	1.82917	0.61712	-0.60509
H	2.06388	1.61464	-0.21820
H	1.93414	0.68620	-1.69300
H	2.62052	-0.06133	-0.26899
C	-1.47606	1.28650	-0.48829
H	-1.24774	2.28222	-0.09443
H	-2.43241	0.98075	-0.05064
H	-1.65838	1.41001	-1.56072
C	-0.39960	-1.91363	-0.53476
H	0.31909	-2.58824	-0.05817
H	-0.34847	-2.11641	-1.60957
H	-1.39770	-2.22796	-0.21180
py–AlMe$_3$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Al	-0.00439	-0.00457	-0.15155
N	0.02215	-0.00976	1.90255
C	-1.08546	-0.36823	2.55519
C	-1.16064	-0.37579	3.93359
C	-0.04443	0.00353	4.66298
C	1.10474	0.37357	3.98496
C	1.09753	0.35310	2.60252
H	-1.92869	-0.65098	1.93682
H	-2.07897	-0.67333	4.42116
H	1.99872	0.67606	4.51320
H	-0.07153	0.01042	5.74560
H	1.96595	0.63089	2.01883
C	1.82643	0.61682	-0.59286
H	2.06018	1.61592	-0.20771
H	1.93115	0.68484	-1.68155
H	2.61851	-0.06182	-0.25683
C	-1.47416	1.28381	-0.48413
H	-1.24625	2.28088	-0.09206
H	-2.43283	0.97931	-0.04928
H	-1.65272	1.40419	-1.55818
C	-0.40060	-1.91053	-0.52544
H	0.31789	-2.58611	-0.04883
H	-0.34832	-2.11168	-1.60113
H	-1.40000	-2.22457	-0.20439
py–AlMe$_3$(THF), B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Al	0.05975	0.28139	-1.07095
C	-0.35787	2.22950	-0.97285
C	1.96857	-0.26787	-1.30774
C	-1.41162	-1.05977	-1.31038
N	0.09266	-0.02584	1.08172
C	0.67203	-1.13152	1.56220
C	0.64693	-1.46347	2.90656

C	-0.00563	-0.61515	3.79165
C	-0.60809	0.53154	3.29481
C	-0.53620	0.78898	1.93419
H	1.16859	-1.75777	0.83456
H	1.13023	-2.36780	3.24686
H	-1.12578	1.22146	3.94543
H	-0.04277	-0.84402	4.84804
H	-0.98773	1.67008	1.50224
H	-2.04333	0.25383	-5.92488
H	1.02813	-0.00081	-5.19735
H	-0.97572	1.90366	-4.67011
C	-1.83747	-0.09746	-4.91457
C	0.47814	-0.49072	-4.38554
H	-0.60371	-1.64541	-5.89198
C	-1.22460	1.03034	-4.06075
O	-0.01952	0.50445	-3.48675
C	-0.76399	-1.20771	-4.90780
H	-2.77340	-0.45398	-4.48987
H	1.16150	-1.12301	-3.82634
H	-1.85803	1.34787	-3.23796
H	-1.04602	-2.00334	-4.22128
H	2.58534	0.01278	-0.44791
H	2.41705	0.21834	-2.17788
H	2.10397	-1.34625	-1.44995
H	0.27282	2.74069	-0.23734
H	-1.39761	2.45725	-0.71188
H	-0.16415	2.71894	-1.93030
H	-1.84810	-1.39589	-0.36523
H	-1.05589	-1.95936	-1.82403
H	-2.24191	-0.67202	-1.90852

py–AlMe$_3$(THF), PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Al	0.05769	0.29179	-1.12090
C	-0.35446	2.23961	-0.99462
C	1.96744	-0.26312	-1.33733
C	-1.43564	-1.04142	-1.24273
N	0.10600	-0.01827	1.03332
C	0.68112	-1.12269	1.50666
C	0.63937	-1.47254	2.84367
C	-0.02758	-0.63969	3.72768
C	-0.62604	0.50858	3.23750
C	-0.53569	0.78030	1.88366
H	1.19099	-1.73767	0.77511
H	1.12211	-2.38064	3.17927
H	-1.15675	1.18967	3.88934
H	-0.07926	-0.88230	4.78204
H	-0.98594	1.66554	1.45248
H	-1.95907	0.24958	-5.89788
H	1.00724	0.00304	-5.15905
H	-1.00251	1.90926	-4.58634
C	-1.81165	-0.10288	-4.87639
C	0.47782	-0.48343	-4.32982
H	-0.60168	-1.70495	-5.77788
C	-1.22769	1.01330	-3.99918
O	-0.01586	0.50972	-3.44193
C	-0.75833	-1.21627	-4.81630
H	-2.77656	-0.44423	-4.50326
H	1.18061	-1.09987	-3.77385
H	-1.87128	1.29680	-3.16832
H	-1.04391	-1.97502	-4.08750
H	2.56671	0.00432	-0.46004

H	2.43451	0.24089	-2.18898
H	2.11114	-1.33904	-1.49567
H	0.27057	2.73218	-0.24057
H	-1.39676	2.46903	-0.74262
H	-0.14422	2.75000	-1.93893
H	-2.06797	-1.01561	-0.34871
H	-1.05231	-2.06702	-1.31627
H	-2.10911	-0.90337	-2.09408

py–$AlCl_2OSi(OSiH_3)_3$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Al	-0.05038	-0.04947	-0.04209
Cl	-0.51803	1.92961	-0.66806
Cl	1.87740	-0.76490	-0.56578
O	-1.30464	-1.18734	-0.24405
N	0.02811	0.07945	1.93950
C	0.22190	-1.06311	2.62301
C	0.24811	-1.09052	4.00330
C	0.07666	0.09816	4.70114
C	-0.11769	1.27550	3.99231
C	-0.13854	1.22991	2.61062
H	0.33976	-1.95933	2.03277
H	0.39450	-2.02999	4.51447
H	-0.25693	2.22016	4.49622
H	0.09052	0.10518	5.78230
H	-0.29956	2.10809	2.00330
Si	-2.52709	-2.02838	0.32139
O	-3.63705	-1.07893	1.05808
O	-1.97334	-3.07916	1.44759
O	-3.28813	-2.85421	-0.84003
Si	-3.74977	-0.00929	2.28812
Si	-4.77105	-3.18742	-1.45169
Si	-2.46922	-4.16513	2.56335
H	-3.21654	1.30985	1.88160
H	-5.16724	0.12456	2.67927
H	-2.96289	-0.48922	3.45172
H	-1.40648	-4.26772	3.59056
H	-2.68443	-5.49259	1.94879
H	-3.72261	-3.71410	3.21103
H	-4.60287	-4.14443	-2.56407
H	-5.41953	-1.95327	-1.94622
H	-5.62688	-3.79489	-0.40559

py–$AlCl_2OSi(OSiH_3)_3$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Al	-0.05707	-0.05035	-0.02980
Cl	-0.51625	1.92190	-0.65558
Cl	1.85772	-0.77337	-0.55737
O	-1.31380	-1.18331	-0.22281
N	0.03965	0.08948	1.94340
C	0.24191	-1.04384	2.62885
C	0.28766	-1.06266	4.00662
C	0.12571	0.12889	4.69602
C	-0.07799	1.29862	3.98289
C	-0.11713	1.24083	2.60457
H	0.35424	-1.94563	2.04055
H	0.44315	-1.99978	4.52272
H	-0.20967	2.24899	4.48114
H	0.15523	0.14418	5.77842
H	-0.28408	2.11592	1.98976
Si	-2.53411	-2.03449	0.32242
O	-3.66046	-1.10072	1.04623
O	-1.98513	-3.08647	1.44357
O	-3.27072	-2.85737	-0.85274

Si	-3.77827	-0.03536	2.27537
Si	-4.75710	-3.16891	-1.45845
Si	-2.48474	-4.17060	2.55443
H	-3.24572	1.29119	1.87074
H	-5.20196	0.09503	2.66306
H	-2.99196	-0.51629	3.44679
H	-1.42316	-4.27447	3.58982
H	-2.69687	-5.50242	1.93641
H	-3.74566	-3.72017	3.19973
H	-4.60212	-4.12386	-2.58080
H	-5.39676	-1.92153	-1.94580
H	-5.61986	-3.77601	-0.41083

py–AlMe$_2$OSi(OSiH$_3$)$_3$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Al	1.29638	0.85445	0.87635
C	0.69329	2.68321	1.29438
C	3.15891	0.49592	0.36036
O	0.13330	-0.08972	-0.02340
N	1.11334	-0.12237	2.66998
C	1.24464	-1.45753	2.69593
C	1.10346	-2.18668	3.86257
C	0.82414	-1.51285	5.04417
C	0.69216	-0.13163	5.01619
C	0.84033	0.52806	3.80914
H	1.44392	-1.93515	1.74863
H	1.20463	-3.26127	3.83620
H	0.46830	0.43097	5.91038
H	0.70508	-2.05691	5.97097
H	0.73167	1.59910	3.72698
Si	-1.13541	-1.03045	-0.04911
O	-2.33006	-0.53113	0.95925
O	-0.72196	-2.53886	0.44541
O	-1.79579	-1.13236	-1.52714
H	0.64084	3.28396	0.38169
H	1.36545	3.21808	1.97289
H	-0.30793	2.70606	1.73473
H	3.38243	0.90303	-0.63013
H	3.38555	-0.57378	0.31410
H	3.87437	0.94760	1.05436
Si	-2.64913	-0.08567	2.49339
Si	-3.25696	-1.16278	-2.26165
Si	-1.31021	-3.90381	1.11591
H	-2.16105	1.28554	2.76490
H	-4.10937	-0.13751	2.71392
H	-1.98128	-1.00647	3.44583
H	-0.20117	-4.57655	1.83330
H	-1.83995	-4.81841	0.08089
H	-2.38222	-3.59350	2.08997
H	-3.05245	-1.52089	-3.68102
H	-3.91713	0.15979	-2.17943
H	-4.13470	-2.17477	-1.62611

py–AlMe$_2$OSi(OSiH$_3$)$_3$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Al	1.29053	0.84747	0.88913
C	0.70577	2.67741	1.31481
C	3.14042	0.48321	0.34511
O	0.11468	-0.08804	0.00240
N	1.12516	-0.12135	2.67823
C	1.25966	-1.45075	2.70777
C	1.13264	-2.17532	3.87614
C	0.86249	-1.49814	5.05462
C	0.72674	-0.12027	5.02216

C	0.86223	0.53162	3.81221
H	1.45347	-1.93121	1.75745
H	1.23858	-3.25118	3.85324
H	0.51065	0.44740	5.91681
H	0.75429	-2.03911	5.98645
H	0.75222	1.60459	3.72359
Si	-1.14565	-1.03347	-0.04680
O	-2.35956	-0.54848	0.93915
O	-0.73028	-2.53984	0.43844
O	-1.77881	-1.12837	-1.53390
H	0.64472	3.27308	0.39836
H	1.39167	3.21294	1.97998
H	-0.29057	2.71116	1.76783
H	3.34518	0.89618	-0.64770
H	3.36224	-0.58749	0.28656
H	3.87027	0.92881	1.02857
Si	-2.67840	-0.08936	2.46627
Si	-3.24122	-1.15952	-2.25835
Si	-1.32266	-3.90021	1.10640
H	-2.19606	1.29255	2.72419
H	-4.14308	-0.14585	2.68751
H	-2.00549	-1.00087	3.43374
H	-0.21186	-4.58195	1.82310
H	-1.85912	-4.81485	0.06794
H	-2.39620	-3.58733	2.08598
H	-3.04106	-1.50680	-3.68588
H	-3.90999	0.16324	-2.16391
H	-4.11479	-2.18340	-1.62486

$AlCl_4^-$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Al	0.00005	0.00030	-0.00031
Cl	-0.00001	-0.00002	2.16549
Cl	-0.03263	2.04197	-0.72172
Cl	1.78429	-0.99294	-0.72176
Cl	-1.75169	-1.04925	-0.72177

$AlCl_4^-$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Al	-0.00003	-0.00007	-0.00001
Cl	0.00004	0.00012	2.15559
Cl	-0.03240	2.03204	-0.71842
Cl	1.77606	-0.98797	-0.71854
Cl	-1.74369	-1.04414	-0.71861

$AlCl_3OSiH_3^-$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Al	-0.02722	-0.01579	-0.03416
Cl	-1.79180	0.99300	-0.80129
Cl	0.02793	-2.04829	-0.79925
Cl	1.75321	1.04943	-0.66328
O	-0.09222	-0.05215	1.68864
Si	-0.69034	-0.41587	3.12466
H	0.17215	0.12007	4.21787
H	-0.79755	-1.88480	3.35753
H	-2.05165	0.14983	3.34828

$AlCl_3OSiH_3^-$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Al	-0.02294	-0.01339	-0.03208
Cl	-1.78351	0.98726	-0.78959
Cl	0.02715	-2.03824	-0.78836
Cl	1.74543	1.04471	-0.67156
O	-0.07598	-0.04285	1.68960
Si	-0.70112	-0.42171	3.10645
H	0.14416	0.10289	4.22456
H	-0.81462	-1.89734	3.32370
H	-2.06998	0.14457	3.31318

$AlCl_2(OSiH_3)_2^-$, B3LYP-D3/cc-pVTZ	*x*	*y*	*z*
Al	-0.06273	0.00918	-0.04169
Cl	-1.73069	1.13895	-0.87102
Cl	-0.29320	-2.09874	-0.56664
O	-0.05777	0.16792	1.67983
O	1.42174	0.59375	-0.70588
Si	-0.65774	-0.18088	3.12004
H	-0.59733	0.99976	4.03134
H	0.10070	-1.26830	3.80479
H	-2.08325	-0.61536	3.08861
Si	2.55975	0.62206	-1.82745
H	3.14941	1.98644	-1.96456
H	2.07444	0.23556	-3.18267
H	3.69881	-0.28794	-1.50929
$AlCl_2(OSiH_3)_2^-$, PBE0-D3/cc-pVTZ	*x*	*y*	*z*
Al	-0.05783	0.02066	-0.03641
Cl	-1.71937	1.12986	-0.87648
Cl	-0.28386	-2.08265	-0.53521
O	-0.05258	0.20094	1.68149
O	1.42511	0.60337	-0.69954
Si	-0.66920	-0.20933	3.09534
H	-0.53267	0.90646	4.08428
H	0.02161	-1.38786	3.70629
H	-2.12395	-0.55077	3.04382
Si	2.54037	0.61328	-1.83941
H	3.26333	1.92386	-1.87418
H	1.99607	0.39646	-3.21512
H	3.59070	-0.43169	-1.62904
$AlCl(OSiH_3)_3^-$, B3LYP-D3/cc-pVTZ	*x*	*y*	*z*
Al	-1.08678	0.32977	0.76137
Cl	-2.25417	1.71760	-0.44914
O	-2.08057	-0.27724	2.04500
O	0.28396	1.17342	1.41553
O	-0.54160	-0.98038	-0.23319
Si	1.71875	1.25009	2.10665
H	2.57946	2.30325	1.49134
H	2.49079	-0.02477	2.01601
H	1.63709	1.58362	3.55986
Si	0.04119	-2.16926	-1.11313
H	1.32701	-1.81545	-1.78476
H	-0.89080	-2.59185	-2.20006
H	0.32003	-3.39607	-0.30841
Si	-2.68307	-1.08820	3.27415
H	-3.01092	-2.50435	2.93240
H	-3.94871	-0.48198	3.78297
H	-1.75442	-1.14823	4.44217
$AlCl(OSiH_3)_3^-$, PBE0-D3/cc-pVTZ	*x*	*y*	*z*
Al	-1.08505	0.33122	0.75652
Cl	-2.25330	1.70778	-0.44501
O	-2.07240	-0.27533	2.04084
O	0.28163	1.17971	1.40448
O	-0.54132	-0.97692	-0.23533
Si	1.70399	1.23838	2.11510
H	2.57074	2.31600	1.54126
H	2.48565	-0.03372	1.99608
H	1.60407	1.52808	3.58117
Si	0.03786	-2.16417	-1.11324
H	1.33670	-1.81828	-1.77380
H	-0.89023	-2.57504	-2.21402
H	0.29952	-3.40113	-0.31000

Si	-2.67053	-1.07719	3.27321
H	-2.95995	-2.51146	2.95320
H	-3.96159	-0.49192	3.75503
H	-1.75517	-1.09387	4.45883

$Al(OSiH_3)_4^-$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Al	-0.08304	-0.00606	-0.03301
O	-0.06754	0.04353	1.70567
O	-0.69415	-1.54748	-0.57335
O	1.53836	0.22215	-0.62231
O	-1.11357	1.26559	-0.64229
Si	2.63264	0.61716	-1.71015
H	2.05024	1.10790	-2.99489
H	3.54398	1.69868	-1.22926
H	3.51787	-0.53127	-2.06925
Si	-1.97591	1.92708	-1.80958
H	-1.28726	3.09395	-2.43828
H	-3.28537	2.44423	-1.31076
H	-2.29580	0.98433	-2.92163
Si	-1.75793	-2.66368	-0.97049
H	-2.06185	-3.59265	0.15871
H	-1.27557	-3.52369	-2.09237
H	-3.06959	-2.10337	-1.41215
Si	-0.60048	-0.29162	3.16871
H	-0.81281	-1.75092	3.40320
H	-1.90077	0.37102	3.48770
H	0.35900	0.16072	4.22030

$Al(OSiH_3)_4^-$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Al	-0.08089	-0.00476	-0.03209
O	-0.05705	0.04984	1.70302
O	-0.69297	-1.54372	-0.56556
O	1.53706	0.21558	-0.62288
O	-1.10750	1.26774	-0.63548
Si	2.62068	0.62054	-1.71260
H	2.02985	1.14980	-2.98356
H	3.55484	1.68167	-1.21677
H	3.48913	-0.53397	-2.10940
Si	-1.96720	1.92000	-1.80545
H	-1.27660	3.08718	-2.44209
H	-3.28081	2.44161	-1.30916
H	-2.28810	0.96923	-2.91677
Si	-1.75426	-2.65770	-0.96149
H	-2.08373	-3.57009	0.17999
H	-1.25671	-3.54062	-2.06455
H	-3.05942	-2.09637	-1.43573
Si	-0.61019	-0.29758	3.15211
H	-0.82610	-1.76307	3.37383
H	-1.91846	0.36408	3.46119
H	0.33761	0.14718	4.22357

$AlCl_3OSi(OSiH_3)_3^-$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Al	-0.10638	-0.02870	0.07394
Cl	-0.25169	-0.04060	2.25542
Cl	-0.09094	1.99891	-0.65699
Cl	1.67695	-1.08076	-0.53488
O	-1.52094	-0.86110	-0.48404
Si	-2.62281	-1.84463	0.08885
O	-3.71236	-1.08496	1.04610
O	-2.00601	-3.09302	0.93241
O	-3.48758	-2.50851	-1.13142
Si	-3.92051	0.26840	1.93767
Si	-4.96120	-3.10639	-1.44891

Si	-1.09013	-3.60147	2.18053
H	-3.16213	1.41433	1.39956
H	-5.37076	0.59730	1.90035
H	-3.55294	0.03181	3.35167
H	0.33973	-3.30070	1.97825
H	-1.25371	-5.07764	2.26619
H	-1.55448	-3.02516	3.46349
H	-4.92400	-3.79466	-2.76183
H	-5.98477	-2.03439	-1.51833
H	-5.39508	-4.08870	-0.42349

$AlCl_3OSi(OSiH_3)_3^-$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Al	-0.10925	-0.03381	0.07438
Cl	-0.25956	-0.05397	2.24541
Cl	-0.10029	1.98806	-0.64597
Cl	1.67438	-1.06649	-0.53279
O	-1.51777	-0.86790	-0.49010
Si	-2.61761	-1.84462	0.08879
O	-3.70678	-1.08705	1.04125
O	-2.00882	-3.09370	0.93020
O	-3.47938	-2.50749	-1.12954
Si	-3.90679	0.26946	1.92325
Si	-4.95562	-3.09645	-1.43236
Si	-1.09645	-3.59294	2.17988
H	-3.14220	1.41436	1.37555
H	-5.36033	0.60442	1.88594
H	-3.53734	0.03874	3.34318
H	0.34034	-3.29831	1.97519
H	-1.26566	-5.07236	2.27613
H	-1.56030	-3.00508	3.46377
H	-4.93290	-3.78604	-2.75016
H	-5.97889	-2.01702	-1.49312
H	-5.38704	-4.08125	-0.40146

Table S51 Equilibrium geometries of structures with Si as the central atom.

$SiCl_4$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Si	0.00001	0.00017	0.00007
Cl	0.96551	1.21896	1.31089
Cl	1.25822	-1.47956	-0.60300
Cl	-1.62476	-0.82031	0.90744
Cl	-0.59898	1.08079	-1.61539
$SiCl_4$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Si	-0.00002	0.00000	0.00003
Cl	0.95994	1.21191	1.30338
Cl	1.25118	-1.47102	-0.59961
Cl	-1.61554	-0.81543	0.90229
Cl	-0.59557	1.07456	-1.60609
$SiCl_3OSiH_3$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Si	-1.16578	-0.06508	-0.57671
Cl	-1.33142	-2.00481	-1.17233
Cl	-2.80190	0.43553	0.54191
Cl	-1.09327	1.13554	-2.22037
O	0.16640	0.11811	0.28899
Si	0.87942	0.61935	1.69363
H	2.33293	0.67202	1.45092
H	0.57008	-0.34814	2.76527
H	0.36701	1.95644	2.05538
$SiCl_3OSiH_3$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Si	-1.16617	0.00743	-0.59668
Cl	-1.61096	-1.96413	-0.74455
Cl	-2.72583	0.96935	0.27836
Cl	-0.87168	0.76270	-2.45072
O	0.15932	0.20323	0.27024
Si	0.87568	0.55895	1.71085
H	2.15932	1.23337	1.41585
H	1.11502	-0.70273	2.44913
H	-0.01124	1.45083	2.49422
$SiCl_2(OSiH_3)_2$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Si	-1.14475	-0.42997	-0.62896
O	0.06362	-0.38521	0.42301
O	-1.23268	-1.88988	-1.28103
Cl	-2.90710	0.01566	0.31923
Cl	-0.84467	0.97027	-2.09441
Si	0.78789	0.53073	1.59113
H	2.21284	0.68341	1.23767
H	0.65852	-0.17082	2.88359
H	0.13642	1.85502	1.66448
Si	-2.03804	-2.88800	-2.31908
H	-1.71529	-4.27661	-1.93925
H	-1.58922	-2.61898	-3.70030
H	-3.49220	-2.65015	-2.20676
$SiCl_2(OSiH_3)_2$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Si	-1.06514	-0.40621	-0.70357
O	0.07820	-0.39368	0.41575
O	-1.27163	-1.90201	-1.22800
Cl	-2.80953	0.30212	0.07689
Cl	-0.53369	0.80197	-2.25384
Si	0.73322	0.50755	1.62948
H	2.13764	0.81766	1.27614
H	0.68710	-0.28939	2.87683
H	-0.04006	1.76183	1.79432
Si	-2.08215	-2.89304	-2.26136
H	-1.48827	-4.24283	-2.13594

H	-1.93385	-2.39225	-3.64886
H	-3.51650	-2.92626	-1.88851
$SiCl(OSiH_3)_3$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Si	-1.35078	-0.09252	-1.25389
Cl	-1.65474	1.46699	-2.56530
O	-0.30284	0.37208	-0.12808
O	-0.76220	-1.35225	-2.06660
O	-2.75956	-0.48927	-0.58637
Si	1.19602	0.97359	0.18593
H	1.45610	2.14432	-0.67824
H	2.21289	-0.06877	-0.06939
H	1.23026	1.37291	1.60666
Si	-1.13195	-2.46264	-3.22544
H	-2.50018	-2.97936	-3.00588
H	-0.15250	-3.56183	-3.11830
H	-1.04585	-1.83773	-4.56206
Si	-4.11855	0.07333	0.15175
H	-5.00456	0.70227	-0.84994
H	-3.75828	1.06588	1.18744
H	-4.79831	-1.08037	0.77318
$SiCl(OSiH_3)_3$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Si	-1.34597	-0.10507	-1.26946
Cl	-1.61937	1.46175	-2.55799
O	-0.31639	0.33841	-0.12217
O	-0.75094	-1.35706	-2.08222
O	-2.76267	-0.50588	-0.62799
Si	1.16042	0.98281	0.19198
H	1.37900	2.18033	-0.65551
H	2.21321	-0.02397	-0.08677
H	1.18965	1.36041	1.62364
Si	-1.13616	-2.47848	-3.21947
H	-2.49301	-3.01798	-2.95609
H	-0.13278	-3.56432	-3.13385
H	-1.09918	-1.86034	-4.56699
Si	-4.08696	0.08536	0.14287
H	-4.95090	0.80187	-0.82616
H	-3.67392	1.01490	1.22338
H	-4.81906	-1.06612	0.71827
$Si(OSiH_3)_4$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Si	-1.73301	0.73359	-2.19691
O	-0.41166	1.23519	-1.41206
O	-1.45920	-0.71055	-2.88331
O	-2.98593	0.62174	-1.17345
O	-2.07866	1.81243	-3.33938
Si	0.63084	0.85098	-0.20741
H	1.98736	1.28879	-0.59286
H	0.62364	-0.61465	0.01306
H	0.22174	1.52839	1.04189
Si	-1.14593	-2.30006	-2.64065
H	-1.84056	-2.76698	-1.41874
H	0.30921	-2.50873	-2.47923
H	-1.63323	-3.05808	-3.81078
Si	-3.64290	-0.26071	0.04152
H	-4.55226	0.61064	0.81265
H	-2.57207	-0.77359	0.92756
H	-4.39973	-1.40397	-0.51359
Si	-3.05444	2.10806	-4.62453
H	-3.14049	3.57109	-4.80821
H	-4.40553	1.55495	-4.37899
H	-2.48576	1.48627	-5.84000

$Si(OSiH_3)_4$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Si	-1.73163	0.73206	-2.19352
O	-0.41732	1.24090	-1.40940
O	-1.45228	-0.70478	-2.88293
O	-2.98612	0.61896	-1.17862
O	-2.07440	1.81101	-3.33190
Si	0.62406	0.85349	-0.20986
H	1.98345	1.29857	-0.59497
H	0.62233	-0.61849	0.00485
H	0.21243	1.52514	1.04743
Si	-1.14281	-2.29189	-2.64438
H	-1.83668	-2.76224	-1.41674
H	0.31726	-2.50518	-2.48860
H	-1.63795	-3.04888	-3.81785
Si	-3.64181	-0.26237	0.03283
H	-4.56156	0.60939	0.80015
H	-2.56993	-0.77064	0.92912
H	-4.39417	-1.41422	-0.52405
Si	-3.05168	2.10162	-4.61180
H	-3.09572	3.56621	-4.83190
H	-4.42119	1.59488	-4.34032
H	-2.51285	1.43126	-5.82097
$SiCl_3OSi(OSiH_3)_3$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Si	-0.83676	-0.39991	0.09898
Cl	-0.43903	-2.39326	-0.05051
Cl	-2.33506	-0.13994	1.46725
Cl	-1.43232	0.31400	-1.70673
O	0.47064	0.39294	0.57413
Si	1.37091	0.68344	1.90433
O	2.90957	0.71055	1.43959
O	1.14495	-0.49133	2.98775
O	0.91038	2.10608	2.50197
Si	0.22428	-1.10863	4.20138
H	-0.51572	-2.28410	3.70168
H	-0.72638	-0.08143	4.67855
H	1.12294	-1.50909	5.30370
Si	0.93467	3.21687	3.70643
H	-0.29146	4.03387	3.61523
H	2.12729	4.07865	3.56051
H	0.98510	2.53232	5.01819
Si	4.46966	0.70711	1.95057
H	5.32160	1.14618	0.82837
H	4.85587	-0.65420	2.37824
H	4.62361	1.63908	3.09156
$SiCl_3OSi(OSiH_3)_3$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Si	-0.83634	-0.39270	0.09703
Cl	-0.45145	-2.37599	-0.06306
Cl	-2.33336	-0.13509	1.44915
Cl	-1.41686	0.32965	-1.69772
O	0.47103	0.39189	0.57771
Si	1.36689	0.67708	1.90693
O	2.90089	0.70991	1.43828
O	1.15200	-0.50035	2.98456
O	0.90351	2.09404	2.50595
Si	0.23734	-1.11008	4.20170
H	-0.50699	-2.29224	3.70847
H	-0.71632	-0.07807	4.67973
H	1.14219	-1.50626	5.30679
Si	0.93599	3.20814	3.70178
H	-0.29569	4.02571	3.61391

H	2.13022	4.07367	3.54225
H	0.99638	2.52981	5.02206
Si	4.45469	0.70926	1.95565
H	5.31609	1.12121	0.82423
H	4.83497	-0.64863	2.41534
H	4.60959	1.66820	3.08044
Me_3SiCl, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Si	-0.01853	0.02886	-0.02249
Cl	1.27653	-1.49301	-0.64872
C	0.92360	1.10949	1.17522
C	-1.48505	-0.78751	0.79877
H	-2.21092	-0.03447	1.11465
H	-1.17823	-1.35428	1.67860
H	-1.98395	-1.47193	0.11178
C	-0.53024	0.97809	-1.54792
H	-1.19533	1.80427	-1.28570
H	-1.05539	0.33039	-2.25121
H	0.34040	1.39258	-2.05777
H	1.22295	0.54566	2.05954
H	0.30212	1.94725	1.50021
H	1.82411	1.51564	0.71269
Me_3SiCl, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Si	-0.01654	0.02641	-0.02338
Cl	1.27041	-1.48583	-0.64594
C	0.92340	1.10381	1.17089
C	-1.47861	-0.78819	0.79555
H	-2.20435	-0.03403	1.11137
H	-1.17000	-1.35499	1.67568
H	-1.97683	-1.47257	0.10678
C	-0.52613	0.97249	-1.54507
H	-1.19168	1.79898	-1.28228
H	-1.05116	0.32285	-2.24785
H	0.34638	1.38644	-2.05381
H	1.22211	0.53825	2.05527
H	0.30095	1.94187	1.49547
H	1.82420	1.50925	0.70651
$Me_3SiOSiH_3$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Si	0.12849	-0.14920	0.00380
O	1.20389	-1.33079	-0.41619
C	0.94396	0.97323	1.26021
C	-1.37062	-0.99257	0.73249
H	-2.12601	-0.25911	1.02319
H	-1.10639	-1.57086	1.61959
H	-1.82501	-1.67330	0.01060
C	-0.33248	0.81977	-1.53045
H	-1.02437	1.63096	-1.29321
H	-0.81293	0.17950	-2.27284
H	0.55013	1.26409	-1.99550
H	1.22554	0.41899	2.15751
H	0.27570	1.78233	1.56315
H	1.84929	1.42661	0.85111
Si	2.57492	-1.73711	-1.19440
H	2.77735	-3.19760	-1.07694
H	3.74107	-1.03736	-0.60215
H	2.49236	-1.37319	-2.63001
$Me_3SiOSiH_3$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Si	0.13109	-0.15291	0.00334
O	1.19610	-1.34249	-0.40897
C	0.94931	0.96557	1.25393
C	-1.36822	-0.98564	0.73060

H	-2.12124	-0.24751	1.01786
H	-1.10562	-1.56222	1.62012
H	-1.82303	-1.66696	0.00851
C	-0.32157	0.80913	-1.53162
H	-1.00990	1.62490	-1.29672
H	-0.80501	0.16665	-2.27115
H	0.56444	1.24776	-1.99742
H	1.22559	0.41070	2.15332
H	0.28399	1.77950	1.55256
H	1.85831	1.41253	0.84390
Si	2.56704	-1.72287	-1.19269
H	2.78723	-3.18659	-1.09025
H	3.73141	-1.01438	-0.59505
H	2.47852	-1.34479	-2.62939

$Me_3SiOSi(OSiH_3)_3$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Si	-0.81479	1.43320	0.12412
O	-0.06369	-0.04078	0.00487
C	0.24915	2.54784	1.18362
C	-2.47807	1.12470	0.91318
H	-3.04079	2.05473	1.01833
H	-2.36705	0.68583	1.90636
H	-3.07379	0.43865	0.30837
C	-1.00899	2.14450	-1.59480
H	-1.53088	3.10345	-1.56639
H	-1.57967	1.46897	-2.23452
H	-0.03799	2.30665	-2.06667
H	0.40336	2.11486	2.17355
H	-0.21152	3.52953	1.31275
H	1.23105	2.69398	0.72955
Si	1.30044	-0.72105	-0.48197
O	1.25512	-2.29785	-0.12130
O	2.56723	-0.03251	0.26921
O	1.46911	-0.53135	-2.08889
Si	4.17538	-0.04786	0.56539
Si	2.02382	-3.73878	-0.18894
Si	2.60314	-0.59282	-3.27024
H	4.90806	-0.51000	-0.63642
H	4.47548	-0.95758	1.69241
H	4.60268	1.32508	0.90581
H	1.80307	-4.37161	-1.50813
H	1.48906	-4.61086	0.87662
H	3.47993	-3.54745	0.01321
H	3.49760	0.58272	-3.17642
H	1.91657	-0.59342	-4.57767
H	3.41304	-1.82517	-3.12805

$Me_3SiOSi(OSiH_3)_3$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Si	-0.80926	1.42837	0.12266
O	-0.05830	-0.04193	0.00334
C	0.24845	2.54224	1.18056
C	-2.46716	1.11500	0.90923
H	-3.03222	2.04421	1.01524
H	-2.35339	0.67487	1.90226
H	-3.05995	0.42742	0.30206
C	-1.00529	2.13904	-1.59089
H	-1.53013	3.09707	-1.55991
H	-1.57553	1.46180	-2.23052
H	-0.03391	2.30431	-2.06281
H	0.40264	2.10809	2.17084
H	-0.21615	3.52282	1.30940
H	1.23073	2.69117	0.72605

Si	1.30368	-0.71908	-0.48298
O	1.25254	-2.29173	-0.12161
O	2.56601	-0.03107	0.26771
O	1.46824	-0.52976	-2.08653
Si	4.17051	-0.04703	0.56339
Si	2.01638	-3.73099	-0.18832
Si	2.60017	-0.59254	-3.26454
H	4.90837	-0.50960	-0.64182
H	4.47165	-0.96017	1.69396
H	4.59852	1.33032	0.90636
H	1.79361	-4.36636	-1.51150
H	1.47664	-4.60396	0.88060
H	3.47837	-3.54511	0.01544
H	3.49851	0.58675	-3.17248
H	1.91094	-0.59338	-4.57602
H	3.41316	-1.82944	-3.12324

Me_2SiCl_2, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Si	0.02216	0.03986	-0.04666
Cl	1.29116	-1.48040	-0.65489
Cl	-1.61639	-0.83507	0.87074
C	0.90729	1.09264	1.20021
C	-0.56000	0.96203	-1.54917
H	-1.25397	1.75399	-1.26300
H	-1.07083	0.29004	-2.23850
H	0.28807	1.41053	-2.06884
H	1.21893	0.49660	2.05746
H	0.25058	1.88943	1.55332
H	1.79404	1.54512	0.75331

Me_2SiCl_2, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Si	0.02143	0.03784	-0.04607
Cl	1.28229	-1.47365	-0.65106
Cl	-1.60603	-0.83422	0.86560
C	0.90455	1.08599	1.19838
C	-0.55945	0.95535	-1.54529
H	-1.24742	1.75375	-1.25961
H	-1.07727	0.28092	-2.22850
H	0.29072	1.39521	-2.07062
H	1.18348	0.49379	2.07059
H	0.26022	1.90467	1.52562
H	1.81153	1.50872	0.76112

$Me_2SiClOSiH_3$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Si	-0.97536	1.43105	0.39943
O	0.28441	0.63993	-0.26862
Cl	-2.32954	-0.00323	1.08384
C	-0.39480	2.41539	1.86376
C	-1.82199	2.45331	-0.89794
H	-2.66791	2.99540	-0.47336
H	-2.19345	1.82156	-1.70521
H	-1.12505	3.17882	-1.32170
H	0.05575	1.76385	2.61324
H	-1.22234	2.95059	2.33108
H	0.35515	3.14499	1.55140
Si	1.10634	-0.77100	-0.41659
H	1.43021	-1.32195	0.91864
H	2.35804	-0.48775	-1.14986
H	0.30306	-1.75790	-1.17034

$Me_2SiClOSiH_3$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Si	-0.97438	1.43054	0.39826
O	0.28621	0.65067	-0.27492
Cl	-2.31122	-0.00418	1.07539

C	-0.39747	2.40887	1.86151
C	-1.82517	2.44972	-0.89139
H	-2.67388	2.98557	-0.46244
H	-2.19449	1.81651	-1.69960
H	-1.13170	3.18041	-1.31369
H	0.05728	1.75466	2.60736
H	-1.22875	2.93722	2.33181
H	0.34830	3.14415	1.55016
Si	1.08730	-0.76935	-0.40546
H	1.40321	-1.31406	0.93979
H	2.34832	-0.50826	-1.14046
H	0.27191	-1.75785	-1.15390
$Me_2Si(OSiH_3)_2$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Si	0.04718	0.14483	0.02941
O	1.11750	-1.04128	-0.31661
O	-1.27305	-0.59213	0.65180
C	0.78947	1.27860	1.30443
C	-0.42092	1.04240	-1.53430
H	-1.11521	1.85955	-1.32745
H	-0.90276	0.36712	-2.24355
H	0.45709	1.47065	-2.02213
H	1.06221	0.72208	2.20270
H	0.08981	2.06476	1.59548
H	1.69205	1.75858	0.92125
Si	2.32624	-1.66241	-1.21493
H	2.39008	-3.12293	-0.99532
H	3.61900	-1.05348	-0.82261
H	2.09525	-1.39365	-2.65453
Si	-2.74003	-0.53901	1.35872
H	-3.07541	-1.88234	1.87642
H	-3.76900	-0.12224	0.37718
H	-2.73556	0.43167	2.47942
$Me_2Si(OSiH_3)_2$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Si	0.04443	0.13557	0.03058
O	1.11564	-1.04578	-0.31198
O	-1.26880	-0.61154	0.64814
C	0.77881	1.26688	1.30465
C	-0.42469	1.02893	-1.52915
H	-1.12155	1.84472	-1.32199
H	-0.90469	0.35039	-2.23774
H	0.45340	1.45917	-2.01675
H	1.05183	0.70866	2.20268
H	0.07600	2.05126	1.59563
H	1.68109	1.74939	0.92193
Si	2.32449	-1.64864	-1.21513
H	2.40153	-3.11456	-1.00437
H	3.61768	-1.02995	-0.82107
H	2.08852	-1.37266	-2.65773
Si	-2.73000	-0.52121	1.35487
H	-3.09544	-1.85883	1.88022
H	-3.75506	-0.08466	0.37035
H	-2.70544	0.45659	2.47592
$PhMe_2SiCl$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Si	0.00684	0.03728	-0.02864
Cl	0.05028	-0.10640	2.05609
C	-0.43891	1.79981	-0.45694
C	-1.29019	-1.15018	-0.66603
C	1.70339	-0.40898	-0.66749
H	1.73433	-0.34341	-1.75721
H	1.97329	-1.42582	-0.38176

H	2.45635	0.27190	-0.26836
H	-1.41032	2.06356	-0.03808
H	-0.49579	1.91756	-1.54137
H	0.30376	2.50038	-0.07293
C	-1.30693	-1.47079	-2.02967
C	-2.27897	-2.31030	-2.55877
C	-3.25701	-2.84710	-1.72945
C	-3.25577	-2.54199	-0.37380
C	-2.28106	-1.70193	0.15129
H	-2.28659	-1.47737	1.20944
H	-4.01470	-3.50211	-2.13864
H	-4.01331	-2.95919	0.27644
H	-0.55324	-1.06458	-2.69400
H	-2.27312	-2.54643	-3.61473

$PhMe_2SiCl$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Si	0.00624	0.03659	-0.02831
Cl	0.04401	-0.11081	2.04308
C	-0.43872	1.79457	-0.45278
C	-1.28853	-1.14911	-0.66562
C	1.69917	-0.40850	-0.66215
H	1.73228	-0.34186	-1.75256
H	1.96697	-1.42651	-0.37537
H	2.45046	0.27341	-0.25938
H	-1.41178	2.05554	-0.03386
H	-0.49407	1.91369	-1.53791
H	0.30459	2.49384	-0.06541
C	-1.30590	-1.46918	-2.02576
C	-2.27659	-2.30730	-2.55203
C	-3.25135	-2.84215	-1.72257
C	-3.24896	-2.53704	-0.36995
C	-2.27561	-1.69840	0.15220
H	-2.27832	-1.47173	1.21208
H	-4.01047	-3.49852	-2.13095
H	-4.00683	-2.95458	0.28213
H	-0.55141	-1.06228	-2.69188
H	-2.27215	-2.54473	-3.60921

$PhMe_2SiOSiH_3$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Si	0.02011	0.05090	-0.06843
O	-0.04827	0.03270	1.57956
C	-0.31951	1.78290	-0.68634
C	-1.30085	-1.13125	-0.66140
C	1.71191	-0.51950	-0.62743
H	1.77039	-0.55258	-1.71748
H	1.92766	-1.52109	-0.25250
H	2.49616	0.15386	-0.27475
H	-1.29181	2.13306	-0.33649
H	-0.32873	1.81277	-1.77795
H	0.44095	2.48598	-0.34025
C	-1.50326	-1.34732	-2.02995
C	-2.47899	-2.22555	-2.48370
C	-3.27563	-2.90813	-1.57074
C	-3.09115	-2.70740	-0.20821
C	-2.11256	-1.82709	0.23961
H	-1.97516	-1.67603	1.30222
H	-4.03599	-3.59362	-1.92116
H	-3.70943	-3.23571	0.50582
H	-0.89304	-0.82438	-2.75771
H	-2.61887	-2.37837	-3.54587
Si	0.65056	0.50666	2.97411
H	-0.17781	0.03283	4.10352

H	0.75459	1.98454	3.03020
H	2.01282	-0.06535	3.09303
$PhMe_2SiOSiH_3$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Si	0.01716	0.04844	-0.06302
O	-0.06268	0.02282	1.58162
C	-0.32259	1.77706	-0.67510
C	-1.30114	-1.13109	-0.66098
C	1.70540	-0.52147	-0.61569
H	1.76535	-0.55372	-1.70646
H	1.91708	-1.52449	-0.24004
H	2.49002	0.15117	-0.26018
H	-1.29788	2.12293	-0.32712
H	-0.32724	1.80866	-1.76747
H	0.43639	2.48064	-0.32440
C	-1.50006	-1.34585	-2.02677
C	-2.47294	-2.22233	-2.48115
C	-3.26925	-2.90316	-1.57121
C	-3.08794	-2.70300	-0.21125
C	-2.11220	-1.82450	0.23724
H	-1.97529	-1.67231	1.30173
H	-4.02998	-3.58968	-1.92344
H	-3.70845	-3.23201	0.50251
H	-0.88709	-0.82230	-2.75451
H	-2.61141	-2.37548	-3.54495
Si	0.65667	0.51033	2.95709
H	-0.15761	0.04609	4.10664
H	0.76212	1.99357	2.99841
H	2.02546	-0.06149	3.06324
$PhMe_2SiOSi(OSiH_3)_3$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Si	0.42778	-0.36868	-1.55832
O	-0.02015	-0.08874	0.01312
C	0.73841	1.27191	-2.39744
C	-1.00100	-1.28000	-2.34295
C	1.97502	-1.41612	-1.58800
H	2.25459	-1.67038	-2.61240
H	1.82491	-2.34681	-1.03950
H	2.81234	-0.88656	-1.13088
H	-0.15443	1.89823	-2.37267
H	1.01938	1.12958	-3.44300
H	1.54586	1.81489	-1.90207
C	-0.89042	-1.78001	-3.64601
C	-1.93987	-2.46348	-4.24627
C	-3.12673	-2.66096	-3.54944
C	-3.25670	-2.17229	-2.25480
C	-2.20270	-1.48866	-1.65889
H	-2.30934	-1.11564	-0.64864
H	-3.94575	-3.19454	-4.01352
H	-4.17863	-2.32615	-1.70940
H	0.02824	-1.64156	-4.20500
H	-1.83314	-2.84387	-5.25377
Si	0.58656	0.56520	1.34515
O	-0.38073	0.22174	2.59491
O	0.69556	2.17779	1.17479
O	2.07832	-0.02846	1.60321
Si	-0.54219	0.01720	4.21041
Si	3.41245	0.18305	2.53085
Si	0.74435	3.57333	2.03257
H	4.05946	1.47354	2.20405
H	4.34776	-0.92770	2.26314
H	3.03382	0.18563	3.96305

H	0.21710	-1.17067	4.66006
H	-1.97597	-0.16696	4.51325
H	-0.03588	1.21346	4.92217
H	1.27299	4.63886	1.15735
H	1.62844	3.41025	3.21044
H	-0.61205	3.93480	2.50008
$PhMe_2SiOSi(OSiH_3)_3$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Si	0.42980	-0.36281	-1.55603
O	-0.01582	-0.09306	0.01428
C	0.72747	1.27694	-2.39012
C	-0.99778	-1.27613	-2.33605
C	1.97485	-1.40386	-1.59815
H	2.24455	-1.65662	-2.62648
H	1.83008	-2.33577	-1.04871
H	2.81626	-0.87190	-1.14903
H	-0.17061	1.89701	-2.36294
H	1.00790	1.13641	-3.43686
H	1.53332	1.82394	-1.89462
C	-0.89378	-1.76412	-3.64064
C	-1.94123	-2.44870	-4.23634
C	-3.11845	-2.65847	-3.53278
C	-3.24141	-2.18130	-2.23638
C	-2.18932	-1.49668	-1.64500
H	-2.28949	-1.13076	-0.62941
H	-3.93876	-3.19482	-3.99488
H	-4.15922	-2.34542	-1.68416
H	0.02088	-1.61437	-4.20681
H	-1.84018	-2.82134	-5.24888
Si	0.58890	0.56252	1.34260
O	-0.38853	0.22752	2.58243
O	0.70489	2.17021	1.16556
O	2.07175	-0.03807	1.61022
Si	-0.54684	0.02239	4.19452
Si	3.40382	0.17855	2.53322
Si	0.74486	3.56097	2.02494
H	4.06401	1.46249	2.18482
H	4.33327	-0.94724	2.28177
H	3.02606	0.20647	3.97078
H	0.21596	-1.16924	4.64474
H	-1.98478	-0.16357	4.49931
H	-0.03919	1.22223	4.91024
H	1.26847	4.63407	1.14789
H	1.63378	3.40221	3.20641
H	-0.61781	3.91539	2.49501
H_3SiO^-, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
O	0.00156	-0.00212	0.03153
Si	-0.00083	0.00121	1.59091
H	-0.80235	1.09954	2.29365
H	1.34837	0.14757	2.29880
H	-0.55171	-1.23908	2.29878
H_3SiO^-, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
O	0.00156	-0.00212	0.03355
Si	-0.00083	0.00121	1.58952
H	-0.80386	1.10161	2.29572
H	1.35087	0.14784	2.30096
H	-0.55272	-1.24136	2.30096
$(H_3SiO)_3SiO^-$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
O	0.07361	-0.02002	1.55802
Si	0.04482	0.03085	0.02885
O	0.29476	-1.42232	-0.79423

O	1.17582	1.02236	-0.73806
O	-1.38279	0.57040	-0.69499
Si	2.48404	0.76677	-1.64570
Si	-0.53601	-2.41160	-1.75439
Si	-1.74585	1.61322	-1.87104
H	2.18365	0.09727	-2.94110
H	3.52242	-0.05270	-0.96521
H	3.10770	2.07835	-1.97496
H	-1.70661	-3.03490	-1.07939
H	0.35101	-3.52010	-2.20296
H	-1.05056	-1.74612	-2.98320
H	-1.58678	3.03435	-1.45824
H	-3.17228	1.43227	-2.25888
H	-0.93403	1.42795	-3.10424

$(H_3SiO)_3SiO^-$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
O	0.06672	-0.01956	1.55292
Si	0.04353	0.03194	0.02681
O	0.31511	-1.41523	-0.79166
O	1.16449	1.03197	-0.73375
O	-1.38420	0.55684	-0.69602
Si	2.45857	0.74990	-1.64965
Si	-0.52595	-2.39139	-1.75241
Si	-1.72949	1.60724	-1.86689
H	2.13285	0.10623	-2.95778
H	3.48017	-0.10957	-0.98385
H	3.11861	2.05214	-1.96533
H	-1.70771	-3.00424	-1.07772
H	0.35266	-3.51227	-2.20146
H	-1.03203	-1.71822	-2.98661
H	-1.55758	3.02926	-1.44659
H	-3.16060	1.44117	-2.26136
H	-0.91389	1.41801	-3.10331

Table S52 Equilibrium geometries of structures with P as the central atom.

PCl_3, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
P	0.04911	-0.13607	-0.02751
Cl	2.10001	-0.41125	-0.08321
Cl	-0.50222	-1.62896	1.29631
Cl	-0.50221	-0.99712	-1.82746
PCl_3, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
P	0.05087	-0.14100	-0.02853
Cl	2.07862	-0.41704	-0.08434
Cl	-0.49228	-1.62007	1.27853
Cl	-0.49232	-0.99585	-1.80765
PCl_2OSiH_3, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
P	0.02190	-0.07848	-0.02068
O	1.60993	-0.18727	-0.02288
Cl	-0.48794	-1.62505	1.31385
Cl	-0.46183	-1.02752	-1.82996
Si	2.79153	-1.38362	-0.01451
H	3.96387	-0.77973	-0.67117
H	2.31049	-2.56204	-0.75588
H	3.09282	-1.72481	1.38702
PCl_2OSiH_3, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
P	0.01852	-0.08455	-0.02407
O	1.60395	-0.17655	-0.03129
Cl	-0.46290	-1.62110	1.29042
Cl	-0.45529	-1.02609	-1.80890
Si	2.76260	-1.38849	-0.00453
H	3.94983	-0.80847	-0.66686
H	2.26626	-2.57370	-0.73637
H	3.05727	-1.71953	1.40630
$PCl(OSiH_3)_2$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
P	-0.00493	-0.07507	0.01828
O	1.39628	-0.81948	-0.26766
Cl	0.07339	-0.00126	2.16175
O	-1.04762	-1.27585	-0.18504
Si	2.75673	-1.34850	0.53819
H	3.67234	-1.82244	-0.51651
H	2.40470	-2.45615	1.44761
H	3.36262	-0.23503	1.29124
Si	-1.07482	-2.92746	0.07440
H	-0.21787	-3.58931	-0.92986
H	-2.47864	-3.34318	-0.09152
H	-0.58724	-3.23468	1.43214
$PCl(OSiH_3)_2$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
P	-0.00488	-0.07684	0.02586
O	1.38487	-0.82559	-0.27432
Cl	0.08841	-0.02096	2.13690
O	-1.05210	-1.26576	-0.18098
Si	2.73309	-1.34089	0.55293
H	3.66109	-1.83031	-0.49048
H	2.37501	-2.44134	1.47761
H	3.33421	-0.21279	1.29830
Si	-1.06040	-2.91314	0.08068
H	-0.19994	-3.57138	-0.93023
H	-2.46589	-3.34299	-0.07757
H	-0.56279	-3.21621	1.44200
$P(OSiH_3)_3$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
P	-1.36807	4.43124	-2.54946
O	0.00814	3.69239	-2.99724
O	-1.00031	4.91970	-1.04583

O	-2.28769	3.13253	-2.14149
Si	1.20519	2.76875	-2.31269
H	2.16632	2.45352	-3.38574
H	0.62871	1.52112	-1.76463
H	1.87164	3.51506	-1.22572
Si	-2.56398	1.58460	-2.65844
H	-1.63641	1.24483	-3.75745
H	-3.96101	1.48089	-3.12680
H	-2.34616	0.67076	-1.51847
Si	-1.22128	4.26690	0.46729
H	-2.66008	4.15853	0.77866
H	-0.55803	5.18658	1.41084
H	-0.59367	2.92994	0.54416
$P(OSiH_3)_3$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
P	-1.36532	4.42599	-2.54448
O	0.00162	3.69510	-3.00436
O	-0.98348	4.92107	-1.05471
O	-2.27083	3.13351	-2.11674
Si	1.18852	2.77261	-2.30798
H	2.16459	2.46065	-3.37491
H	0.60363	1.51742	-1.77027
H	1.84449	3.51839	-1.20738
Si	-2.55324	1.59577	-2.65060
H	-1.64988	1.27681	-3.78269
H	-3.96602	1.49437	-3.08568
H	-2.30328	0.66222	-1.52673
Si	-1.23108	4.25488	0.44547
H	-2.67922	4.16079	0.74092
H	-0.56619	5.16274	1.40664
H	-0.61616	2.90574	0.52087
$PCl_2OSi(OSiH_3)_3$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
P	0.08177	-0.15357	-0.07322
O	0.91402	0.17440	-1.38307
Cl	-1.85271	0.46742	-0.63781
Cl	-0.16962	-2.23452	-0.25419
Si	0.72277	0.25085	-3.03726
O	2.19510	0.11291	-3.65771
O	0.11913	1.68818	-3.40389
O	-0.23739	-0.93338	-3.51593
Si	3.49836	-0.86454	-3.87497
Si	-1.21734	2.61029	-3.65903
Si	-1.19541	-2.24126	-3.75159
H	-2.41009	-2.12580	-2.92310
H	-0.45142	-3.46755	-3.40071
H	-1.56477	-2.27862	-5.18279
H	4.07362	-1.23076	-2.56300
H	4.49216	-0.12327	-4.67537
H	3.08412	-2.09037	-4.59192
H	-2.39056	1.74677	-3.91233
H	-0.95998	3.46105	-4.83901
H	-1.46339	3.45800	-2.47555
$PCl_2OSi(OSiH_3)_3$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
P	0.08081	-0.15898	-0.07806
O	0.91627	0.15738	-1.38486
Cl	-1.82290	0.46928	-0.63767
Cl	-0.19039	-2.21028	-0.25464
Si	0.72034	0.24700	-3.03164
O	2.18970	0.12345	-3.65453
O	0.11732	1.68351	-3.38906
O	-0.23282	-0.93270	-3.52563

Si	3.48342	-0.85968	-3.87287
Si	-1.22195	2.59154	-3.65294
Si	-1.18238	-2.24170	-3.76264
H	-2.40920	-2.12487	-2.94221
H	-0.43615	-3.46867	-3.39696
H	-1.54059	-2.28808	-5.20101
H	4.07126	-1.21769	-2.55874
H	4.47649	-0.12772	-4.69115
H	3.05795	-2.09494	-4.57735
H	-2.39231	1.71578	-3.90916
H	-0.96672	3.44341	-4.83838
H	-1.48063	3.44432	-2.46950
$POCl_3$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
P	-1.59967	-0.03027	2.43141
O	-2.27826	0.82954	3.38600
Cl	0.27739	0.53996	1.96102
Cl	-1.37810	-1.94627	3.02283
Cl	-2.50898	-0.19137	0.63772
$POCl_3$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
P	-1.59720	-0.03356	2.42781
O	-2.27404	0.82396	3.37988
Cl	0.26187	0.53149	1.96210
Cl	-1.37775	-1.93106	3.01405
Cl	-2.49793	-0.19264	0.65141
$POCl_2OSiH_3$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
P	-0.02421	-0.07585	-0.01225
O	-0.51336	1.26876	0.22918
O	1.52543	-0.25757	-0.01280
Cl	-0.67859	-1.45530	1.33153
Cl	-0.60846	-0.86469	-1.78735
Si	2.66456	-1.49193	0.01567
H	3.91259	-0.87527	-0.45964
H	2.21679	-2.57373	-0.87976
H	2.79017	-1.97060	1.40269
$POCl_2OSiH_3$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
P	-0.02359	-0.07871	-0.01633
O	-0.52227	1.25747	0.22925
O	1.52425	-0.24199	-0.02235
Cl	-0.65285	-1.45333	1.31469
Cl	-0.60290	-0.86099	-1.77302
Si	2.63431	-1.49696	0.02699
H	3.89688	-0.91327	-0.46620
H	2.16089	-2.59082	-0.84942
H	2.75669	-1.95323	1.42723
$POCl(OSiH_3)_2$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
P	0.04932	-0.21512	0.01581
O	0.02635	1.00893	-0.76517
O	1.39914	-1.02209	0.03483
Cl	-0.30245	0.10641	2.01173
O	-1.01088	-1.29797	-0.37409
Si	2.96670	-0.69388	0.52816
H	3.84450	-1.38229	-0.43335
H	3.13625	-1.24878	1.88365
H	3.18922	0.76238	0.52273
Si	-1.48487	-2.77250	0.26647
H	-0.30402	-3.46718	0.81269
H	-2.07267	-3.51985	-0.85744
H	-2.48114	-2.52693	1.32363
$POCl(OSiH_3)_2$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
P	0.05588	-0.22393	0.02094

O	0.04235	1.00205	-0.75045
O	1.39707	-1.03528	0.03909
Cl	-0.30335	0.08408	1.99603
O	-1.00341	-1.29515	-0.38340
Si	2.95645	-0.67370	0.52310
H	3.84600	-1.37616	-0.42475
H	3.13379	-1.19624	1.89595
H	3.16059	0.78990	0.48210
Si	-1.49079	-2.75083	0.27865
H	-0.31750	-3.43888	0.86275
H	-2.06150	-3.52360	-0.84327
H	-2.50967	-2.48051	1.31530
$PO(OSiH_3)_3$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
P	-1.18056	3.90048	-2.36416
O	-1.99239	4.90974	-3.03568
O	0.24209	3.65102	-2.98148
O	-0.83957	4.17973	-0.84449
O	-1.84049	2.46158	-2.33243
Si	1.74104	3.28209	-2.35346
H	2.59599	2.98359	-3.51544
H	1.63552	2.10621	-1.46683
H	2.26230	4.44168	-1.60512
Si	-3.25081	1.94458	-3.07027
H	-3.16719	2.15073	-4.52741
H	-4.40421	2.66628	-2.50132
H	-3.33419	0.50706	-2.75182
Si	-1.68607	4.77438	0.46378
H	-2.84682	5.55251	-0.00332
H	-0.74235	5.61418	1.22298
H	-2.12603	3.62836	1.28418
$PO(OSiH_3)_3$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
P	-1.18269	3.79987	-2.31077
O	-2.03721	4.85907	-2.83551
O	0.23479	3.67706	-2.96100
O	-0.86081	3.91593	-0.76770
O	-1.78700	2.35511	-2.46053
Si	1.75679	3.39595	-2.35136
H	2.65037	3.34209	-3.52699
H	1.77095	2.10949	-1.61819
H	2.14003	4.50517	-1.44915
Si	-3.29772	1.98034	-3.07350
H	-3.39604	2.41143	-4.48415
H	-4.34654	2.61888	-2.24782
H	-3.38363	0.50704	-2.96999
Si	-1.64247	4.91304	0.32647
H	-1.36937	6.32995	0.00606
H	-1.06220	4.55085	1.63795
H	-3.09523	4.63274	0.30245
$POClOSi(OSiH_3)_3$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
P	0.41917	-0.16989	0.01098
O	1.05699	0.31602	1.22028
Cl	-1.47619	0.52483	-0.25883
Cl	0.16342	-2.18489	-0.02839
O	1.14229	0.13701	-1.33366
Si	0.74582	0.23535	-2.95323
O	2.12453	0.05841	-3.74629
O	0.13137	1.68472	-3.23301
O	-0.31155	-0.91729	-3.27722
Si	3.47830	-0.85948	-3.94309
Si	-1.21983	2.60242	-3.43371

Si	-1.23105	-2.25185	-3.51536
H	-2.29551	-2.29017	-2.49450
H	-0.38401	-3.45808	-3.41280
H	-1.82594	-2.17077	-4.86537
H	4.08805	-1.13543	-2.62579
H	4.41445	-0.10341	-4.79614
H	3.10944	-2.13269	-4.59895
H	-2.41638	1.73342	-3.44211
H	-1.10724	3.31420	-4.72259
H	-1.31002	3.57116	-2.32420

POClOSi(OSiH$_3$)$_3$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
P	0.41716	-0.17353	0.00614
O	1.04838	0.32789	1.20797
Cl	-1.46400	0.49802	-0.26900
Cl	0.18081	-2.17090	-0.01331
O	1.14181	0.12646	-1.33485
Si	0.73729	0.23313	-2.94602
O	2.10731	0.05593	-3.74789
O	0.13580	1.68594	-3.21799
O	-0.32546	-0.90827	-3.27591
Si	3.46122	-0.85643	-3.93305
Si	-1.20367	2.60634	-3.44551
Si	-1.23575	-2.24353	-3.52065
H	-2.30189	-2.29266	-2.49412
H	-0.37938	-3.45004	-3.42501
H	-1.83537	-2.15868	-4.87330
H	4.07161	-1.12121	-2.60820
H	4.39983	-0.10133	-4.79248
H	3.09893	-2.14062	-4.58235
H	-2.38431	1.73189	-3.65880
H	-0.98348	3.45247	-4.64107
H	-1.41678	3.45774	-2.25271

Table S53 Equilibrium geometries of structures with Ti as the central atom.

$TiCl_4$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Ti	0.10888	-0.32165	-0.04310
Cl	2.28924	-0.31020	0.00763
Cl	-0.64595	-1.69943	1.46959
Cl	-0.56849	-0.96516	-2.01381
Cl	-0.63965	1.68612	0.36307
$TiCl_4$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Ti	0.10886	-0.32212	-0.04341
Cl	2.27372	-0.30975	0.00758
Cl	-0.64066	-1.68943	1.45919
Cl	-0.56395	-0.96048	-2.00019
Cl	-0.63394	1.67164	0.36032
$TiCl_3OSiH_3$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Ti	-0.09241	-0.31737	-0.01925
Cl	-1.32266	-1.25129	1.54527
Cl	-0.95487	-0.72183	-2.00064
Cl	0.04633	1.85080	0.31677
O	1.52121	-1.00635	0.03930
Si	3.05328	-1.64954	0.07283
H	4.00570	-0.55635	0.35063
H	3.32646	-2.25830	-1.24402
H	3.10351	-2.66915	1.13927
$TiCl_3OSiH_3$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Ti	-0.09195	-0.31763	-0.01942
Cl	-1.31274	-1.24547	1.53505
Cl	-0.94784	-0.71934	-1.98748
Cl	0.04621	1.83572	0.31449
O	1.51093	-1.00197	0.03859
Si	3.03876	-1.64372	0.07269
H	3.99432	-0.54726	0.35208
H	3.31337	-2.25408	-1.24846
H	3.08831	-2.66685	1.14236
$TiCl_2(OSiH_3)_2$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Ti	0.06554	-0.23109	-0.07931
Cl	-1.19932	-0.97457	1.57950
Cl	-0.87501	-0.66733	-2.03660
O	1.64081	-1.03720	-0.00132
O	0.28739	1.51875	0.09092
Si	3.02831	-1.91640	0.19511
H	4.12858	-0.99320	0.54417
H	3.33033	-2.61237	-1.07255
H	2.81939	-2.89457	1.28249
Si	0.69926	3.11125	0.26312
H	-0.09413	3.68860	1.36749
H	0.40640	3.81470	-1.00261
H	2.14222	3.19912	0.57289
$TiCl_2(OSiH_3)_2$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Ti	0.06215	-0.23177	-0.07850
Cl	-1.19447	-0.97091	1.56872
Cl	-0.86775	-0.66698	-2.02417
O	1.62884	-1.02961	0.00037
O	0.28310	1.50696	0.09033
Si	3.01841	-1.89781	0.19229
H	4.11850	-0.96433	0.53462
H	3.31994	-2.59798	-1.07867
H	2.81986	-2.87714	1.28695
Si	0.70837	3.09112	0.26232
H	-0.07778	3.67639	1.37401

H	0.41555	3.80127	-1.00519
H	2.15792	3.16690	0.56737
$TiCl(OSiH_3)_3$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Ti	0.73588	0.03221	-0.15676
Cl	-0.24978	-0.30011	-2.12910
O	2.45123	-0.45420	-0.26872
O	-0.08146	-0.96089	1.08204
O	0.62289	1.76038	0.28226
Si	3.95916	-1.11692	-0.27021
H	4.95207	-0.06006	0.02098
H	4.22779	-1.70703	-1.59887
H	4.03115	-2.16751	0.76930
Si	0.61073	3.35920	0.67532
H	0.03432	3.52030	2.02820
H	-0.20993	4.09414	-0.31074
H	1.99660	3.87688	0.65970
Si	-0.80883	-1.88478	2.23520
H	-1.15832	-1.03123	3.39181
H	0.12535	-2.94824	2.66475
H	-2.03313	-2.48897	1.66819
$TiCl(OSiH_3)_3$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Ti	0.73452	0.03241	-0.15858
Cl	-0.24353	-0.29744	-2.11807
O	2.43968	-0.45049	-0.26704
O	-0.07675	-0.95408	1.07369
O	0.62340	1.74949	0.27975
Si	3.94279	-1.11271	-0.26504
H	4.93953	-0.05338	0.02845
H	4.21515	-1.70609	-1.59683
H	4.01231	-2.16605	0.77876
Si	0.61275	3.34344	0.67358
H	0.03404	3.50469	2.03072
H	-0.20903	4.08342	-0.31495
H	2.00373	3.86110	0.65953
Si	-0.79648	-1.87628	2.22644
H	-1.14511	-1.02039	3.38770
H	0.14432	-2.94097	2.65525
H	-2.02550	-2.48591	1.66293
$Ti(OSiH_3)_4$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Ti	0.94040	-0.14596	-0.23637
O	2.67969	-0.57576	-0.05741
O	-0.03099	-0.98762	1.02374
O	0.35882	-0.64116	-1.86602
O	0.73845	1.63326	-0.05811
Si	4.29911	-0.81211	0.05353
H	4.97800	0.48556	0.27151
H	4.79736	-1.42227	-1.19995
H	4.59010	-1.71527	1.18962
Si	0.39275	3.23619	-0.00111
H	-0.89876	3.44184	0.69272
H	0.30161	3.77167	-1.37846
H	1.46426	3.94636	0.73238
Si	-0.96772	-1.75254	2.13189
H	-1.49236	-0.76608	3.10322
H	-0.16158	-2.76616	2.84880
H	-2.09980	-2.41753	1.44768
Si	-0.24055	-1.03369	-3.34179
H	-1.37733	-0.14315	-3.66863
H	-0.70558	-2.43902	-3.33079
H	0.81794	-0.87437	-4.36427

$Ti(OSiH_3)_4$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Ti	0.94023	-0.14596	-0.23706
O	2.66900	-0.57277	-0.05841
O	-0.02473	-0.98241	1.01595
O	0.36242	-0.63895	-1.85663
O	0.73954	1.62255	-0.05951
Si	4.28391	-0.80826	0.05292
H	4.96527	0.49348	0.27129
H	4.78501	-1.42075	-1.20388
H	4.57580	-1.71374	1.19307
Si	0.39570	3.22122	-0.00163
H	-0.89891	3.42847	0.69610
H	0.30256	3.75961	-1.38280
H	1.47164	3.93304	0.73330
Si	-0.95940	-1.74507	2.12069
H	-1.48615	-0.75556	3.09496
H	-0.15132	-2.76212	2.84028
H	-2.09498	-2.41254	1.43443
Si	-0.23645	-1.02996	-3.32802
H	-1.37634	-0.13576	-3.65555
H	-0.70420	-2.43934	-3.31720
H	0.82449	-0.87086	-4.35477
$TiCl_3OSi(OSiH_3)_3$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Ti	-0.16893	-0.25518	-0.11812
Cl	-2.19656	0.59014	-0.20475
Cl	-0.27915	-2.42696	0.20945
Cl	1.00589	0.71539	1.46394
O	0.58717	0.02597	-1.67620
Si	0.78487	0.24916	-3.30464
O	2.34881	0.18856	-3.65066
O	0.20669	1.69810	-3.69050
O	-0.02878	-0.92375	-4.05390
Si	3.66966	-0.77495	-3.83003
Si	-1.11849	2.65882	-3.49915
Si	-1.02934	-2.21260	-3.83485
H	-2.00444	-1.89641	-2.76959
H	-0.23611	-3.39617	-3.44371
H	-1.72946	-2.46642	-5.10898
H	4.20695	-1.12683	-2.49848
H	4.67925	-0.02450	-4.60125
H	3.28979	-2.00876	-4.55186
H	-2.34676	1.85387	-3.67626
H	-1.05492	3.71896	-4.52392
H	-1.10816	3.25683	-2.14846
$TiCl_3OSi(OSiH_3)_3$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Ti	-0.17550	-0.25918	-0.12231
Cl	-2.20230	0.55232	-0.17303
Cl	-0.24706	-2.41389	0.22813
Cl	1.00088	0.73121	1.42475
O	0.55683	0.01980	-1.68141
Si	0.78047	0.25358	-3.30015
O	2.34660	0.18818	-3.62030
O	0.22357	1.70677	-3.68751
O	-0.02456	-0.90338	-4.07620
Si	3.64180	-0.80172	-3.80892
Si	-1.10050	2.66437	-3.50892
Si	-1.02258	-2.18981	-3.85885
H	-1.99412	-1.87923	-2.78032
H	-0.22615	-3.38186	-3.48040
H	-1.73507	-2.43437	-5.13334

H	4.17835	-1.17248	-2.47684
H	4.66820	-0.06816	-4.58330
H	3.23079	-2.02778	-4.53719
H	-2.33231	1.85549	-3.68861
H	-1.03268	3.72292	-4.54177
H	-1.09899	3.27242	-2.15664
Cp_2TiCl_2, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Ti	-0.35288	-0.47277	0.57936
Cl	1.95209	-0.31213	0.91628
Cl	-0.27041	-1.22684	-1.63121
C	-0.66516	1.66211	1.59654
C	0.03589	1.93280	0.39422
C	-0.78921	1.58188	-0.67845
C	-2.01633	1.09914	-0.15503
H	-0.51728	1.60573	-1.71751
H	1.05188	2.27444	0.32636
C	-1.95041	1.19323	1.24838
H	-0.28606	1.80562	2.59423
H	-2.84437	0.72740	-0.73393
H	-2.72988	0.92337	1.93737
H	0.84210	-1.84527	3.05613
C	-0.02764	-1.98254	2.44030
H	0.71965	-3.32395	0.83296
C	-0.09433	-2.77299	1.26986
H	-1.52966	-0.67924	3.41287
C	-1.27005	-1.35084	2.61322
C	-1.39550	-2.65482	0.74035
C	-2.11948	-1.76205	1.54996
H	-1.75060	-3.11048	-0.16539
H	-3.13986	-1.45709	1.39558
Cp_2TiCl_2, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Ti	-0.47843	-0.48958	0.52274
Cl	1.84002	-0.42501	0.34577
Cl	-0.84864	-1.31495	-1.62086
C	-0.96426	1.53062	1.65813
C	0.01209	1.84981	0.69996
C	-0.53530	1.61984	-0.57418
C	-1.87207	1.20053	-0.40693
H	-0.00934	1.68974	-1.51206
H	1.02478	2.14994	0.90583
C	-2.13874	1.13699	0.96807
H	-0.84655	1.61058	2.72604
H	-2.54779	0.91958	-1.19732
H	-3.07548	0.85651	1.42006
H	1.13819	-1.70331	2.79764
C	0.17971	-1.88856	2.34310
H	0.68197	-3.30392	0.70722
C	-0.06255	-2.74027	1.24475
H	-1.17366	-0.55798	3.48252
C	-1.02735	-1.25929	2.67804
C	-1.42878	-2.66430	0.92776
C	-2.02862	-1.73117	1.79064
H	-1.91690	-3.17629	0.11684
H	-3.06983	-1.45482	1.79868
$Cp_2TiClOSiH_3$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Ti	-0.33566	-0.47819	0.61257
Cl	1.96179	-0.22531	1.06188
O	-0.15968	-1.06851	-1.12995
C	-0.66703	1.70259	1.59759
C	-0.02360	1.95044	0.35568

C	-0.88878	1.55589	-0.66886
C	-2.06735	1.04026	-0.07929
H	-0.66305	1.55636	-1.72043
H	0.97992	2.31430	0.23340
C	-1.94238	1.18021	1.32287
H	-0.24614	1.88410	2.57195
H	-2.91577	0.63610	-0.60551
H	-2.68402	0.90931	2.05229
H	0.85121	-1.87270	3.10328
C	-0.01256	-2.01125	2.47956
H	0.76856	-3.31779	0.85844
C	-0.05933	-2.78638	1.29419
H	-1.53862	-0.74553	3.45961
C	-1.26415	-1.40407	2.65413
C	-1.35392	-2.67678	0.75529
C	-2.09590	-1.80289	1.57202
H	-1.69357	-3.11213	-0.16825
H	-3.11923	-1.50826	1.41559
Si	-0.11023	-1.47987	-2.69335
H	1.27542	-1.80362	-3.10486
H	-0.61109	-0.36641	-3.54309
H	-0.97287	-2.66542	-2.94122

$Cp_2TiClOSiH_3$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Ti	-0.36855	-0.47301	0.60894
Cl	1.92747	-0.24133	1.00375
O	-0.22083	-1.06516	-1.12860
C	-0.67347	1.66922	1.60835
C	-0.02886	1.91574	0.37062
C	-0.89575	1.53278	-0.65349
C	-2.07760	1.02850	-0.06731
H	-0.66799	1.53231	-1.70676
H	0.97978	2.27149	0.24999
C	-1.95150	1.16046	1.33184
H	-0.24908	1.84065	2.58519
H	-2.92839	0.62866	-0.59692
H	-2.69649	0.89107	2.06169
H	0.87674	-1.83714	3.06534
C	0.00260	-1.98010	2.45358
H	0.76494	-3.28249	0.82216
C	-0.06007	-2.75490	1.27236
H	-1.50933	-0.71662	3.45585
C	-1.24498	-1.37705	2.64581
C	-1.36015	-2.64964	0.75427
C	-2.09004	-1.77716	1.57844
H	-1.71194	-3.08428	-0.16732
H	-3.11803	-1.48431	1.43602
Si	-0.09544	-1.48390	-2.68101
H	1.30742	-1.83959	-3.01967
H	-0.52855	-0.36258	-3.56619
H	-0.96995	-2.65715	-2.97139

$Cp_2Ti(OSiH_3)_2$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Ti	-0.26611	-0.49211	0.57638
O	1.54169	-0.26954	0.97032
O	-0.09168	-1.08126	-1.18889
C	-0.69861	1.67907	1.56367
C	-0.03330	1.97906	0.34916
C	-0.84752	1.56364	-0.70824
C	-2.02939	1.00318	-0.16486
H	-0.59268	1.59294	-1.75255
H	0.95645	2.39160	0.26168

C	-1.95017	1.11544	1.23892
H	-0.32168	1.86375	2.55571
H	-2.84656	0.58285	-0.72687
H	-2.70467	0.80807	1.93989
H	0.89604	-1.87643	3.07457
C	0.03954	-2.04189	2.44515
H	0.86101	-3.32631	0.82852
C	0.02115	-2.80965	1.25996
H	-1.52080	-0.79748	3.40339
C	-1.22410	-1.44977	2.60045
C	-1.27271	-2.72166	0.70362
C	-2.04128	-1.87315	1.51538
H	-1.59345	-3.16805	-0.22152
H	-3.06795	-1.59724	1.34738
Si	-0.39585	-1.40808	-2.73987
H	0.86806	-1.57084	-3.49826
H	-1.18039	-0.31234	-3.37315
H	-1.18970	-2.65940	-2.87344
Si	3.02764	0.26636	1.29769
H	3.55036	-0.37006	2.53598
H	3.02871	1.73931	1.51501
H	3.95837	-0.03778	0.18344

$Cp_2Ti(OSiH_3)_2$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Ti	-0.29343	-0.48662	0.58388
O	1.51382	-0.25635	0.94943
O	-0.12862	-1.08413	-1.17250
C	-0.71970	1.64814	1.57321
C	-0.05062	1.94398	0.36360
C	-0.85923	1.52867	-0.69410
C	-2.04252	0.97360	-0.15502
H	-0.59931	1.55483	-1.73944
H	0.94420	2.35046	0.27955
C	-1.96861	1.08773	1.24539
H	-0.34361	1.83098	2.56796
H	-2.85822	0.55003	-0.72042
H	-2.72659	0.77988	1.94563
H	0.92335	-1.83433	3.05433
C	0.05936	-2.00571	2.43320
H	0.87032	-3.28463	0.80829
C	0.03101	-2.77404	1.25216
H	-1.49433	-0.76853	3.40985
C	-1.20329	-1.42230	2.60329
C	-1.26681	-2.69382	0.71268
C	-2.02893	-1.85081	1.53119
H	-1.59596	-3.14025	-0.21179
H	-3.06126	-1.58172	1.37437
Si	-0.36836	-1.38288	-2.73524
H	0.92594	-1.60056	-3.43602
H	-1.07136	-0.24560	-3.40329
H	-1.21480	-2.59863	-2.92225
Si	3.00745	0.24546	1.26974
H	3.49931	-0.35488	2.54469
H	3.05654	1.73065	1.42732
H	3.94468	-0.13640	0.17892

$Cp_2TiClOSi(OSiH_3)_3$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Ti	-0.43620	-0.48834	0.62871
Cl	1.90397	-0.29138	0.59561
O	-0.62591	-1.11981	-1.11830
C	-0.76469	1.60578	1.74344
C	-0.11037	1.93451	0.53156

C	-0.96563	1.60845	-0.52923
C	-2.16284	1.08480	0.01482
H	-0.72515	1.66095	-1.57656
H	0.89461	2.30247	0.44312
C	-2.04829	1.11245	1.41896
H	-0.35884	1.72868	2.73320
H	-2.99878	0.70863	-0.55063
H	-2.80327	0.80238	2.11895
H	1.12185	-1.77821	2.95676
C	0.18804	-1.97000	2.46036
H	0.78982	-3.31979	0.79739
C	0.01136	-2.79314	1.32036
H	-1.23775	-0.70385	3.58095
C	-1.04631	-1.38502	2.77039
C	-1.34324	-2.74340	0.95506
C	-2.00063	-1.84763	1.82016
H	-1.78345	-3.23346	0.10551
H	-3.04581	-1.59342	1.78878
Si	-1.25188	-1.30102	-2.57526
O	-0.74623	-2.70935	-3.22597
O	-0.84218	-0.07945	-3.56012
O	-2.87879	-1.33024	-2.48681
Si	0.36082	-3.84726	-2.79677
H	-0.05769	-4.51330	-1.54121
H	1.69414	-3.24046	-2.60060
H	0.41622	-4.84868	-3.88139
Si	-0.12998	0.22811	-5.00528
H	0.19618	1.66875	-5.04965
H	-1.05394	-0.10278	-6.11326
H	1.10889	-0.56767	-5.15229
Si	-4.10908	-2.37001	-2.20574
H	-5.08726	-1.70487	-1.31589
H	-3.61128	-3.59411	-1.53389
H	-4.77098	-2.74419	-3.47327

$Cp_2TiClOSi(OSiH_3)_3$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Ti	-0.49325	-0.50274	0.62147
Cl	1.83944	-0.39329	0.55321
O	-0.71429	-1.14601	-1.11590
C	-0.69698	1.59082	1.70959
C	-0.05923	1.86865	0.47967
C	-0.95104	1.55857	-0.55137
C	-2.15218	1.09290	0.02863
H	-0.73353	1.58314	-1.60673
H	0.95782	2.19875	0.35983
C	-2.00398	1.14535	1.42606
H	-0.26050	1.71138	2.68865
H	-3.01697	0.73744	-0.51056
H	-2.75380	0.87914	2.15261
H	1.06069	-1.76702	2.93082
C	0.11730	-1.94683	2.44380
H	0.67966	-3.33130	0.79792
C	-0.08552	-2.78012	1.31951
H	-1.27013	-0.63281	3.55473
C	-1.09970	-1.33164	2.75190
C	-1.43816	-2.70632	0.96309
C	-2.06874	-1.78406	1.81612
H	-1.89286	-3.20336	0.12241
H	-3.10900	-1.50240	1.78470
Si	-1.24994	-1.28959	-2.60833
O	-0.64765	-2.63839	-3.29294

O	-0.84226	-0.01758	-3.52519
O	-2.87546	-1.38557	-2.62488
Si	0.38371	-3.81119	-2.79113
H	-0.16666	-4.51369	-1.60031
H	1.70713	-3.24113	-2.43896
H	0.52925	-4.78423	-3.89954
Si	-0.13415	0.27892	-4.97288
H	0.12817	1.73596	-5.05077
H	-1.03520	-0.12174	-6.08309
H	1.14509	-0.46501	-5.09076
Si	-4.01116	-2.46764	-2.17364
H	-4.69684	-1.98059	-0.94648
H	-3.39133	-3.78607	-1.87113
H	-5.00831	-2.62558	-3.25815

Table S54 Equilibrium geometries of structures with V as the central atom.

VCl_4, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
V	-0.92504	-1.56332	0.67631
Cl	0.75061	-2.56522	1.56413
Cl	-2.14639	-3.07911	-0.22365
Cl	-0.27187	-0.13811	-0.78719
Cl	-2.02933	-0.47033	2.15471
VCl_4, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
V	-0.92422	-1.56315	0.67685
Cl	0.73737	-2.55875	1.55724
Cl	-2.13602	-3.06685	-0.21639
Cl	-0.27824	-0.14896	-0.77576
Cl	-2.02093	-0.47837	2.14238
VCl_3OSiH_3, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
V	0.57316	1.26819	-0.29239
Cl	2.56147	0.65795	0.27290
Cl	-0.64104	-0.48912	-0.66252
Cl	0.66192	2.38060	-2.15016
O	-0.31502	2.23278	0.83589
Si	-1.76656	2.97639	1.20615
H	-2.80817	1.93329	1.27348
H	-2.07270	3.95923	0.14813
H	-1.59328	3.64249	2.51070
VCl_3OSiH_3, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
V	0.56805	1.27106	-0.28143
Cl	2.55601	0.68163	0.24627
Cl	-0.63125	-0.48266	-0.61443
Cl	0.61194	2.35667	-2.13686
O	-0.30102	2.23480	0.84441
Si	-1.75537	2.97329	1.19543
H	-2.80960	1.93346	1.20517
H	-2.02631	3.99278	0.15579
H	-1.61268	3.60076	2.52783
$VCl_2(OSiH_3)_2$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
V	0.64477	1.38709	-0.21836
O	2.22742	0.85637	0.27660
Cl	-0.50749	-0.38982	-0.75467
Cl	0.83139	2.52263	-2.07551
O	-0.32836	2.30777	0.89612
Si	-1.82728	2.95881	1.22367
H	-2.79653	1.85182	1.34759
H	-2.21191	3.86546	0.12314
H	-1.71919	3.70313	2.49389
Si	3.60582	-0.05137	0.06644
H	4.56927	0.35470	1.10909
H	4.15646	0.21045	-1.27849
H	3.25045	-1.47714	0.21487
$VCl_2(OSiH_3)_2$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
V	0.65488	1.39722	-0.19874
O	2.22494	0.86912	0.29965
Cl	-0.48382	-0.36353	-0.74897
Cl	0.84811	2.53068	-2.03646
O	-0.31587	2.30630	0.90955
Si	-1.81968	2.94655	1.21331
H	-2.78295	1.82890	1.34784
H	-2.20583	3.83565	0.09240
H	-1.72747	3.71370	2.47679
Si	3.58723	-0.04840	0.06130
H	4.57742	0.35134	1.08776

H	4.11638	0.20800	-1.29853
H	3.22150	-1.47564	0.21845
$VCl(OSiH_3)_3$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
V	0.63692	0.88792	-0.12574
Cl	0.44095	1.95998	-2.03347
O	2.24355	1.21094	0.50174
O	0.13137	-0.77293	-0.39926
O	-0.56403	1.67165	0.93121
Si	-1.73676	2.83959	0.87737
H	-2.40265	2.86526	2.19768
H	-2.72643	2.51640	-0.17338
H	-1.12906	4.15982	0.60100
Si	3.34207	2.35376	0.98978
H	2.67448	3.32970	1.87812
H	3.88314	3.03754	-0.20303
H	4.42361	1.66142	1.72009
Si	-1.14246	-1.67937	-0.95937
H	-0.92330	-1.96507	-2.39214
H	-2.40505	-0.93104	-0.77755
H	-1.18172	-2.93646	-0.18434
$VCl(OSiH_3)_3$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
V	0.64217	0.87901	-0.11226
Cl	0.43386	1.95597	-1.99660
O	2.24250	1.19779	0.50221
O	0.14141	-0.77148	-0.38743
O	-0.54428	1.65202	0.94906
Si	-1.71877	2.81145	0.87488
H	-2.38768	2.85305	2.19859
H	-2.71110	2.46831	-0.17444
H	-1.11574	4.13524	0.57925
Si	3.32432	2.35448	0.98057
H	2.64624	3.32895	1.87084
H	3.85388	3.04296	-0.22079
H	4.42078	1.67645	1.71147
Si	-1.14141	-1.64980	-0.95939
H	-0.89931	-1.96396	-2.38737
H	-2.39208	-0.86406	-0.81560
H	-1.23017	-2.89726	-0.16427
$V(OSiH_3)_4$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
V	0.02675	1.74141	-1.29010
O	1.50294	2.00207	-0.31721
O	-0.51573	0.05338	-1.04245
O	0.50501	1.96258	-2.98145
O	-1.24957	2.77962	-0.63706
Si	-2.00902	3.30392	0.73147
H	-2.84937	2.21392	1.27685
H	-2.85604	4.46313	0.38057
H	-1.00395	3.70202	1.74247
Si	2.71848	1.32264	0.56023
H	2.41706	1.45563	2.00274
H	3.97908	2.02921	0.24529
H	2.86962	-0.11350	0.22561
Si	-0.31497	-1.25788	-0.06648
H	-1.62257	-1.92879	0.09978
H	0.19209	-0.84302	1.26386
H	0.65163	-2.19447	-0.68163
Si	1.61306	1.49824	-4.11451
H	1.97094	2.67420	-4.93558
H	1.02660	0.44544	-4.97200
H	2.82559	0.97038	-3.44642

$V(OSiH_3)_4$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
V	0.07895	1.78487	-1.25594
O	1.49658	2.06960	-0.22410
O	-0.42073	0.08834	-1.07280
O	0.59985	2.05789	-2.91547
O	-1.25426	2.76403	-0.65637
Si	-2.02420	3.29071	0.70029
H	-2.92338	2.22119	1.20377
H	-2.82019	4.49160	0.34975
H	-1.02965	3.63318	1.74888
Si	2.70621	1.35734	0.62841
H	2.35711	1.34316	2.07132
H	3.95235	2.13682	0.42461
H	2.92474	-0.03951	0.16442
Si	-0.22630	-1.22736	-0.10808
H	-1.54170	-1.89377	0.05678
H	0.28854	-0.82640	1.22960
H	0.73607	-2.16688	-0.73666
Si	1.53496	1.43484	-4.11951
H	2.10485	2.55917	-4.90058
H	0.69891	0.58071	-4.99853
H	2.63892	0.62059	-3.54578
$VCl_3OSi(OSiH_3)_3$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
V	-0.07411	1.38974	-0.14440
Cl	2.05441	1.08178	-0.24908
Cl	-1.07075	-0.50988	0.18500
Cl	-0.78231	2.14243	-2.05117
O	-0.65921	2.47810	1.06551
Si	-2.07696	3.28131	1.39759
O	-3.30097	2.30342	1.04230
O	-2.13895	4.60215	0.48771
O	-2.03593	3.65616	2.95592
Si	-4.31131	1.07562	1.46591
H	-4.61530	0.28864	0.25671
H	-5.55491	1.65554	2.01771
H	-3.66900	0.22175	2.48659
Si	-2.27676	4.73706	4.16988
H	-1.01705	4.89231	4.92461
H	-3.33573	4.21619	5.05891
H	-2.69222	6.03970	3.60600
Si	-2.59642	5.25888	-0.95307
H	-1.39305	5.54496	-1.75766
H	-3.31752	6.51582	-0.66397
H	-3.48481	4.32467	-1.67487
$VCl_3OSi(OSiH_3)_3$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
V	-0.05998	1.34950	-0.19998
Cl	2.03914	0.95599	-0.28380
Cl	-1.12477	-0.50624	0.03837
Cl	-0.69913	2.18465	-2.07805
O	-0.62127	2.41926	1.02167
Si	-2.00886	3.23696	1.40892
O	-3.26294	2.29683	1.07405
O	-2.07557	4.58058	0.53746
O	-1.90642	3.58032	2.97251
Si	-4.30069	1.10288	1.51312
H	-4.67425	0.34414	0.29910
H	-5.50662	1.72178	2.11646
H	-3.65515	0.20723	2.50300
Si	-2.28305	4.73321	4.08113
H	-1.32387	5.85977	3.98464

H	-2.20059	4.10929	5.42103
H	-3.65961	5.23401	3.83958
Si	-2.57159	5.26349	-0.87440
H	-1.38481	5.57917	-1.70141
H	-3.29855	6.51108	-0.53891
H	-3.47113	4.33386	-1.59894
$VOCl_3$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
V	-0.85857	-1.59984	0.71209
O	0.39101	-2.26809	1.35168
Cl	-2.06735	-3.13694	-0.17596
Cl	-0.19319	-0.20798	-0.78197
Cl	-1.95013	-0.58184	2.25627
$VOCl_3$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
V	-0.86202	-1.59800	0.71054
O	0.37576	-2.25977	1.34372
Cl	-2.05676	-3.12822	-0.16891
Cl	-0.19477	-0.21875	-0.77098
Cl	-1.94045	-0.58997	2.24775
$VOCl_2OSiH_3$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
V	-0.97522	-1.41091	0.55487
O	0.57586	-1.59264	0.55167
Cl	-1.89588	-3.29124	0.00991
Cl	-1.59886	-0.78111	2.52827
O	-1.38285	-0.19029	-0.61630
Si	-0.70129	0.83066	-1.75156
H	0.76772	0.69499	-1.69330
H	-1.12083	2.20547	-1.41712
H	-1.21807	0.43146	-3.07500
$VOCl_2OSiH_3$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
V	-0.98079	-1.39957	0.55047
O	0.55813	-1.55760	0.54762
Cl	-1.85981	-3.28106	0.00381
Cl	-1.60346	-0.78795	2.51229
O	-1.39697	-0.19096	-0.61316
Si	-0.70333	0.81914	-1.74393
H	0.76818	0.65356	-1.69365
H	-1.09468	2.20537	-1.40120
H	-1.23668	0.43547	-3.07080
V	-0.98079	-1.39957	0.55047
O	0.55813	-1.55760	0.54762
Cl	-1.85981	-3.28106	0.00381
Cl	-1.60346	-0.78795	2.51229
O	-1.39697	-0.19096	-0.61316
Si	-0.70333	0.81914	-1.74393
$VOCl(OSiH_3)_2$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
V	-1.25422	-1.22744	0.57988
O	0.01743	-2.09949	0.29629
O	-2.67597	-2.23190	0.37345
Cl	-1.14936	-0.48837	2.62607
O	-1.29471	0.11344	-0.54599
Si	-0.56445	0.96854	-1.76636
H	0.68269	0.28599	-2.17062
H	-0.27306	2.32613	-1.26238
H	-1.50735	1.03431	-2.90199
Si	-3.20191	-3.77353	0.04061
H	-2.03586	-4.63705	-0.23959
H	-4.09128	-3.70681	-1.13738
H	-3.94488	-4.26834	1.21728
$VOCl(OSiH_3)_2$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
V	-1.27524	-1.21889	0.57582

O	-0.02142	-2.08745	0.28233
O	-2.69180	-2.21285	0.37563
Cl	-1.14705	-0.49599	2.60930
O	-1.31520	0.11618	-0.53973
Si	-0.56792	0.95219	-1.75666
H	0.66490	0.23710	-2.16676
H	-0.23949	2.30566	-1.25064
H	-1.51421	1.04421	-2.89374
Si	-3.18567	-3.75969	0.04009
H	-1.99914	-4.60311	-0.24242
H	-4.07815	-3.70803	-1.14223
H	-3.92253	-4.27382	1.21825
$VO(OSiH_3)_3$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
V	-1.98195	-1.09678	0.40785
O	-0.64323	-1.76010	0.90253
O	-3.05296	-2.36894	-0.19175
O	-2.73584	-0.25194	1.76195
O	-1.60992	0.05009	-0.88184
Si	-0.40284	0.71618	-1.79681
H	0.91386	0.28152	-1.28250
H	-0.51911	2.18813	-1.71879
H	-0.57254	0.27277	-3.19727
Si	-3.13008	-4.01670	-0.34861
H	-1.85506	-4.52496	-0.89898
H	-4.24259	-4.33446	-1.26774
H	-3.38127	-4.62319	0.97680
Si	-2.62573	0.13018	3.36752
H	-1.24820	-0.11279	3.84797
H	-3.58148	-0.70807	4.12312
H	-2.97513	1.55771	3.52729
$VO(OSiH_3)_3$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
V	-1.98906	-1.08107	0.40137
O	-0.64843	-1.72858	0.86463
O	-3.05680	-2.35299	-0.16965
O	-2.71742	-0.24382	1.76053
O	-1.65055	0.05586	-0.89151
Si	-0.45058	0.71551	-1.81192
H	0.87312	0.29768	-1.28717
H	-0.57878	2.19223	-1.75727
H	-0.61410	0.24909	-3.21072
Si	-3.13877	-3.99511	-0.32525
H	-1.77099	-4.55845	-0.44559
H	-3.92595	-4.30439	-1.54323
H	-3.81459	-4.56111	0.86840
Si	-2.56689	0.09948	3.36692
H	-1.16371	-0.11147	3.80197
H	-3.47376	-0.78926	4.13441
H	-2.95682	1.51504	3.57480
$VOCl_2OSi(OSiH_3)_3$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
V	-0.18902	-2.47195	1.45846
O	1.14074	-3.27119	1.29355
Cl	-1.61921	-3.66425	2.55653
Cl	0.19368	-0.61403	2.50348
O	-0.80971	-2.09500	-0.12300
Si	-2.05228	-1.20399	-0.76071
O	-1.48899	0.26429	-1.09764
O	-3.24915	-1.15220	0.31557
O	-2.52789	-1.94705	-2.09581
Si	-4.01830	-0.46374	1.59437
H	-3.17144	-0.56923	2.79913

H	-5.29203	-1.17965	1.80142
H	-4.27932	0.96117	1.29605
Si	-0.74580	1.62332	-0.54180
H	0.69655	1.36320	-0.36276
H	-1.34913	2.01690	0.74950
H	-0.95095	2.68948	-1.54208
Si	-3.71718	-2.37102	-3.14554
H	-3.70357	-3.83875	-3.30786
H	-3.46084	-1.71817	-4.44554
H	-5.02890	-1.93635	-2.61696

$VOCl_2OSi(OSiH_3)_3$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
V	-0.18921	-2.49735	1.46301
O	1.10558	-3.31747	1.26540
Cl	-1.60237	-3.66624	2.57742
Cl	0.26724	-0.67550	2.50910
O	-0.82757	-2.10290	-0.09474
Si	-2.04266	-1.20304	-0.75552
O	-1.45883	0.25118	-1.10099
O	-3.26010	-1.12668	0.29045
O	-2.50306	-1.95013	-2.09053
Si	-4.03065	-0.43907	1.56360
H	-3.17870	-0.53179	2.77345
H	-5.30220	-1.16670	1.77694
H	-4.30451	0.98708	1.25865
Si	-0.75673	1.62541	-0.54252
H	0.69856	1.40749	-0.36883
H	-1.36703	2.00013	0.75792
H	-0.99700	2.69383	-1.53958
Si	-3.70370	-2.37123	-3.12209
H	-3.65036	-3.83601	-3.33682
H	-3.50045	-1.66534	-4.40923
H	-5.01899	-1.99387	-2.54674

Table S55 Equilibrium geometries of structures with Zn as the central atom and THF.

$ZnCl_2$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Zn	-0.02457	-0.12560	0.16156
Cl	-2.08393	0.11059	-0.13419
Cl	2.03484	-0.36125	0.45740
$ZnCl_2$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Zn	-0.04076	-0.29982	0.13511
Cl	-2.08502	-0.06562	-0.15851
Cl	2.00351	-0.53403	0.42872
$ZnCl_2$(THF), B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Zn	0.06961	0.15379	0.31613
Cl	-1.99522	-0.01756	-0.24400
Cl	2.11389	-0.43690	0.03146
O	0.07497	1.43551	1.97997
C	-1.08631	1.46486	2.84988
C	1.22212	1.44365	2.86853
C	0.82764	0.51237	4.01542
H	1.36812	2.47167	3.20596
H	2.08148	1.11716	2.29236
C	-0.72488	0.53088	4.00680
H	1.24310	0.85259	4.96175
H	1.20141	-0.49313	3.83077
H	-1.14292	0.88742	4.94602
H	-1.11958	-0.46767	3.82736
H	-1.94228	1.15487	2.25955
H	-1.22146	2.49585	3.18247
$ZnCl_2$(THF), PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Zn	0.06946	0.15222	0.32000
Cl	-1.98001	-0.01310	-0.23548
Cl	2.09917	-0.42949	0.03767
O	0.07476	1.42466	1.97585
C	-1.07514	1.45951	2.83887
C	1.21076	1.43853	2.85711
C	0.82285	0.51213	4.00146
H	1.35480	2.46854	3.19557
H	2.07544	1.11504	2.28250
C	-0.72024	0.53052	3.99299
H	1.24097	0.85452	4.94715
H	1.19915	-0.49426	3.81826
H	-1.14033	0.88963	4.93164
H	-1.11771	-0.46878	3.81551
H	-1.93633	1.15333	2.24951
H	-1.20803	2.49246	3.17264
$ZnCl_2(THF)_2$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Zn	0.08888	0.39444	0.23132
Cl	-1.99826	-0.18755	-0.14446
Cl	2.01477	-0.65799	0.29616
O	0.04132	1.63561	1.97024
O	0.42304	2.05309	-1.04502
C	-1.08266	1.38829	2.85254
C	1.21030	1.56663	2.82764
C	0.92727	0.41482	3.79827
H	1.29562	2.52639	3.34179
H	2.07292	1.40786	2.18915
C	-0.61408	0.24681	3.75128
H	1.28562	0.65083	4.79867
H	1.42682	-0.49133	3.46342
H	-1.07216	0.29982	4.73712
H	-0.88303	-0.71060	3.30791

H	-1.93990	1.15022	2.23135
H	-1.26982	2.30580	3.41602
C	-0.74109	2.76385	-1.53137
C	1.25040	1.82083	-2.21106
C	-1.05257	2.14920	-2.90061
H	-0.47321	3.81999	-1.60706
H	-1.53484	2.63776	-0.80139
C	0.26224	1.43641	-3.31000
H	-1.34253	2.91903	-3.61368
H	-1.86643	1.43392	-2.81663
H	0.61646	1.74351	-4.29215
H	0.11825	0.35761	-3.32548
H	1.97174	1.05312	-1.94840
H	1.77251	2.75325	-2.43995

$ZnCl_2(THF)_2$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Zn	0.08775	0.38788	0.23086
Cl	-1.98548	-0.18245	-0.13615
Cl	2.00421	-0.64549	0.29241
O	0.03938	1.62362	1.95777
O	0.42079	2.03873	-1.03919
C	-1.07349	1.38918	2.83599
C	1.19672	1.56517	2.80903
C	0.92017	0.42384	3.78360
H	1.28013	2.52914	3.31977
H	2.06473	1.40597	2.17374
C	-0.61202	0.25645	3.73833
H	1.28159	0.66626	4.78255
H	1.42208	-0.48473	3.45329
H	-1.07284	0.31480	4.72377
H	-0.88335	-0.70422	3.29936
H	-1.93703	1.15147	2.21900
H	-1.25680	2.31132	3.39696
C	-0.72779	2.75296	-1.51747
C	1.24213	1.81920	-2.19551
C	-1.04367	2.15158	-2.88439
H	-0.45564	3.81032	-1.58903
H	-1.52586	2.63035	-0.78801
C	0.26181	1.44217	-3.29507
H	-1.33387	2.92736	-3.59254
H	-1.86145	1.43777	-2.80345
H	0.61977	1.75292	-4.27591
H	0.11672	0.36208	-3.31671
H	1.96926	1.05124	-1.93947
H	1.76328	2.75542	-2.42034

$ZnClOSiH_3$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Zn	-0.07258	-0.46581	-0.06867
Cl	-2.13918	-0.20556	-0.20325
O	1.67793	-0.59888	0.03697
Si	2.94220	-1.61151	0.21595
H	4.19188	-0.81776	0.25941
H	3.02805	-2.57388	-0.91241
H	2.83293	-2.39670	1.47249

$ZnClOSiH_3$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Zn	-0.07027	-0.46141	-0.06900
Cl	-2.12384	-0.21624	-0.20130
O	1.67246	-0.59108	0.03575
Si	2.92298	-1.61192	0.21501
H	4.18562	-0.83011	0.26038
H	3.00248	-2.57867	-0.91653
H	2.80610	-2.40023	1.47469

$ZnClOSiH_3(THF)$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Zn	0.02286	-0.20542	-0.25516
Cl	-2.05590	-0.59997	0.07589
O	1.78156	-0.64057	-0.19117
Si	2.67202	-1.85770	0.41163
H	4.08482	-1.69237	-0.01679
H	2.20322	-3.18679	-0.06687
H	2.64638	-1.88988	1.89862
O	0.08606	1.57794	-1.35027
C	-0.98494	1.96508	-2.25094
C	1.32947	1.85769	-2.04233
C	-0.44604	1.70735	-3.67019
H	-1.19582	3.02125	-2.07892
H	-1.85463	1.37451	-1.98051
C	1.05651	1.39782	-3.46640
H	-0.59231	2.58458	-4.29789
H	-0.95992	0.87371	-4.14385
H	1.69262	1.90156	-4.19152
H	1.24323	0.32707	-3.54097
H	2.11046	1.30724	-1.52715
H	1.51556	2.93280	-1.98259
$ZnClOSiH_3(THF)$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Zn	0.02398	-0.20923	-0.26027
Cl	-2.03992	-0.59236	0.06976
O	1.77435	-0.63728	-0.19487
Si	2.65990	-1.84744	0.41620
H	4.07852	-1.68933	-0.01202
H	2.18912	-3.18476	-0.05263
H	2.63322	-1.86935	1.90828
O	0.08987	1.56314	-1.35288
C	-0.97409	1.95831	-2.23684
C	1.31853	1.84847	-2.04125
C	-0.44890	1.71045	-3.65555
H	-1.18159	3.01603	-2.05831
H	-1.84909	1.37126	-1.96618
C	1.04519	1.39842	-3.46159
H	-0.59746	2.59334	-4.27681
H	-0.96876	0.88147	-4.13381
H	1.68164	1.90528	-4.18580
H	1.23157	0.32662	-3.54290
H	2.10733	1.29924	-1.53171
H	1.50361	2.92552	-1.97850
$ZnClOSiH_3(THF)_2$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Zn	-0.05879	-0.10277	0.03174
Cl	-2.08131	-0.89120	-0.22588
O	1.71061	-0.66775	0.01359
Si	2.56493	-2.02107	0.19459
H	4.00925	-1.75879	-0.05469
H	2.14542	-3.11068	-0.73056
H	2.45937	-2.57230	1.57888
O	-0.09424	1.12917	1.79577
O	0.16022	1.52079	-1.29906
C	-1.06624	0.70559	2.78220
C	1.17359	1.17770	2.49907
C	1.13466	0.01914	3.50744
H	1.24030	2.14934	2.99239
H	1.95510	1.07678	1.75416
C	-0.35553	-0.40079	3.55190
H	1.49746	0.34084	4.48206
H	1.75740	-0.80536	3.16962

H	-0.73574	-0.50205	4.56665
H	-0.49997	-1.35272	3.04230
H	-1.95550	0.38789	2.24691
H	-1.30030	1.56374	3.41810
C	-0.94655	1.92228	-2.13726
C	1.34715	1.63863	-2.11617
C	-0.60661	1.39330	-3.53686
H	-1.00600	3.01287	-2.11563
H	-1.84810	1.49453	-1.71016
C	0.91771	1.11125	-3.48310
H	-0.86339	2.12328	-4.30236
H	-1.16085	0.48073	-3.74405
H	1.46246	1.59687	-4.29074
H	1.11081	0.04165	-3.54325
H	2.12515	1.06144	-1.62693
H	1.62510	2.69526	-2.15407

$ZnClOSiH_3(THF)_2$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Zn	-0.04740	-0.11343	0.03039
Cl	-2.05789	-0.89271	-0.20217
O	1.71420	-0.66956	0.00590
Si	2.56703	-2.02057	0.17817
H	4.01289	-1.76124	-0.09181
H	2.13314	-3.11574	-0.74143
H	2.48063	-2.57262	1.56894
O	-0.07747	1.12146	1.77679
O	0.15943	1.50200	-1.29607
C	-1.06441	0.75155	2.75043
C	1.16695	1.15367	2.49537
C	1.08931	0.01226	3.51113
H	1.24576	2.12983	2.98237
H	1.96352	1.03249	1.76598
C	-0.40430	-0.36300	3.54048
H	1.45216	0.33408	4.48692
H	1.69525	-0.83297	3.18812
H	-0.80381	-0.44369	4.55080
H	-0.57173	-1.31573	3.03616
H	-1.96298	0.45610	2.21314
H	-1.27450	1.62743	3.37362
C	-0.94324	1.91039	-2.11401
C	1.33011	1.64155	-2.10990
C	-0.61478	1.40686	-3.51824
H	-1.00667	3.00225	-2.07791
H	-1.84523	1.47641	-1.68767
C	0.90240	1.13448	-3.47805
H	-0.88279	2.14749	-4.27118
H	-1.16738	0.49412	-3.73635
H	1.44257	1.63573	-4.28061
H	1.10276	0.06596	-3.55603
H	2.11968	1.06438	-1.63403
H	1.60140	2.70226	-2.13492

$Zn(OSiH_3)_2$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Zn	-0.10231	-0.82364	-0.11754
O	-1.82720	-0.51549	-0.24641
O	1.64171	-0.97127	0.02612
Si	-3.28055	-1.24187	-0.11578
Si	2.88782	-1.99645	-0.20163
H	-4.34273	-0.23668	-0.34928
H	-3.47243	-1.83473	1.23326
H	-3.43101	-2.33347	-1.11265
H	4.10953	-1.40906	0.39495

H	3.13228	-2.23803	-1.64677
H	2.63236	-3.31332	0.43876
$Zn(OSiH_3)_2$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Zn	-0.10187	-0.82012	-0.11728
O	-1.81893	-0.51542	-0.24692
O	1.63378	-0.96902	0.02668
Si	-3.26298	-1.24785	-0.11613
Si	2.86929	-1.99800	-0.20178
H	-4.33657	-0.24757	-0.34871
H	-3.45269	-1.84455	1.23691
H	-3.40987	-2.34432	-1.11545
H	4.10083	-1.41820	0.39379
H	3.11185	-2.24334	-1.65163
H	2.60776	-3.31822	0.44060
$Zn(OSiH_3)_2$(THF), B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Zn	0.04479	0.23622	0.33575
O	-1.72802	0.21985	-0.00386
O	1.79145	-0.21148	0.24185
Si	-2.74479	-0.55892	-1.00073
Si	2.72429	-1.52598	0.38758
H	-4.13788	-0.12346	-0.72636
H	-2.68589	-2.03570	-0.81833
H	-2.45003	-0.28308	-2.43301
H	4.09819	-1.23460	-0.09245
H	2.20222	-2.69065	-0.37807
H	2.82873	-1.95792	1.81224
O	0.05120	1.55112	1.98967
C	-1.11127	1.57153	2.85263
C	1.20012	1.55987	2.86742
C	0.81453	0.62082	4.01003
H	1.35076	2.58531	3.21306
H	2.05320	1.23579	2.28022
C	-0.73748	0.67013	4.03547
H	1.25730	0.93482	4.95310
H	1.16366	-0.38819	3.79762
H	-1.12340	1.07116	4.97076
H	-1.15564	-0.32649	3.90709
H	-1.95217	1.22754	2.25891
H	-1.27676	2.60457	3.16572
$Zn(OSiH_3)_2$(THF), PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Zn	0.04489	0.23346	0.34171
O	-1.71921	0.21835	0.00498
O	1.78342	-0.20791	0.24176
Si	-2.72816	-0.55585	-0.99548
Si	2.71182	-1.52087	0.37992
H	-4.12855	-0.12627	-0.72317
H	-2.66552	-2.03845	-0.82216
H	-2.43114	-0.27101	-2.43063
H	4.09004	-1.23072	-0.10321
H	2.18550	-2.68580	-0.39198
H	2.82009	-1.96230	1.80657
O	0.05062	1.53963	1.98866
C	-1.10125	1.57005	2.84439
C	1.18738	1.55630	2.86154
C	0.80611	0.62511	4.00326
H	1.33451	2.58465	3.20595
H	2.04744	1.23475	2.27884
C	-0.73643	0.67569	4.02656
H	1.25104	0.94293	4.94532
H	1.15693	-0.38588	3.79513

H	-1.12512	1.08201	4.95974
H	-1.15783	-0.32145	3.90205
H	-1.94845	1.23064	2.25278
H	-1.26178	2.60627	3.15602

$Zn(OSiH_3)_2(THF)_2$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Zn	0.03412	0.50616	0.25750
O	-1.76232	0.10749	0.03607
O	1.72237	-0.23781	0.39843
Si	-2.63811	-0.71792	-1.03535
Si	2.36524	-1.68098	0.71306
H	-4.03113	-0.90839	-0.55150
H	-2.07711	-2.06391	-1.34341
H	-2.72981	0.00024	-2.34434
H	3.85004	-1.59085	0.75790
H	2.01077	-2.71076	-0.30446
H	1.92835	-2.22834	2.03387
O	-0.03982	1.73743	2.01955
O	0.38308	2.13727	-1.04716
C	-1.03851	1.24022	2.94250
C	1.20263	1.80592	2.76374
C	1.13729	0.67758	3.80871
H	1.25780	2.79190	3.22840
H	2.00763	1.68348	2.04705
C	-0.31016	0.14383	3.70759
H	1.35180	1.06308	4.80416
H	1.85841	-0.10485	3.58653
H	-0.75843	-0.05012	4.68026
H	-0.33206	-0.78311	3.13489
H	-1.88124	0.90193	2.34698
H	-1.34222	2.06253	3.59628
C	-0.80087	2.79737	-1.58380
C	1.26806	1.82429	-2.14935
C	-0.80781	2.50729	-3.09419
H	-0.72168	3.86109	-1.36128
H	-1.65521	2.37492	-1.06231
C	0.31849	1.47717	-3.28185
H	-0.59124	3.41418	-3.65820
H	-1.77122	2.12548	-3.42370
H	0.78997	1.54020	-4.26105
H	-0.06144	0.46321	-3.15094
H	1.91932	1.02003	-1.81684
H	1.86600	2.71055	-2.37907

$Zn(OSiH_3)_2(THF)_2$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Zn	0.02847	0.49642	0.25983
O	-1.76073	0.10393	0.05665
O	1.71632	-0.22851	0.38181
Si	-2.63313	-0.71987	-1.01333
Si	2.35742	-1.67089	0.68589
H	-4.02696	-0.92518	-0.52406
H	-2.06176	-2.06397	-1.33375
H	-2.73641	0.00753	-2.32233
H	3.84691	-1.58213	0.72953
H	2.00078	-2.69797	-0.34021
H	1.92054	-2.22923	2.00790
O	-0.03988	1.72500	2.01077
O	0.36848	2.11941	-1.04314
C	-1.03061	1.25344	2.93507
C	1.19019	1.80116	2.74920
C	1.12706	0.68907	3.80179
H	1.24688	2.79292	3.20593

H	2.00032	1.67389	2.03547
C	-0.31463	0.16402	3.70857
H	1.34764	1.08414	4.79340
H	1.84659	-0.09879	3.58520
H	-0.76621	-0.02055	4.68268
H	-0.34345	-0.76889	3.14242
H	-1.88315	0.91594	2.34898
H	-1.32548	2.08643	3.58261
C	-0.79632	2.77692	-1.58745
C	1.26987	1.83465	-2.12230
C	-0.77512	2.51263	-3.09575
H	-0.72926	3.84006	-1.34941
H	-1.66279	2.34570	-1.08809
C	0.35145	1.49393	-3.27347
H	-0.54895	3.42949	-3.64213
H	-1.73283	2.13567	-3.45119
H	0.84304	1.56791	-4.24309
H	-0.02640	0.47535	-3.15953
H	1.92786	1.03323	-1.78894
H	1.86310	2.73149	-2.33150

$ZnEtOSiH_3$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Zn	-0.01391	-0.34883	-0.06173
C	-1.93059	-0.21206	-0.36363
O	1.74596	-0.44466	0.18354
C	-2.38441	-0.57867	-1.78304
Si	3.02203	-1.27088	0.74370
H	4.28062	-0.57615	0.37519
H	3.07837	-2.64828	0.18248
H	2.98775	-1.40051	2.22561
H	-2.41690	-0.85794	0.37071
H	-2.23020	0.80838	-0.11595
H	-2.11024	-1.60113	-2.04681
H	-1.94274	0.07851	-2.53351
H	-3.47035	-0.49885	-1.88132

$ZnEtOSiH_3$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Zn	-0.00999	-0.34836	-0.06293
C	-1.91454	-0.21885	-0.35991
O	1.74115	-0.43444	0.17938
C	-2.37188	-0.58278	-1.77098
Si	3.00352	-1.27134	0.74062
H	4.27335	-0.57427	0.39738
H	3.06343	-2.64497	0.15813
H	2.95255	-1.42552	2.22459
H	-2.40090	-0.86561	0.37607
H	-2.22011	0.80075	-0.10883
H	-2.09708	-1.60502	-2.03885
H	-1.93501	0.07541	-2.52480
H	-3.45895	-0.50585	-1.86752

$ZnEtOSiH_3$(THF), B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Zn	-0.14315	0.02698	0.29799
C	-2.01067	-0.16434	-0.27609
O	1.66317	-0.19287	0.44258
C	-2.22844	-0.76965	-1.66816
Si	2.77322	-1.31228	0.77738
H	4.14275	-0.74915	0.64399
H	2.68537	-2.50664	-0.10818
H	2.64394	-1.81295	2.17948
O	-0.22770	1.47907	2.04733
C	-0.88744	0.92095	3.19709
C	1.04475	1.99113	2.51197

C	1.44388	1.12116	3.72028
H	0.90662	3.03738	2.79189
H	1.73901	1.91329	1.68202
C	0.22666	0.19949	3.94330
H	1.63385	1.74269	4.59425
H	2.34318	0.54520	3.51609
H	-0.00458	0.04707	4.99605
H	0.40382	-0.77506	3.48860
H	-1.69103	0.28237	2.83683
H	-1.31941	1.73204	3.79210
H	-2.52080	-0.77313	0.47654
H	-2.46410	0.82779	-0.21180
H	-1.79740	-1.76913	-1.74421
H	-1.76561	-0.16355	-2.44897
H	-3.29161	-0.85459	-1.91319

$ZnEtOSiH_3(THF)$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Zn	-0.13582	0.02707	0.30541
C	-1.99380	-0.17077	-0.25600
O	1.66285	-0.18607	0.42899
C	-2.21884	-0.76469	-1.64396
Si	2.76289	-1.30997	0.76324
H	4.14092	-0.76008	0.61273
H	2.65665	-2.51546	-0.11309
H	2.64293	-1.80166	2.17502
O	-0.21663	1.46931	2.03797
C	-0.88777	0.92971	3.17521
C	1.03886	1.97774	2.51309
C	1.42209	1.11819	3.72531
H	0.90012	3.02708	2.78829
H	1.74742	1.89935	1.69213
C	0.20616	0.20663	3.93554
H	1.60357	1.74492	4.59879
H	2.32428	0.53875	3.53539
H	-0.04023	0.05610	4.98618
H	0.38425	-0.77165	3.48483
H	-1.69672	0.29530	2.81349
H	-1.31876	1.74897	3.76295
H	-2.49892	-0.78785	0.49562
H	-2.45656	0.81813	-0.18079
H	-1.78323	-1.76224	-1.73162
H	-1.76504	-0.15190	-2.42617
H	-3.28357	-0.85428	-1.88371

$ZnEtOSiH_3(THF)_2$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Zn	-0.16427	0.14901	0.23594
C	-2.03305	-0.43956	-0.07718
O	1.65637	-0.22103	0.40287
C	-2.33073	-0.92317	-1.50376
Si	2.66554	-1.40431	0.79951
H	4.07886	-0.93257	0.75540
H	2.57476	-2.58942	-0.10236
H	2.43532	-1.91851	2.18470
O	-0.24441	1.55399	2.04184
O	0.29546	1.97304	-0.96230
C	-0.89232	0.92856	3.16147
C	1.05247	1.98900	2.51311
C	1.45245	1.01697	3.64110
H	0.95523	3.01430	2.87742
H	1.72428	1.96022	1.66235
C	0.21471	0.11403	3.81751
H	1.67587	1.56302	4.55703

H	2.33244	0.43624	3.37565
H	0.00369	-0.11913	4.85992
H	0.35118	-0.82304	3.27858
H	-1.72463	0.34580	2.77475
H	-1.27655	1.70290	3.83383
C	-0.76380	2.61867	-1.69153
C	1.45424	1.97977	-1.81596
C	-0.49401	2.33618	-3.18357
H	-0.73302	3.68882	-1.47373
H	-1.70287	2.21130	-1.32652
C	0.89397	1.65373	-3.19473
H	-0.48398	3.26388	-3.75379
H	-1.25758	1.69246	-3.61470
H	1.53226	2.01362	-3.99981
H	0.78980	0.57435	-3.30251
H	2.14515	1.24925	-1.40779
H	1.90448	2.97760	-1.78875
H	-2.27986	-1.23360	0.63314
H	-2.69312	0.39593	0.17652
H	-1.71891	-1.78781	-1.76803
H	-2.11528	-0.15071	-2.24596
H	-3.37763	-1.21365	-1.63953

$ZnEtOSiH_3(THF)_2$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Zn	-0.14895	0.16442	0.24421
C	-2.00209	-0.44174	-0.06281
O	1.66394	-0.20401	0.39623
C	-2.29409	-0.93235	-1.48027
Si	2.64929	-1.40232	0.79497
H	4.07410	-0.94974	0.77426
H	2.55430	-2.58273	-0.12011
H	2.39388	-1.92853	2.17714
O	-0.22937	1.55767	2.03063
O	0.29075	1.96224	-0.96672
C	-0.88791	0.94473	3.13623
C	1.05183	1.98314	2.51441
C	1.43780	1.00875	3.63559
H	0.95525	3.00798	2.88561
H	1.73675	1.96055	1.67065
C	0.19871	0.11951	3.79697
H	1.66010	1.54970	4.55615
H	2.31717	0.42243	3.37319
H	-0.02492	-0.11903	4.83657
H	0.33159	-0.81765	3.25311
H	-1.72733	0.37155	2.74466
H	-1.26752	1.72357	3.80882
C	-0.76195	2.60847	-1.68214
C	1.43621	1.97366	-1.81805
C	-0.49517	2.34768	-3.17199
H	-0.73681	3.67796	-1.45243
H	-1.70293	2.19496	-1.32176
C	0.87312	1.64732	-3.18745
H	-0.46574	3.28581	-3.72658
H	-1.26974	1.72568	-3.61870
H	1.51492	1.99175	-3.99787
H	0.75265	0.56732	-3.28693
H	2.13591	1.24597	-1.41356
H	1.88478	2.97436	-1.79567
H	-2.24035	-1.23734	0.65110
H	-2.67660	0.38472	0.19015
H	-1.67082	-1.79013	-1.74433

H	-2.08973	-0.16009	-2.22783
H	-3.33744	-1.23799	-1.61633
$ZnEt_2$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Zn	-0.14793	-0.35427	0.04792
C	-2.08623	-0.06248	-0.17118
C	1.79039	-0.64285	0.26747
C	-2.56850	0.05684	-1.62540
C	2.19794	-1.35827	1.56504
H	-2.61009	-0.88352	0.32759
H	-2.35620	0.84016	0.38507
H	-2.33699	-0.83796	-2.20727
H	-2.10182	0.89969	-2.13982
H	-3.65077	0.20613	-1.68411
H	1.87431	-0.80818	2.45115
H	3.28262	-1.47970	1.64190
H	1.75838	-2.35560	1.63298
H	2.28285	0.33262	0.20883
H	2.15181	-1.20635	-0.59808
$ZnEt_2$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Zn	-0.14793	-0.35512	0.04767
C	-2.07123	-0.06428	-0.17130
C	1.77580	-0.64097	0.26740
C	-2.55706	0.05500	-1.61628
C	2.18614	-1.35284	1.55707
H	-2.59678	-0.88471	0.32993
H	-2.34315	0.83792	0.38758
H	-2.32847	-0.83984	-2.20089
H	-2.09264	0.89789	-2.13451
H	-3.64014	0.20464	-1.67306
H	1.86447	-0.80465	2.44617
H	3.27168	-1.47390	1.63304
H	1.74856	-2.35186	1.62699
H	2.27008	0.33510	0.20715
H	2.13994	-1.20279	-0.59989
$ZnEt_2$(THF), B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Zn	-0.10075	-0.18879	0.04014
C	-2.08120	-0.14643	-0.10229
C	1.79362	-0.71708	0.31936
C	-2.59657	-0.28157	-1.54419
C	2.04547	-1.65297	1.51068
O	0.40891	1.91529	-1.01894
C	-0.59818	2.88285	-1.37055
C	1.33593	1.84756	-2.11079
C	-0.63226	2.94459	-2.91276
H	-0.32685	3.84808	-0.93636
H	-1.53202	2.54697	-0.92811
C	0.45405	1.94174	-3.34840
H	-0.39631	3.94952	-3.26025
H	-1.61076	2.67875	-3.30680
H	1.00111	2.26642	-4.23211
H	0.01341	0.96700	-3.55788
H	1.89211	0.91853	-2.01605
H	2.03693	2.68792	-2.05035
H	-2.49675	-0.95113	0.51023
H	-2.45927	0.78044	0.34066
H	-2.31827	-1.24217	-1.98456
H	-2.18619	0.49144	-2.19846
H	-3.68709	-0.20708	-1.60904
H	1.73033	-1.19895	2.45306
H	3.10357	-1.91322	1.62105

H	1.49476	-2.59152	1.41358
H	2.38705	0.19558	0.42910
H	2.15443	-1.19597	-0.59812

$ZnEt_2(THF)$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Zn	-0.09900	-0.17711	0.02925
C	-2.06829	-0.15237	-0.09444
C	1.78025	-0.70835	0.31037
C	-2.60080	-0.29898	-1.52068
C	2.02351	-1.64349	1.49439
O	0.40506	1.90359	-1.01859
C	-0.59629	2.85996	-1.36972
C	1.33259	1.84865	-2.09561
C	-0.61236	2.94026	-2.90425
H	-0.34014	3.82458	-0.92085
H	-1.53620	2.51418	-0.94212
C	0.46107	1.93451	-3.33238
H	-0.35765	3.94673	-3.23757
H	-1.59088	2.69444	-3.31525
H	1.01098	2.24796	-4.21952
H	0.01561	0.95823	-3.53249
H	1.90282	0.92600	-1.99787
H	2.02412	2.69894	-2.03287
H	-2.46655	-0.96054	0.52771
H	-2.45673	0.76953	0.35371
H	-2.30673	-1.25238	-1.96874
H	-2.22178	0.48479	-2.18380
H	-3.69452	-0.25207	-1.57030
H	1.71480	-1.18831	2.43931
H	3.07908	-1.91693	1.60474
H	1.46266	-2.57724	1.39890
H	2.37921	0.20214	0.42398
H	2.14615	-1.18595	-0.60741

$ZnEt_2(THF)_2$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Zn	-0.10810	-0.09174	0.09786
C	-2.08570	-0.18753	-0.18933
C	1.77714	-0.74863	0.26161
C	-2.53758	-0.40448	-1.64057
C	2.02128	-1.76062	1.38976
O	-0.22965	1.44876	1.95279
O	0.47975	1.96394	-0.98863
C	-1.00607	1.07093	3.09210
C	0.98267	2.02766	2.45287
C	1.29679	1.29525	3.77236
H	0.82231	3.09732	2.61906
H	1.73634	1.89635	1.68286
C	0.00861	0.49393	4.07703
H	1.52650	2.00525	4.56540
H	2.15204	0.63262	3.66150
H	-0.31659	0.59413	5.11135
H	0.16145	-0.56497	3.87344
H	-1.76069	0.36734	2.75002
H	-1.50443	1.95667	3.50333
C	-0.57710	2.87736	-1.33989
C	1.34600	1.84028	-2.12344
C	-0.65666	2.88885	-2.88163
H	-0.33679	3.86559	-0.94095
H	-1.48223	2.51462	-0.86094
C	0.39824	1.85402	-3.31413
H	-0.40909	3.87658	-3.26946
H	-1.65179	2.63157	-3.23773

H	0.89331	2.11686	-4.24780
H	-0.05465	0.86946	-3.42989
H	1.91224	0.92136	-2.00064
H	2.03684	2.69060	-2.15117
H	-2.48679	-0.99574	0.43176
H	-2.53910	0.72934	0.20256
H	-2.13715	-1.33432	-2.05223
H	-2.19186	0.39911	-2.29582
H	-3.62717	-0.45173	-1.74725
H	2.43748	0.11551	0.39408
H	2.08287	-1.19913	-0.68918
H	1.76078	-1.34624	2.36658
H	3.06440	-2.09043	1.45369
H	1.41007	-2.65725	1.26199

$ZnEt_2(THF)_2$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Zn	-0.10501	-0.08346	0.10017
C	-2.07256	-0.19811	-0.16863
C	1.76676	-0.74768	0.23930
C	-2.53672	-0.41486	-1.60815
C	2.01754	-1.76752	1.34906
O	-0.22328	1.44801	1.94198
O	0.46880	1.95489	-0.98116
C	-1.00370	1.08905	3.07057
C	0.97385	2.02436	2.44808
C	1.28061	1.29420	3.76243
H	0.81066	3.09497	2.61756
H	1.73712	1.90027	1.68308
C	-0.00605	0.50399	4.05748
H	1.51166	2.00357	4.55723
H	2.13526	0.62774	3.65494
H	-0.33822	0.60175	5.09090
H	0.14032	-0.55690	3.85091
H	-1.77148	0.39554	2.73100
H	-1.48998	1.98474	3.47937
C	-0.57628	2.86103	-1.33740
C	1.34251	1.84410	-2.09682
C	-0.63943	2.88136	-2.87269
H	-0.34419	3.85031	-0.93123
H	-1.48954	2.49673	-0.86944
C	0.41276	1.85185	-3.29311
H	-0.38453	3.87137	-3.25318
H	-1.63242	2.62970	-3.24304
H	0.91628	2.11047	-4.22452
H	-0.03858	0.86464	-3.40807
H	1.91927	0.92970	-1.97022
H	2.02687	2.70215	-2.11722
H	-2.45736	-1.01510	0.45398
H	-2.53920	0.70969	0.23351
H	-2.12220	-1.33332	-2.03370
H	-2.21878	0.40078	-2.26514
H	-3.62691	-0.48572	-1.70232
H	2.43882	0.10994	0.37046
H	2.06130	-1.19240	-0.71962
H	1.77546	-1.36240	2.33610
H	3.05864	-2.10871	1.39563
H	1.39630	-2.65857	1.22296

$ZnClOSi(OSiH_3)_3(THF)_2$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Zn	0.06372	-0.04314	0.15977
Cl	-1.96294	-0.82546	-0.10047
O	1.80588	-0.68997	0.34374

Si	2.62330	-1.90946	-0.24306
O	3.95412	-2.22928	0.65227
O	3.13189	-1.57124	-1.77093
O	1.74543	-3.28421	-0.30856
O	0.03940	1.23017	1.85277
O	0.32095	1.47846	-1.30266
C	-1.00524	0.97406	2.82142
C	1.27251	1.24543	2.61724
C	1.11142	0.13030	3.65572
H	1.35998	2.23130	3.07900
H	2.08397	1.07777	1.91822
C	-0.42041	-0.10675	3.72822
H	1.52860	0.42685	4.61633
H	1.62683	-0.76748	3.32246
H	-0.81173	-0.03493	4.74147
H	-0.67583	-1.09210	3.34133
H	-1.89149	0.67132	2.27264
H	-1.19717	1.90521	3.36025
C	-0.82915	1.77309	-2.13439
C	1.41775	1.27712	-2.23008
C	-0.68503	0.86570	-3.36247
H	-0.78069	2.83154	-2.39864
H	-1.71839	1.57723	-1.54455
C	0.80778	0.44820	-3.35529
H	-0.96198	1.39433	-4.27275
H	-1.32853	-0.00635	-3.26887
H	1.30408	0.62921	-4.30638
H	0.90471	-0.61081	-3.12450
H	2.21871	0.78451	-1.69205
H	1.74433	2.26127	-2.57582
Si	3.59750	-2.29188	-3.16165
H	3.72630	-1.24161	-4.19557
H	2.59094	-3.28556	-3.60150
H	4.90073	-2.97287	-2.98742
Si	5.57134	-2.00007	0.65825
H	5.91600	-0.65382	0.14181
H	6.24232	-3.01547	-0.18519
H	6.05848	-2.12569	2.04913
Si	1.92015	-4.90677	-0.21809
H	1.97931	-5.35163	1.19310
H	3.16767	-5.33052	-0.90008
H	0.76362	-5.54245	-0.88280

$ZnClOSi(OSiH_3)_3(THF)_2$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Zn	0.13039	-0.10105	0.10626
Cl	-1.91260	-0.81078	-0.08471
O	1.85057	-0.78070	0.22962
Si	2.58848	-2.04075	-0.37377
O	3.92780	-2.41240	0.48753
O	3.06355	-1.73135	-1.91234
O	1.66188	-3.37634	-0.40564
O	0.15819	1.16809	1.79431
O	0.38164	1.41686	-1.34004
C	-0.83396	0.95062	2.80802
C	1.40936	1.20824	2.49976
C	1.30604	0.11297	3.55262
H	1.50671	2.20162	2.94876
H	2.20303	1.04491	1.77578
C	-0.21294	-0.07562	3.74718
H	1.81179	0.40254	4.47336
H	1.76941	-0.80228	3.18640

H	-0.52635	0.08823	4.77773
H	-0.51765	-1.08192	3.46086
H	-1.74243	0.61787	2.31074
H	-1.01435	1.90589	3.31089
C	-0.77067	1.78306	-2.11426
C	1.43330	1.22157	-2.29939
C	-0.69948	0.93038	-3.37875
H	-0.69505	2.85163	-2.33679
H	-1.65126	1.59502	-1.50419
C	0.76884	0.46525	-3.43671
H	-0.98732	1.50886	-4.25617
H	-1.37305	0.07765	-3.30200
H	1.24600	0.67309	-4.39370
H	0.83940	-0.60750	-3.25718
H	2.23620	0.68094	-1.80623
H	1.78477	2.20881	-2.61661
Si	3.60056	-2.52699	-3.23154
H	3.63516	-1.56246	-4.35995
H	2.68592	-3.64676	-3.57674
H	4.96513	-3.06980	-3.00703
Si	5.20169	-1.59758	1.09974
H	4.77471	-0.71177	2.21636
H	5.84616	-0.76083	0.05275
H	6.18330	-2.58372	1.61285
Si	1.77849	-4.99990	-0.28709
H	1.86318	-5.41852	1.13569
H	2.98642	-5.49161	-1.00270
H	0.57018	-5.59995	-0.90228

$ZnEtOSi(OSiH_3)_3(THF)_2$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Zn	-0.21653	0.19254	0.20438
C	-2.08198	-0.38946	-0.12472
O	1.60059	-0.18648	0.37075
C	-2.37292	-0.86318	-1.55575
Si	2.69352	-1.27075	0.67804
O	4.10931	-0.55027	1.09423
O	2.99648	-2.23086	-0.61543
O	2.27468	-2.25577	1.92516
O	-0.28272	1.55423	2.04087
O	0.28272	2.04410	-0.93785
C	-0.95589	0.90891	3.13502
C	1.02308	1.92803	2.53955
C	1.39683	0.87651	3.60146
H	0.94766	2.92940	2.96965
H	1.69769	1.93938	1.69107
C	0.11773	0.02535	3.75756
H	1.66927	1.35763	4.53986
H	2.23966	0.27230	3.27892
H	-0.09844	-0.22988	4.79364
H	0.20684	-0.89980	3.18908
H	-1.80899	0.37411	2.72528
H	-1.31056	1.67100	3.83665
C	-0.75559	2.67287	-1.71119
C	1.47305	2.07004	-1.74886
C	-0.43267	2.37221	-3.18852
H	-0.73776	3.74600	-1.50675
H	-1.70410	2.26524	-1.37189
C	0.96967	1.72250	-3.14414
H	-0.42754	3.29019	-3.77429
H	-1.16712	1.70293	-3.63111
H	1.62915	2.08998	-3.92839

H	0.89592	0.64004	-3.24395
H	2.16322	1.35523	-1.31456
H	1.90118	3.07712	-1.71099
H	-2.33301	-1.18721	0.57990
H	-2.74101	0.44618	0.13077
H	-1.76104	-1.72691	-1.82252
H	-2.15319	-0.08633	-2.29205
H	-3.41955	-1.15122	-1.69768
Si	2.86268	-2.97817	3.26489
H	1.74725	-3.66866	3.94837
H	3.44578	-1.97550	4.18720
H	3.90901	-3.96653	2.91526
Si	5.72896	-0.72935	1.05017
H	6.35286	0.55473	1.43840
H	6.19014	-1.09782	-0.30992
H	6.16482	-1.78201	1.99851
Si	3.66917	-3.67853	-0.96101
H	2.66175	-4.76145	-0.88051
H	4.76415	-3.97827	-0.00700
H	4.21912	-3.63189	-2.33333

$ZnEtOSi(OSiH_3)_3(THF)_2$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Zn	-0.13888	0.21867	0.26963
C	-1.97548	-0.44041	-0.03060
O	1.68354	-0.16016	0.31480
C	-2.21911	-0.96413	-1.44587
Si	2.68105	-1.31106	0.69047
O	4.04849	-0.71061	1.36700
O	3.12405	-2.18200	-0.62042
O	2.06708	-2.36228	1.79270
O	-0.15938	1.60179	2.01949
O	0.21293	1.94486	-1.05036
C	-0.82602	1.00158	3.13086
C	1.14650	1.96669	2.49403
C	1.50983	0.95253	3.58629
H	1.09064	2.98476	2.89064
H	1.82354	1.94112	1.64332
C	0.23378	0.11622	3.75445
H	1.77197	1.46366	4.51310
H	2.36011	0.33894	3.29348
H	0.01905	-0.13321	4.79320
H	0.31119	-0.81400	3.18828
H	-1.69837	0.47515	2.74621
H	-1.15340	1.78893	3.82008
C	-0.86178	2.60429	-1.72386
C	1.36011	2.00822	-1.89821
C	-0.53847	2.54118	-3.22402
H	-0.92153	3.63611	-1.36586
H	-1.78094	2.08678	-1.45205
C	0.79360	1.78283	-3.28321
H	-0.43210	3.54654	-3.63300
H	-1.32209	2.03728	-3.78855
H	1.45137	2.14445	-4.07319
H	0.62613	0.71578	-3.44004
H	2.05393	1.24920	-1.54502
H	1.81964	3.00029	-1.80753
H	-2.20345	-1.23040	0.69214
H	-2.67841	0.37053	0.19347
H	-1.57236	-1.81451	-1.67475
H	-2.00846	-0.20279	-2.20355
H	-3.25227	-1.29264	-1.60494

Si	2.56950	-3.11837	3.14788
H	1.44271	-3.93493	3.66305
H	2.96764	-2.13390	4.18928
H	3.72849	-4.00582	2.86579
Si	5.67289	-0.76079	1.27641
H	6.21479	0.55007	1.71477
H	6.12438	-1.03344	-0.11433
H	6.20538	-1.82460	2.16787
Si	3.80536	-3.62416	-0.95837
H	2.78819	-4.70740	-0.94006
H	4.86090	-3.95022	0.03953
H	4.41710	-3.55417	-2.30820
$ZnCl_3^-$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Zn	0.07690	0.18233	-0.51313
Cl	-1.88698	-0.67309	-1.11069
Cl	1.92135	-1.04956	-0.67492
Cl	0.19571	2.26934	0.24554
$ZnCl_3^-$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Zn	0.07677	0.18239	-0.51322
Cl	-1.87008	-0.66588	-1.10555
Cl	1.90541	-1.03883	-0.67348
Cl	0.19488	2.25134	0.23906
$ZnCl_2OSiH_3^-$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Zn	-0.37247	0.18909	0.12583
Cl	0.53170	2.01944	-0.75939
O	0.10018	-0.31776	1.86823
Si	1.15156	0.15878	2.97245
H	1.10429	-0.72812	4.17953
H	0.92215	1.54305	3.49557
H	2.58065	0.13566	2.52519
Cl	-1.82113	-1.07544	-0.98195
$ZnCl_2OSiH_3^-$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Zn	-0.37213	0.18904	0.12538
Cl	0.52586	2.00388	-0.74848
O	0.09537	-0.31788	1.85879
Si	1.14558	0.16274	2.95622
H	1.10394	-0.72264	4.17022
H	0.91532	1.55217	3.47864
H	2.57878	0.14187	2.50622
Cl	-1.80867	-1.06351	-0.97344
$ZnCl(OSiH_3)_2^-$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Zn	0.05238	0.43545	0.25514
O	-1.50553	1.03109	-0.60619
O	1.70243	0.63456	-0.61582
Si	-1.95873	1.58409	-2.03281
Si	2.29953	1.10329	-2.01880
H	-3.35699	2.12182	-1.99093
H	-1.96809	0.54954	-3.11600
H	-1.12324	2.70652	-2.56640
H	3.60451	0.43064	-2.31984
H	2.59104	2.57112	-2.09218
H	1.42342	0.81385	-3.19744
Cl	-0.05744	-0.47227	2.27176
$ZnCl(OSiH_3)_2^-$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Zn	0.05335	0.43625	0.25289
O	-1.49758	1.02558	-0.60316
O	1.69676	0.63387	-0.60885
Si	-1.95833	1.58068	-2.02167
Si	2.29565	1.09811	-2.00783
H	-3.36422	2.11037	-1.97418

H	-1.96413	0.54947	-3.11467
H	-1.12980	2.71486	-2.55549
H	3.60694	0.42587	-2.30463
H	2.58586	2.57068	-2.08673
H	1.42226	0.80321	-3.19370
Cl	-0.05707	-0.46347	2.25207

$ZnCl_2OSi(OSiH_3)_3^-$, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
Zn	-0.24988	0.19360	0.31052
Cl	1.28711	1.74064	-0.18774
Cl	-1.77150	-0.58491	-1.06814
O	-0.08445	-0.37005	2.09779
Si	1.04024	-0.00759	3.14026
O	0.85251	-0.87699	4.52758
O	1.04628	1.56409	3.62600
O	2.56754	-0.34108	2.64352
Si	0.68778	3.08885	3.18416
H	-0.54084	3.16473	2.36219
H	1.80928	3.73052	2.46647
H	0.44627	3.86348	4.43233
Si	1.54365	-0.89958	5.99512
H	1.48813	-2.27929	6.54034
H	0.82808	-0.01168	6.94681
H	2.96533	-0.47417	5.95619
Si	3.87392	0.19508	1.83910
H	3.88590	-0.27271	0.43646
H	5.07462	-0.37744	2.50948
H	4.00056	1.66880	1.88069

$ZnCl_2OSi(OSiH_3)_3^-$, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
Zn	-0.24647	0.19407	0.31928
Cl	1.28574	1.72563	-0.15928
Cl	-1.74836	-0.57295	-1.05797
O	-0.09007	-0.36584	2.09848
Si	1.03863	-0.00673	3.13237
O	0.84900	-0.87494	4.51551
O	1.05480	1.56005	3.62106
O	2.55982	-0.34934	2.63512
Si	0.68158	3.07589	3.17257
H	-0.55364	3.13925	2.34977
H	1.79967	3.72990	2.44961
H	0.43299	3.85469	4.42222
Si	1.54332	-0.88661	5.97755
H	1.45940	-2.26013	6.54666
H	0.84890	0.03418	6.92089
H	2.97879	-0.49244	5.92794
Si	3.85490	0.19914	1.82669
H	3.86606	-0.26739	0.41822
H	5.06546	-0.36889	2.49348
H	3.97421	1.67880	1.87137

THF, B3LYP-D3/cc-pVTZ	***x***	***y***	***z***
O	0.02315	0.01123	0.00790
C	-0.40158	0.81074	1.11863
C	0.02216	0.06066	2.38196
H	-1.48079	0.96011	1.05335
H	0.08388	1.79078	1.05758
C	1.25525	-0.70646	1.89414
H	-0.75773	-0.63762	2.69220
H	0.22796	0.72863	3.21716
C	0.84557	-1.06522	0.46811
H	1.48814	-1.58148	2.49954
H	2.13032	-0.05383	1.88573

H	0.27228	-1.99955	0.44902
H	1.69212	-1.16900	-0.21205

THF, PBE0-D3/cc-pVTZ	***x***	***y***	***z***
O	0.02598	0.01044	0.01537
C	-0.39357	0.80400	1.11683
C	0.02146	0.05529	2.37486
H	-1.47319	0.96194	1.05146
H	0.09643	1.78405	1.06071
C	1.25274	-0.69937	1.88942
H	-0.75805	-0.64900	2.67674
H	0.21845	0.72097	3.21527
C	0.83775	-1.05933	0.47317
H	1.49643	-1.57203	2.49563
H	2.12315	-0.03859	1.87450
H	0.26144	-1.99399	0.46174
H	1.68259	-1.17322	-0.21004

Table S56 Equilibrium geometries of structures with Sn as the central atom.

$Me_3SnOSiH_3$, B3LYP-D3/cc-pVTZ+aug-cc-pVTZ-PP(Sn)	***x***	***y***	***z***
Si	-0.55080	0.77261	-1.31305
O	0.06279	-0.09821	-0.08759
Sn	0.01526	0.00802	1.91530
C	0.30641	-2.03857	2.50878
H	-0.52166	-2.64178	2.14208
H	0.35633	-2.11688	3.59384
H	1.23529	-2.40857	2.07908
C	-1.92856	0.80958	2.40027
H	-2.70065	0.16579	1.98399
H	-2.02804	1.80645	1.97473
H	-2.05412	0.86946	3.48042
C	1.64308	1.32352	2.43233
H	2.54608	0.98398	1.92914
H	1.80776	1.32001	3.50879
H	1.41128	2.33593	2.10781
H	-0.15131	0.16650	-2.60572
H	-0.06643	2.18111	-1.29018
H	-2.03767	0.82830	-1.26317
$Me_3SnOSiH_3$, PBE0-D3/cc-pVTZ+aug-cc-pVTZ-PP(Sn)	***x***	***y***	***z***
Si	-0.55096	0.77381	-1.28718
O	0.07013	-0.10817	-0.07883
Sn	0.01513	0.00816	1.90998
C	0.30124	-2.01704	2.51028
H	-0.52529	-2.62568	2.14539
H	0.34799	-2.09233	3.59684
H	1.23206	-2.39298	2.08688
C	-1.91206	0.80346	2.38575
H	-2.68775	0.15923	1.97334
H	-2.01588	1.80044	1.95808
H	-2.04026	0.86834	3.46656
C	1.62618	1.31369	2.42365
H	2.53410	0.97418	1.92653
H	1.78932	1.31669	3.50156
H	1.39914	2.32728	2.09508
H	-0.15827	0.18085	-2.59324
H	-0.06683	2.18737	-1.25300
H	-2.04252	0.82877	-1.22878
$Me_3SnOSi(OSiH_3)_3$, B3LYP-D3/cc-pVTZ+aug-cc-pVTZ-PP(Sn)	***x***	***y***	***z***
Si	-0.13196	-0.28299	3.51364
O	-0.23045	-0.93863	2.06151
Sn	0.17969	-0.09100	0.27593
C	-1.17169	1.57732	0.11519
H	-2.16072	1.25663	0.43653
H	-1.22509	1.92928	-0.91385
H	-0.83136	2.38327	0.76071
C	-0.22969	-1.71460	-1.07272
H	-1.25398	-2.05009	-0.92315
H	0.45186	-2.53513	-0.85964
H	-0.10069	-1.39657	-2.10587
C	2.25066	0.48436	0.45106
H	2.36441	1.13631	1.31543
H	2.57215	1.01906	-0.44100
H	2.86949	-0.40063	0.58279
O	-1.36813	-0.74679	4.45366

O	-0.14271	1.35324	3.39653
O	1.24479	-0.70069	4.29326
Si	-1.73997	-0.98402	6.03057
Si	0.62687	2.66092	4.01038
Si	2.84405	-0.98079	4.10686
H	-1.19624	0.11549	6.86207
H	-1.17835	-2.26820	6.50562
H	-3.21227	-1.01342	6.15852
H	3.57812	0.30196	4.00490
H	3.09949	-1.77447	2.88291
H	3.33031	-1.72564	5.28694
H	-0.11305	3.86922	3.58809
H	2.00717	2.72560	3.47566
H	0.68576	2.60189	5.48792

$Me_3SnOSi(OSiH_3)_3$, PBE0-D3/cc-pVTZ+aug-cc-pVTZ-PP(Sn)	***x***	***y***	***z***
Si	-0.11530	-0.25466	3.51025
O	-0.21474	-0.92327	2.06788
Sn	0.16732	-0.07506	0.29053
C	-1.42027	1.32198	0.00746
H	-2.37262	0.79527	0.05506
H	-1.33010	1.81423	-0.96059
H	-1.38160	2.06779	0.79971
C	0.11453	-1.75263	-1.02438
H	-0.85757	-2.23805	-0.94893
H	0.89001	-2.46124	-0.73613
H	0.27954	-1.43957	-2.05533
C	2.11517	0.77342	0.51868
H	2.10545	1.51957	1.31212
H	2.43852	1.24733	-0.40832
H	2.82349	-0.01351	0.77680
O	-1.36598	-0.67996	4.44428
O	-0.09508	1.37700	3.37615
O	1.24476	-0.68932	4.30285
Si	-1.71863	-0.90222	6.02461
Si	0.69119	2.64924	4.03694
Si	2.77640	-1.18845	4.03785
H	-1.20688	0.23290	6.83677
H	-1.10770	-2.16129	6.52052
H	-3.19282	-0.98057	6.16149
H	3.66252	-0.01692	3.80950
H	2.84793	-2.07791	2.84883
H	3.24362	-1.92689	5.23541
H	0.07932	3.88997	3.50204
H	2.12912	2.61485	3.65989
H	0.58161	2.63432	5.51757

Me_3SnCl, B3LYP-D3/cc-pVTZ+aug-cc-pVTZ-PP(Sn)	***x***	***y***	***z***
Sn	0.00018	-0.00022	-0.04555
C	2.08223	0.05277	-0.59989
H	2.53272	0.96450	-0.21382
H	2.18195	0.03003	-1.68438
H	2.58930	-0.80882	-0.17133
C	-1.07940	1.78312	-0.59228
H	-0.55396	2.65417	-0.20660
H	-2.07748	1.74486	-0.16190
H	-1.15366	1.85596	-1.67657
C	-0.99505	-1.83226	-0.59114
H	-0.42546	-2.67640	-0.20863
H	-1.06925	-1.90709	-1.67527
H	-1.99237	-1.84413	-0.15727

Cl	-0.00420	-0.00086	2.34415
Me_3SnCl, PBE0-D3/cc-pVTZ+aug-cc-pVTZ-PP(Sn)	***x***	***y***	***z***
Sn	0.00000	-0.00034	-0.04161
C	2.06247	0.05288	-0.59285
H	2.51606	0.96524	-0.20828
H	2.16621	0.02948	-1.67818
H	2.57436	-0.80773	-0.16461
C	-1.06910	1.76593	-0.58722
H	-0.54614	2.64063	-0.20271
H	-2.06969	1.73171	-0.15896
H	-1.14377	1.84084	-1.67253
C	-0.98621	-1.81444	-0.58607
H	-0.41936	-2.66270	-0.20485
H	-1.06099	-1.89123	-1.67120
H	-1.98573	-1.83005	-0.15404
Cl	-0.00336	-0.00079	2.32358
$SnMe_4$, B3LYP-D3/cc-pVTZ+aug-cc-pVTZ-PP(Sn)	***x***	***y***	***z***
Sn	-0.00093	0.00027	-0.00219
C	2.04744	0.04777	-0.71599
H	2.53706	0.96107	-0.38085
H	2.06696	0.01682	-1.80437
H	2.59786	-0.80849	-0.32857
C	-1.06667	1.74332	-0.72931
H	-0.57379	2.65436	-0.39244
H	-2.08968	1.73950	-0.35496
H	-1.09175	1.73944	-1.81823
C	-0.98221	-1.79152	-0.72962
H	-0.43763	-2.67644	-0.40285
H	-1.01551	-1.78325	-1.81838
H	-2.00112	-1.84508	-0.34810
C	0.00865	-0.00146	2.16703
H	0.48523	0.90405	2.54019
H	0.55851	-0.86590	2.53697
H	-1.01081	-0.04524	2.54760
$SnMe_4$, PBE0-D3/cc-pVTZ+aug-cc-pVTZ-PP(Sn)	***x***	***y***	***z***
Sn	-0.00093	0.00025	-0.00217
C	2.02935	0.04747	-0.70987
H	2.52213	0.96088	-0.37590
H	2.05175	0.01663	-1.79933
H	2.58302	-0.80869	-0.32365
C	-1.05710	1.72803	-0.72299
H	-0.56572	2.64177	-0.38752
H	-2.08169	1.72711	-0.34962
H	-1.08393	1.72645	-1.81300
C	-0.97353	-1.77578	-0.72321
H	-0.43034	-2.66339	-0.39762
H	-1.00832	-1.77015	-1.81308
H	-1.99389	-1.83208	-0.34276
C	0.00845	-0.00150	2.14797
H	0.48510	0.90403	2.52437
H	0.55835	-0.86594	2.52119
H	-1.01092	-0.04526	2.53213
$SnMe_3Et$, B3LYP-D3/cc-pVTZ+aug-cc-pVTZ-PP(Sn)	***x***	***y***	***z***
Sn	0.00595	-0.00745	-0.00446
C	2.05367	0.07337	-0.71846
H	2.52560	0.99733	-0.38733
H	2.06993	0.04023	-1.80685
H	2.62256	-0.77070	-0.33115
C	-1.08319	1.73114	-0.71321
H	-0.59917	2.64680	-0.37577

H	-2.10307	1.71298	-0.33130
H	-1.11719	1.73273	-1.80183
C	-0.96203	-1.79390	-0.76691
H	-0.40772	-2.68023	-0.46103
H	-1.00148	-1.76311	-1.85507
H	-1.97878	-1.86504	-0.38249
C	-0.04298	-0.03429	2.17428
C	-1.40911	0.34646	2.74831
H	0.73106	0.64580	2.53344
H	0.24493	-1.03739	2.49340
H	-1.68838	1.36590	2.47580
H	-1.42144	0.28799	3.83989
H	-2.19837	-0.31299	2.38096

$SnMe_3Et$, PBE0-D3/cc-pVTZ+aug-cc-pVTZ-PP(Sn)	***x***	***y***	***z***
Sn	0.00504	-0.00719	-0.00336
C	2.03473	0.07336	-0.71017
H	2.50951	0.99764	-0.38013
H	2.05419	0.04044	-1.79967
H	2.60685	-0.77053	-0.32403
C	-1.07340	1.71678	-0.70608
H	-0.59020	2.63485	-0.37026
H	-2.09521	1.70221	-0.32558
H	-1.10893	1.72034	-1.79583
C	-0.95439	-1.77866	-0.75753
H	-0.40091	-2.66722	-0.45248
H	-0.99602	-1.75139	-1.84686
H	-1.97244	-1.85267	-0.37367
C	-0.04225	-0.03451	2.15684
C	-1.40103	0.34375	2.73116
H	0.73369	0.64461	2.51825
H	0.24742	-1.03830	2.47726
H	-1.68240	1.36426	2.46055
H	-1.41289	0.28459	3.82349
H	-2.19292	-0.31505	2.36512

$SnCl_4$, B3LYP-D3/cc-pVTZ+aug-cc-pVTZ-PP(Sn)	***x***	***y***	***z***
Sn	-0.00019	0.00000	-0.00010
Cl	0.00015	0.00028	2.31500
Cl	1.04580	1.91593	-0.77133
Cl	1.13701	-1.86308	-0.77178
Cl	-2.18229	-0.05313	-0.77154

$SnCl_4$, PBE0-D3/cc-pVTZ+aug-cc-pVTZ-PP(Sn)	***x***	***y***	***z***
Sn	-0.00008	-0.00003	-0.00005
Cl	-0.00003	0.00028	2.29269
Cl	1.03545	1.89748	-0.76402
Cl	1.12592	-1.84515	-0.76443
Cl	-2.16107	-0.05249	-0.76410

$SnCl_3OSiH_3$, B3LYP-D3/cc-pVTZ+aug-cc-pVTZ-PP(Sn)	***x***	***y***	***z***
Sn	-0.02114	0.00187	-0.01817
Cl	1.05870	1.92172	-0.74040
Cl	1.15530	-1.86596	-0.72647
Cl	-2.18557	-0.05577	-0.81885
O	-0.11383	0.00701	1.91923
Si	0.98800	0.01107	3.15243
H	0.22175	0.02697	4.41479
H	1.85268	1.20987	3.06619
H	1.83816	-1.19926	3.08772

$SnCl_3OSiH_3$, PBE0-D3/cc-pVTZ+aug-cc-pVTZ-PP(Sn)	***x***	***y***	***z***
Sn	-0.02167	0.00188	-0.01680
Cl	1.04923	1.90235	-0.73132

Cl	1.14486	-1.84714	-0.71739
Cl	-2.16293	-0.05522	-0.81668
O	-0.11739	0.00695	1.90750
Si	0.98832	0.01106	3.13025
H	0.22974	0.02697	4.40270
H	1.85602	1.21368	3.03897
H	1.84175	-1.20303	3.06062

$SnCl_2(OSiH_3)_2$, B3LYP-D3/cc-pVTZ+aug-cc-pVTZ-PP(Sn)	***x***	***y***	***z***
Sn	-0.03303	0.01598	0.01273
Cl	0.05527	0.09404	2.31801
Cl	-2.00027	0.95923	-0.75227
O	0.07044	-1.84367	-0.53925
Si	0.66563	-2.66048	-1.84334
H	-0.36535	-3.60707	-2.31847
H	1.88634	-3.39787	-1.45349
H	1.00187	-1.71173	-2.93302
O	1.45581	1.01993	-0.72245
Si	2.85091	0.72461	-1.54931
H	2.62972	0.91038	-3.00002
H	3.31054	-0.66418	-1.30700
H	3.87697	1.67455	-1.07093

$SnCl_2(OSiH_3)_2$, PBE0-D3/cc-pVTZ+aug-cc-pVTZ-PP(Sn)	***x***	***y***	***z***
Sn	-0.03173	0.01585	0.01216
Cl	0.05536	0.09756	2.29560
Cl	-1.98326	0.94393	-0.74547
O	0.07320	-1.83304	-0.53055
Si	0.66309	-2.63527	-1.83991
H	-0.36711	-3.58918	-2.31680
H	1.89584	-3.36948	-1.46335
H	0.98689	-1.67400	-2.93041
O	1.44200	1.01895	-0.72162
Si	2.83452	0.70853	-1.53746
H	2.62246	0.88889	-2.99529
H	3.28440	-0.68798	-1.28542
H	3.87086	1.65427	-1.05833

$SnCl(OSiH_3)_3$, B3LYP-D3/cc-pVTZ+aug-cc-pVTZ-PP(Sn)	***x***	***y***	***z***
Sn	-0.02265	0.01139	0.06597
Cl	0.01725	0.00995	2.36205
O	0.11875	-1.81832	-0.58130
Si	0.16084	-2.50330	-2.07986
H	-1.15562	-3.09388	-2.40597
H	1.19974	-3.55443	-2.09063
H	0.48983	-1.47692	-3.10070
O	1.47226	1.04568	-0.61653
Si	2.29219	1.22382	-2.03333
H	1.35171	1.48342	-3.14919
H	3.06727	0.00059	-2.34452
H	3.21040	2.37095	-1.87682
O	-1.70185	0.80047	-0.51828
Si	-2.33559	1.22158	-1.98071
H	-3.72946	1.65513	-1.75416
H	-2.31886	0.06581	-2.91073
H	-1.55586	2.32384	-2.58908

$SnCl(OSiH_3)_3$, PBE0-D3/cc-pVTZ+aug-cc-pVTZ-PP(Sn)	***x***	***y***	***z***
Sn	-0.02410	0.01051	0.06202
Cl	0.02179	0.01342	2.33753

O	0.11399	-1.80954	-0.57397
Si	0.15944	-2.48713	-2.07044
H	-1.16195	-3.07329	-2.40689
H	1.19766	-3.54555	-2.08305
H	0.49754	-1.45408	-3.09036
O	1.46078	1.03897	-0.61415
Si	2.29026	1.21820	-2.01942
H	1.35752	1.47007	-3.15058
H	3.08017	-0.00425	-2.32100
H	3.20250	2.37542	-1.85783
O	-1.69463	0.79351	-0.51132
Si	-2.32766	1.21278	-1.96905
H	-3.72556	1.64933	-1.74280
H	-2.31298	0.05281	-2.90241
H	-1.54508	2.31780	-2.58147

$Sn(OSiH_3)_4$, B3LYP-D3/cc-pVTZ+aug-cc-pVTZ-PP(Sn)	***x***	***y***	***z***
Sn	-0.09059	-0.08988	0.07010
O	-0.17241	-0.08764	2.01068
Si	0.97999	-0.13809	3.18752
H	2.16819	-0.88753	2.71021
H	0.40529	-0.82019	4.36575
H	1.40199	1.23135	3.55934
O	1.75719	0.21501	-0.47593
Si	-0.31412	-2.86604	-1.72875
H	0.64800	-2.23352	-2.66477
H	0.33179	-4.04079	-1.10352
H	-1.51724	-3.29251	-2.47401
O	-0.76753	-1.79214	-0.56410
Si	3.09630	-0.73282	-0.62538
H	3.60087	-0.65621	-2.01337
H	2.75980	-2.14315	-0.30877
H	4.13824	-0.26150	0.31226
O	-1.20377	1.32769	-0.63098
Si	-1.02193	2.96071	-0.78150
H	-0.53411	3.29712	-2.13770
H	-0.05180	3.46811	0.21850
H	-2.34023	3.59081	-0.55883

$Sn(OSiH_3)_4$, PBE0-D3/cc-pVTZ+aug-cc-pVTZ-PP(Sn)	***x***	***y***	***z***
Sn	-0.08956	-0.09094	0.07083
O	-0.17465	-0.08486	1.99834
Si	0.97688	-0.13383	3.16902
H	2.17116	-0.88214	2.68745
H	0.40684	-0.82129	4.35230
H	1.39819	1.24045	3.54325
O	1.74360	0.21783	-0.47542
Si	-0.30274	-2.84544	-1.72208
H	0.66878	-2.20283	-2.65052
H	0.34082	-4.03017	-1.10160
H	-1.50370	-3.26743	-2.48270
O	-0.76165	-1.78369	-0.55538
Si	3.07390	-0.73482	-0.62326
H	3.56971	-0.67971	-2.02057
H	2.73381	-2.14536	-0.28424
H	4.12918	-0.25517	0.30291
O	-1.19906	1.31435	-0.62721
Si	-1.01006	2.94156	-0.77480
H	-0.52650	3.28048	-2.13712
H	-0.02744	3.44358	0.22361
H	-2.32669	3.58251	-0.54196

$SnCl_3OSi(OSiH_3)_3$, B3LYP-D3/cc-pVTZ+aug-cc-pVTZ-PP(Sn)	***x***	***y***	***z***
Sn	0.01111	0.14632	0.08072
Cl	0.03209	2.43638	-0.24271
Cl	2.02342	-0.77167	-0.62523
Cl	-1.74067	-0.80821	-1.08220
O	-0.26184	-0.26201	1.96050
Si	0.84965	-0.19648	3.14667
O	0.15010	0.43451	4.45524
O	2.08237	0.74394	2.65748
O	1.39670	-1.68639	3.45192
Si	0.42061	0.88620	6.00953
H	-0.83793	0.73660	6.76597
H	0.87171	2.29336	6.05176
H	1.46786	0.02232	6.60444
Si	2.41119	-2.65268	4.30184
H	2.90271	-3.72167	3.40983
H	1.68701	-3.24431	5.44690
H	3.55581	-1.86038	4.80832
Si	3.69665	0.84118	2.35971
H	3.90034	1.68257	1.16501
H	4.24997	-0.51100	2.13169
H	4.36504	1.45423	3.52775
$SnCl_3OSi(OSiH_3)_3$, PBE0-D3/cc-pVTZ+aug-cc-pVTZ-PP(Sn)	***x***	***y***	***z***
Sn	0.01530	0.14322	0.08778
Cl	0.04483	2.41282	-0.22335
Cl	2.00083	-0.77096	-0.62620
Cl	-1.72518	-0.78732	-1.06897
O	-0.25942	-0.27390	1.95264
Si	0.84864	-0.19922	3.13513
O	0.14342	0.43020	4.43743
O	2.06922	0.74912	2.64196
O	1.40129	-1.68221	3.44306
Si	0.41958	0.88721	5.98500
H	-0.85092	0.78064	6.73796
H	0.91218	2.28592	6.01855
H	1.44209	-0.00279	6.59709
Si	2.41059	-2.64316	4.29798
H	2.90746	-3.71740	3.40725
H	1.68013	-3.23443	5.44549
H	3.55779	-1.84735	4.80893
Si	3.68279	0.85043	2.36065
H	3.89470	1.70465	1.16994
H	4.24371	-0.50333	2.12409
H	4.34292	1.45699	3.54294

Table S57 Equilibrium geometries of structures with Sb as the central atom.

$SbCl_3$, B3LYP-D3/cc-pVTZ+aug-cc-pVTZ-PP(Sb)	***x***	***y***	***z***
Sb	0.03266	-0.07727	0.00413
Cl	-1.40684	-1.95160	0.12585
Cl	1.45007	-0.64602	1.81206
Cl	1.42246	-0.85442	-1.74613
$SbCl_3$, B3LYP-D3/cc-pVTZ+aug-cc-pVTZ-PP(Sb)	***x***	***y***	***z***
Sb	0.03329	-0.07855	0.00435
Cl	-1.38115	-1.93907	0.12473
Cl	1.43589	-0.65134	1.78791
Cl	1.40877	-0.85720	-1.72160
$SbCl_2OSiH_3$, B3LYP-D3/cc-pVTZ+aug-cc-pVTZ-PP(Sb)	***x***	***y***	***z***
Sb	0.02947	-0.03849	0.01584
Cl	-0.87256	-2.16631	0.58704
Cl	2.21645	-0.78783	-0.53871
O	0.41661	0.55812	1.82707
Si	0.99669	-0.15334	3.21025
H	1.92305	-1.25586	2.87812
H	-0.13046	-0.67521	4.01238
H	1.70736	0.89466	3.97254
$SbCl_2OSiH_3$, B3LYP-D3/cc-pVTZ+aug-cc-pVTZ-PP(Sb)	***x***	***y***	***z***
Sb	0.03141	-0.04098	0.01629
Cl	-0.84841	-2.14430	0.59968
Cl	2.19411	-0.78613	-0.52256
O	0.41750	0.56102	1.81204
Si	0.98676	-0.17118	3.18376
H	1.90619	-1.28359	2.84066
H	-0.14952	-0.69132	3.98335
H	1.71034	0.86384	3.96074
$SbCl(OSiH_3)_2$, B3LYP-D3/cc-pVTZ+aug-cc-pVTZ-PP(Sb)	***x***	***y***	***z***
Sb	-0.27566	0.24543	0.17557
Cl	-1.43373	-1.85245	0.17903
O	0.91286	-0.12012	1.68036
O	0.98320	-0.20785	-1.24353
Si	1.33544	-1.42993	-2.29596
H	2.39410	-0.93081	-3.20020
H	0.13982	-1.79188	-3.09022
H	1.82255	-2.62482	-1.57419
Si	1.73087	-1.45170	2.22740
H	2.88931	-0.96703	3.00835
H	2.20387	-2.27968	1.09630
H	0.85572	-2.26880	3.09576
$SbCl(OSiH_3)_2$, B3LYP-D3/cc-pVTZ+aug-cc-pVTZ-PP(Sb)	***x***	***y***	***z***
Sb	-0.27339	0.24116	0.17457
Cl	-1.39617	-1.84405	0.18272
O	0.90719	-0.11140	1.67027
O	0.98221	-0.20575	-1.23018
Si	1.31631	-1.42645	-2.28343
H	2.37412	-0.93109	-3.19816
H	0.10854	-1.78123	-3.07218
H	1.80307	-2.63101	-1.56670
Si	1.70308	-1.45283	2.21325
H	2.87496	-0.98456	2.99292
H	2.16228	-2.29260	1.07780
H	0.81561	-2.25882	3.08799

$Sb(OSiH_3)_3$, B3LYP-D3/cc-pVTZ+aug-cc-pVTZ-PP(Sb)	***x***	***y***	***z***
Sb	-0.01468	0.01692	-0.00784
O	-1.65268	-0.82719	-0.66002
O	0.51162	-1.60938	0.96732
O	1.10674	-0.31136	-1.58222
Si	1.57604	-1.62965	-2.45904
H	1.81428	-2.79545	-1.58075
H	2.83037	-1.27880	-3.16139
H	0.53980	-1.98425	-3.45536
Si	1.78964	-2.14091	1.85381
H	2.74824	-2.87227	0.99665
H	1.29005	-3.03630	2.91911
H	2.49699	-0.99124	2.47514
Si	-2.17373	-2.39119	-0.76749
H	-1.10960	-3.27279	-1.29787
H	-3.32804	-2.40694	-1.69244
H	-2.60283	-2.89732	0.55584
$Sb(OSiH_3)_3$, PBE0-D3/cc-pVTZ+aug-cc-pVTZ-PP(Sb)	***x***	***y***	***z***
Sb	-0.00884	0.00981	-0.01206
O	-1.63981	-0.81634	-0.66251
O	0.49805	-1.62586	0.92802
O	1.09670	-0.30195	-1.58152
Si	1.56399	-1.61250	-2.46349
H	1.82499	-2.78170	-1.58647
H	2.80994	-1.24765	-3.18303
H	0.51582	-1.97707	-3.45125
Si	1.74858	-2.13676	1.85859
H	2.77592	-2.81764	1.03052
H	1.22798	-3.07708	2.88052
H	2.38867	-0.97634	2.54129
Si	-2.13773	-2.38683	-0.73236
H	-1.06918	-3.26802	-1.27006
H	-3.31122	-2.43157	-1.63950
H	-2.53897	-2.87836	0.61047
$SbCl_2OSi(OSiH_3)_3$, B3LYP-D3/cc-pVTZ+aug-cc-pVTZ-PP(Sb)	***x***	***y***	***z***
Sb	0.49031	-0.00778	-0.13729
Cl	-1.56439	-0.10928	-1.35157
Cl	0.18070	-1.95074	1.17605
O	1.59255	-0.90344	-1.48557
Si	1.78380	-0.41805	-3.03242
O	3.34753	-0.42770	-3.41468
O	1.20914	1.10347	-3.10691
O	0.97820	-1.38040	-4.04984
Si	4.50587	-1.12256	-4.34775
Si	0.23160	2.09181	-3.98930
Si	-0.30765	-2.39915	-4.19656
H	-1.48551	-1.64386	-4.67159
H	-0.60539	-3.03913	-2.89981
H	0.05326	-3.42637	-5.19619
H	4.46708	-2.59388	-4.20048
H	5.81574	-0.60862	-3.89947
H	4.28891	-0.76572	-5.76690
H	-0.86380	1.31402	-4.60282
H	1.02433	2.75573	-5.04704
H	-0.31825	3.10786	-3.06910
$SbCl_2OSi(OSiH_3)_3$, PBE0-D3/cc-pVTZ+aug-cc-pVTZ-PP(Sb)	***x***	***y***	***z***
Sb	0.48296	-0.00799	-0.14227

Cl	-1.54675	-0.13070	-1.34267
Cl	0.18914	-1.94194	1.14036
O	1.58649	-0.89112	-1.47866
Si	1.78945	-0.39553	-3.01552
O	3.35602	-0.39126	-3.38275
O	1.20858	1.11928	-3.08820
O	1.01199	-1.36039	-4.04848
Si	4.42155	-1.17160	-4.35678
Si	0.23924	2.09711	-3.98505
Si	-0.25325	-2.40090	-4.18617
H	-1.44946	-1.66461	-4.66159
H	-0.53745	-3.04391	-2.88164
H	0.12419	-3.42807	-5.18649
H	4.33515	-2.63841	-4.14737
H	5.77938	-0.69431	-4.00653
H	4.13308	-0.86082	-5.77911
H	-0.85423	1.31074	-4.60485
H	1.04206	2.75702	-5.04405
H	-0.32395	3.12109	-3.07389

Ph_3SbCl_2, B3LYP-D3/cc-pVTZ+aug-cc-pVTZ-PP(Sb)	***x***	***y***	***z***
Sb	-0.44570	-0.18238	-0.02458
Cl	-0.67708	2.30050	0.06726
Cl	-0.29266	-2.67810	-0.14693
C	2.11112	0.16557	-4.19470
C	1.15813	-0.83485	-4.04576
C	2.33296	1.07474	-3.16669
C	0.43412	-0.94091	-2.86392
C	1.59634	0.99260	-1.99099
C	0.65563	-0.02132	-1.84459
C	-2.56860	-0.36241	-0.12709
C	-3.27526	0.47734	-0.98044
C	-4.65345	0.33172	-1.08955
C	-5.31712	-0.62425	-0.33009
C	-4.60290	-1.44814	0.53230
C	-3.22101	-1.33120	0.62669
C	0.63956	-0.18830	1.82026
C	0.39818	0.78725	2.78203
C	1.60855	-1.16557	2.02441
C	1.12803	0.77276	3.96534
C	2.34767	-1.15650	3.20142
C	2.10529	-0.19343	4.17299
H	1.77531	-1.93724	1.28840
H	2.67767	-0.19549	5.09089
H	3.10837	-1.90942	3.35722
H	-0.33354	1.55942	2.60197
H	0.93651	1.52404	4.71940
H	-2.76462	1.24370	-1.54479
H	-5.20658	0.97212	-1.76314
H	-6.39079	-0.72822	-0.41066
H	-5.11794	-2.19217	1.12467
H	-2.66297	-2.00182	1.26325
H	1.74261	1.71728	-1.20425
H	2.68075	0.23661	-5.11154
H	3.07487	1.85353	-3.27976
H	0.98129	-1.54192	-4.84493
H	-0.28111	-1.73989	-2.73696

Ph_3SbCl_2, PBE0-D3/cc-pVTZ+aug-cc-pVTZ-PP(Sb)	***x***	***y***	***z***
Sb	-0.44541	-0.18212	-0.02447
Cl	-0.66867	2.27050	0.06583
Cl	-0.28888	-2.64535	-0.14887

C	2.09666	0.15976	-4.17855
C	1.14750	-0.83964	-4.02692
C	2.31663	1.07098	-3.15611
C	0.42644	-0.94321	-2.84687
C	1.58171	0.99191	-1.98278
C	0.64543	-0.02201	-1.83173
C	-2.55122	-0.36047	-0.12409
C	-3.25969	0.48827	-0.96302
C	-4.63440	0.34107	-1.07392
C	-5.29372	-0.62517	-0.32935
C	-4.57921	-1.45801	0.51920
C	-3.20064	-1.34021	0.61368
C	0.62788	-0.18727	1.80710
C	0.39512	0.79308	2.76270
C	1.58725	-1.16910	2.01780
C	1.12196	0.77834	3.94408
C	2.32442	-1.16014	3.19225
C	2.08931	-0.19243	4.15655
H	1.74811	-1.94618	1.28269
H	2.66186	-0.19433	5.07617
H	3.08043	-1.91893	3.35260
H	-0.33188	1.57172	2.57717
H	0.93556	1.53559	4.69560
H	-2.74873	1.26469	-1.51761
H	-5.19025	0.98994	-1.73952
H	-6.36875	-0.73046	-0.41094
H	-5.09331	-2.21230	1.10208
H	-2.63868	-2.02000	1.24080
H	1.72678	1.72038	-1.19614
H	2.66682	0.22904	-5.09702
H	3.05849	1.85144	-3.27213
H	0.97127	-1.55007	-4.82524
H	-0.28867	-1.74465	-2.71551

$Ph_3SbClOSiH_3$, B3LYP-D3/cc-pVTZ+aug-cc-pVTZ-PP(Sb)	***x***	***y***	***z***
Sb	-0.00623	0.05233	-0.03464
O	-0.08801	-0.07159	1.99457
Cl	0.10688	0.21777	-2.54221
C	2.37779	4.32342	0.35749
C	1.44349	4.14539	-0.65597
C	2.63688	3.29198	1.25229
C	0.77363	2.93443	-0.78507
C	1.95392	2.08649	1.14316
C	1.02578	1.91013	0.12153
C	-2.13831	0.00887	-0.07112
C	-2.82873	0.40326	1.07290
C	-4.21871	0.39766	1.06648
C	-4.91238	-0.01635	-0.06475
C	-4.21606	-0.42012	-1.19756
C	-2.82608	-0.39965	-1.20921
C	1.13193	-1.74268	-0.13295
C	0.76533	-2.82985	0.65366
C	2.25199	-1.80844	-0.95433
C	1.52694	-3.99249	0.61703
C	3.01977	-2.96671	-0.97068
C	2.65668	-4.05792	-0.18946
H	2.51355	-0.97423	-1.58878
H	3.25298	-4.96014	-0.21085
H	3.89696	-3.01659	-1.60143
H	-0.10163	-2.77282	1.29607

H	1.23858	-4.84132	1.22208
H	-2.28555	0.69576	1.95789
H	-4.75740	0.71320	1.94995
H	-5.99420	-0.02466	-0.06297
H	-4.75181	-0.74630	-2.07882
H	-2.28415	-0.68612	-2.09728
H	2.14809	1.29447	1.84967
H	2.90523	5.26352	0.44795
H	3.36794	3.42363	2.03849
H	1.23990	4.94584	-1.35438
H	0.07442	2.78470	-1.59406
Si	0.63784	-0.63962	3.32699
H	0.07029	-1.94625	3.74926
H	0.45394	0.32355	4.44135
H	2.09909	-0.83226	3.12631

$Ph_3SbClOSiH_3$, PBE0-D3/cc-pVTZ+aug-cc-pVTZ-PP(Sb)	***x***	***y***	***z***
Sb	-0.00589	0.05021	-0.03537
O	-0.08868	-0.07525	1.97916
Cl	0.10605	0.21478	-2.50817
C	2.35955	4.30680	0.35573
C	1.43213	4.12529	-0.65927
C	2.61479	3.28116	1.25359
C	0.76637	2.91566	-0.78765
C	1.93449	2.07764	1.14565
C	1.01404	1.89583	0.12150
C	-2.12113	0.01123	-0.07259
C	-2.81104	0.40768	1.06789
C	-4.19787	0.40832	1.05968
C	-4.89004	-0.00228	-0.06994
C	-4.19573	-0.40847	-1.19944
C	-2.80889	-0.39322	-1.20913
C	1.12452	-1.73082	-0.13259
C	0.77034	-2.81007	0.66630
C	2.23375	-1.80258	-0.96400
C	1.53164	-3.96931	0.63133
C	3.00221	-2.95664	-0.97801
C	2.65031	-4.03903	-0.18490
H	2.48686	-0.97077	-1.60874
H	3.24930	-4.94136	-0.20443
H	3.87436	-3.01049	-1.61789
H	-0.09275	-2.74879	1.31757
H	1.25096	-4.81481	1.24722
H	-2.26593	0.69935	1.95472
H	-4.73723	0.72708	1.94339
H	-5.97342	-0.00598	-0.06960
H	-4.73259	-0.73304	-2.08244
H	-2.26449	-0.68194	-2.09793
H	2.12592	1.28582	1.85720
H	2.88623	5.24911	0.44591
H	3.34297	3.41644	2.04386
H	1.23060	4.92457	-1.36190
H	0.06970	2.76124	-1.60102
Si	0.64349	-0.64706	3.30320
H	0.06589	-1.95176	3.73555
H	0.47626	0.32287	4.42068
H	2.10670	-0.85296	3.09083

$Ph_3Sb(OSiH_3)_2$, B3LYP-D3/cc-pVTZ+aug-cc-pVTZ-PP(Sb)	***x***	***y***	***z***
Sb	0.02026	-0.07747	-0.06761

O	-0.04252	-0.26472	1.97983
O	0.13209	0.15233	-2.10175
C	2.26415	4.23773	0.58895
C	2.70946	3.37605	-0.40661
C	1.17520	3.88549	1.37750
C	2.06580	2.16228	-0.61804
C	0.53872	2.66605	1.18082
C	0.98427	1.80564	0.18156
C	-2.10270	-0.15417	-0.09041
C	-2.82083	0.10016	1.07617
C	-4.21025	0.07065	1.04745
C	-4.88016	-0.22611	-0.13391
C	-4.16006	-0.49651	-1.29158
C	-2.77087	-0.45738	-1.27370
C	1.10700	-1.89329	-0.25878
C	1.08991	-2.80558	0.79247
C	1.80251	-2.18057	-1.43096
C	1.77545	-4.00878	0.66948
C	2.49496	-3.38122	-1.54058
C	2.48107	-4.29477	-0.49312
H	1.78251	-1.47588	-2.24728
H	3.01637	-5.23051	-0.58460
H	3.03957	-3.60358	-2.44854
H	0.53924	-2.58449	1.69413
H	1.75448	-4.72089	1.48328
H	-2.29315	0.29882	1.99604
H	-4.76836	0.27498	1.95152
H	-5.96161	-0.25093	-0.15103
H	-4.67730	-0.73701	-2.21064
H	-2.21044	-0.66553	-2.17239
H	-0.29383	2.38722	1.81091
H	2.76575	5.18218	0.75127
H	0.82380	4.55521	2.15073
H	3.55837	3.64699	-1.01964
H	2.40576	1.49843	-1.39976
Si	1.07768	-0.10429	3.14951
H	1.11846	-1.33468	3.98167
H	0.75537	1.03967	4.04006
H	2.43935	0.11209	2.59492
Si	-0.30417	1.33579	-3.12892
H	0.87487	1.82861	-3.88604
H	-0.91045	2.49292	-2.42107
H	-1.29972	0.82845	-4.10810

$Ph_3Sb(OSiH_3)_2$, PBE0-D3/cc-pVTZ+aug-cc-pVTZ-PP(Sb)	***x***	***y***	***z***
Sb	0.02000	-0.07690	-0.06926
O	-0.04859	-0.25840	1.96095
O	0.13298	0.14776	-2.08726
C	2.25965	4.21760	0.58158
C	2.70233	3.35852	-0.41321
C	1.17525	3.86591	1.37119
C	2.05988	2.14740	-0.62346
C	0.54046	2.64870	1.17631
C	0.98219	1.79006	0.17710
C	-2.08807	-0.15605	-0.09677
C	-2.80970	0.08244	1.06793
C	-4.19580	0.04800	1.03563
C	-4.85991	-0.23834	-0.14792
C	-4.13767	-0.49352	-1.30404
C	-2.75174	-0.44903	-1.28225

C	1.09610	-1.88188	-0.25305
C	1.08739	-2.78369	0.80399
C	1.77943	-2.18145	-1.42635
C	1.76888	-3.98619	0.68667
C	2.46799	-3.38124	-1.53070
C	2.46249	-4.28273	-0.47684
H	1.75245	-1.48297	-2.25075
H	2.99682	-5.22113	-0.56460
H	3.00475	-3.61318	-2.44269
H	0.54241	-2.55320	1.70980
H	1.75425	-4.69175	1.50822
H	-2.28359	0.27381	1.99282
H	-4.75758	0.24071	1.94175
H	-5.94274	-0.26743	-0.16788
H	-4.65250	-0.72746	-2.22784
H	-2.18645	-0.64825	-2.18303
H	-0.29310	2.36846	1.80854
H	2.76183	5.16369	0.74272
H	0.82484	4.53666	2.14603
H	3.55107	3.63036	-1.02867
H	2.39959	1.48197	-1.40711
Si	1.08338	-0.08947	3.11504
H	1.13300	-1.32015	3.95510
H	0.76762	1.06141	4.00727
H	2.44380	0.12610	2.54357
Si	-0.30673	1.35441	-3.08277
H	0.87534	1.88098	-3.82158
H	-0.93323	2.48884	-2.34552
H	-1.29277	0.85994	-4.08540

$Ph_3SbClOSi(OSiH_3)_3$, B3LYP-D3/cc-pVTZ+aug-cc-pVTZ-PP(Sb)	***x***	***y***	***z***
Sb	0.02628	0.06765	-0.01088
O	0.07579	-0.03186	2.02588
Cl	-0.00774	0.05231	-2.51817
C	2.25368	4.44947	0.17922
C	1.73707	3.98998	-1.02565
C	2.14187	3.66856	1.32272
C	1.11506	2.74869	-1.09447
C	1.51262	2.42988	1.26843
C	1.00609	1.97033	0.05430
C	-2.10037	-0.06917	0.11073
C	-2.71904	0.29575	1.30494
C	-4.10018	0.19613	1.41826
C	-4.85669	-0.27896	0.35357
C	-4.23280	-0.64468	-0.83259
C	-2.85223	-0.53318	-0.96347
C	1.16764	-1.71578	-0.09553
C	0.66319	-2.88282	0.46508
C	2.42493	-1.69470	-0.68475
C	1.43090	-4.04102	0.44045
C	3.19436	-2.85248	-0.69142
C	2.69748	-4.02362	-0.13106
H	2.80648	-0.79124	-1.14000
H	3.29843	-4.92281	-0.14003
H	4.17999	-2.83769	-1.13629
H	-0.31593	-2.89513	0.92392
H	1.04183	-4.95101	0.87645
H	-2.12623	0.63980	2.13745
H	-4.58167	0.48614	2.34255
H	-5.93113	-0.36273	0.44825

H	-4.81812	-1.01487	-1.66346
H	-2.37356	-0.79488	-1.89475
H	1.41275	1.84285	2.16555
H	2.74128	5.41396	0.22744
H	2.53954	4.01973	2.26535
H	1.81613	4.59411	-1.91942
H	0.72472	2.38969	-2.03360
Si	0.73450	-0.63750	3.34276
O	-0.31408	-1.59272	4.14091
O	1.14234	0.59049	4.33487
O	2.07340	-1.51107	3.03657
Si	-1.28659	-2.88600	3.90166
H	-2.06949	-2.72267	2.65480
H	-2.20761	-2.99261	5.05207
H	-0.48307	-4.12537	3.79368
Si	1.33216	1.00580	5.90608
H	1.91981	2.36235	5.94573
H	2.24131	0.05977	6.59286
H	0.02723	1.01597	6.60437
Si	3.69081	-1.32677	2.87099
H	3.99422	-0.39984	1.75739
H	4.28718	-2.64776	2.59141
H	4.27321	-0.77562	4.11719

$Ph_3SbClOSi(OSiH_3)_3$, PBE0-D3/cc-pVTZ+aug-cc-pVTZ-PP(Sb)	***x***	***y***	***z***
Sb	0.02902	0.06381	0.00086
O	0.08334	-0.04253	2.02411
Cl	-0.02900	0.05480	-2.47356
C	2.24839	4.42559	0.18295
C	1.78794	3.93760	-1.02995
C	2.08202	3.67564	1.33680
C	1.16639	2.69942	-1.09536
C	1.45499	2.43919	1.28488
C	1.00283	1.95031	0.06341
C	-2.07975	-0.07078	0.12593
C	-2.69821	0.32728	1.30648
C	-4.07648	0.23297	1.42192
C	-4.83087	-0.27234	0.37367
C	-4.20825	-0.67290	-0.79838
C	-2.83099	-0.56470	-0.93208
C	1.16376	-1.70463	-0.10400
C	0.66682	-2.87669	0.44739
C	2.41148	-1.67844	-0.70857
C	1.43101	-4.03314	0.39754
C	3.17765	-2.83427	-0.73950
C	2.68713	-4.00943	-0.18922
H	2.78809	-0.76807	-1.15945
H	3.28701	-4.91075	-0.21829
H	4.15831	-2.81542	-1.19868
H	-0.30940	-2.89447	0.91804
H	1.04542	-4.95009	0.82591
H	-2.10377	0.69408	2.13125
H	-4.55901	0.55116	2.33805
H	-5.90688	-0.35305	0.47043
H	-4.79437	-1.06849	-1.61884
H	-2.35043	-0.85279	-1.85739
H	1.31477	1.87100	2.19209
H	2.73644	5.39166	0.22936
H	2.43669	4.05073	2.28916
H	1.91020	4.51943	-1.93534

H	0.81332	2.31755	-2.04307
Si	0.73763	-0.63770	3.34578
O	-0.30933	-1.58308	4.15011
O	1.13348	0.59964	4.32562
O	2.07364	-1.51217	3.05420
Si	-1.28315	-2.87083	3.91032
H	-2.07733	-2.69955	2.66480
H	-2.20037	-2.98149	5.06938
H	-0.48021	-4.11578	3.79230
Si	1.30733	1.00567	5.89790
H	1.86938	2.37784	5.94905
H	2.23581	0.07122	6.58513
H	-0.00428	0.98644	6.59371
Si	3.68734	-1.32353	2.88721
H	3.99169	-0.37949	1.78071
H	4.28576	-2.64578	2.58988
H	4.27477	-0.78783	4.14375