Electronic Supplementary Material (ESI) for Dalton Transactions.

Reactivity of an Amidinato Silylene and Germylene toward Germanium(II), Tin(II) and Lead(II) Halides

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1. Selected X-ray crystallographic data refinement.

Compound **6** crystallized in P-1 space group with a formula of 'C23 H45 Cl2 Ge N3 O0.50 Si2 Sn' or 'C19 H37 Cl2 Ge N3 Si2 Sn . 0.50 (C4 H8 O)' which is reasonable and correct. If the Z value is 1, the formula would be doubled and thus contains two Ge complex molecules and one THF molecule.

For compound **2**, the following restraints were used to restrain the geometry and thermal parameters of the toluene molecules.
sadi c57 c59 c57 c63
RIGU C43 > C63
SIMU 0.02 C43 > C63
ISOR 0.02 C43 > C63

2. **Theoretical studies**.
Compounds **2**, **3**, **5** and **6** were investigated using DFT[1] M06-2X[2] method with the LanL08d for Sn, Pb and 6-311+g(d) for other atoms level.[3] All calculations were carried out using the Gaussian 09 packages.[4] The NBO analyses were performed using the NBO 5.0 program at the same level.[5] The optimized geometries are in good agreement with their X-ray crystallographic data.

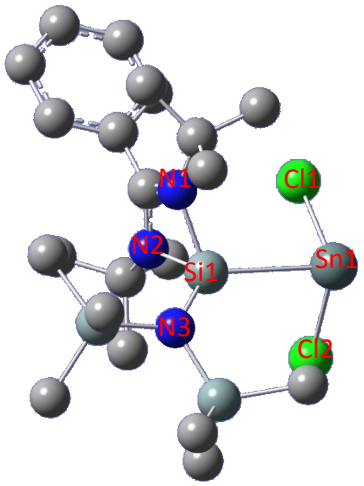


Figure S1. Molecular structure of calculated compound **2**. Hydrogen atoms are omitted for clarity. Selected bond lengths (Å) and angles (°): Si1-Sn1 2.786, Si1-N1 1.853, Si1-N2 1.851, Si1-N3 1.736; Cl1-Sn1-Cl2 96.70, Cl1-Sn1-Si1 86.38, Cl2-Sn1-Si1 87.68, Sn1-Si1-N1 108.86, Sn1-Si1-N2 113.23, Sn1-Si1-N3 125.47, N1-Si1-N2 70.62, N1-Si1-N3 112.62, N2-Si1-N3 112.90.

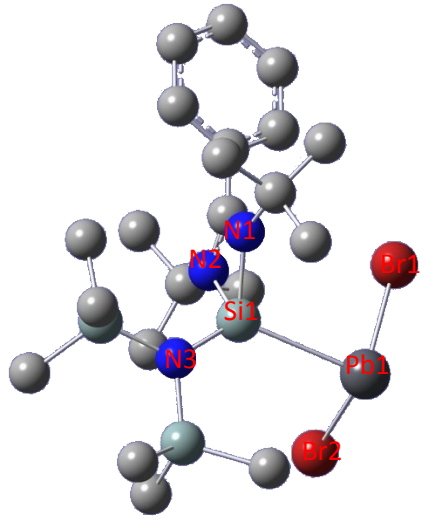


Figure S2. Molecular structure of calculated compound **3**. Hydrogen atoms are omitted for clarity. Selected bond lengths (Å) and angles (°): Si1-Pb1 2.844, Si1-N1 1.857, Si1-N2 1.852, Si1-N3 1.739; Br1-Pb1-Br2 101.93, Br1-Pb1-Si1 86.81, Br2-Pb1-Si1 88.65, Pb1-Si1-N1 110.41, Pb1-Si1-N2 114.75, Pb1-Si1-N3 124.09, N1-Si1-N2 70.54, N1-Si1-N3 111.98, N2-Si1-N3 112.64.

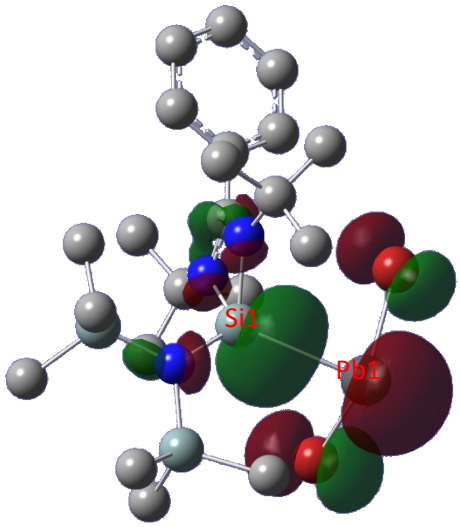


Figure S3. HOMO of calculated compound **3** showing the donor−acceptor interaction between the Si(II) and Pb(II) centres (isovalue = 0.04)

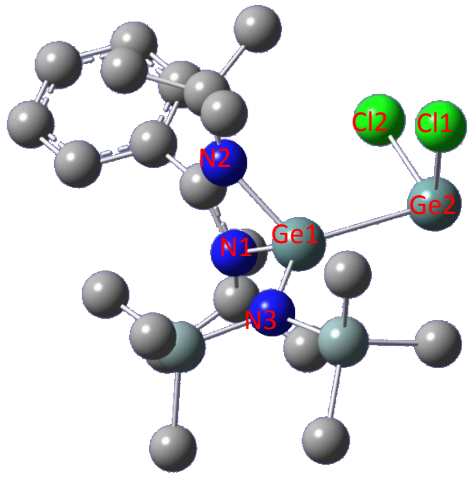


Figure S4. Molecular structure of calculated compound **5**. Hydrogen atoms are omitted for clarity. Selected bond lengths (Å) and angles (°): Ge1–Ge2 2.614, Ge1–N1 1.974, Ge1–N2 1.970, Ge1–N3 1.847; Cl1-Ge2-Cl2 98.90, Cl1-Ge2-Ge1 89.52, Cl2-Ge2-Ge1 87.68, N1-Ge1-N2 66.64, N1-Ge1-N3 111.40, N2-Ge1-N3 111.44, N1-Ge1-Ge2 109.90, N2-Ge1-Ge2 113.79, N3-Ge1-Ge2 127.54.

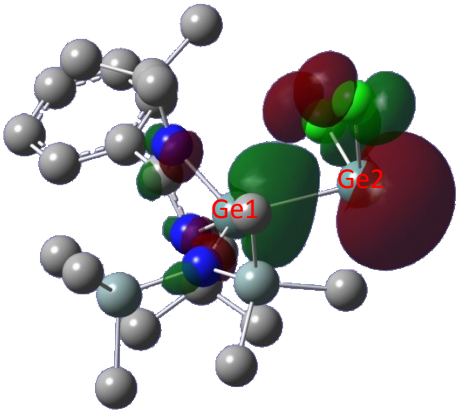


Figure S5. HOMO of calculated compound **5** showing the donor−acceptor interaction between the Ge(II) centres (isovalue = 0.04)

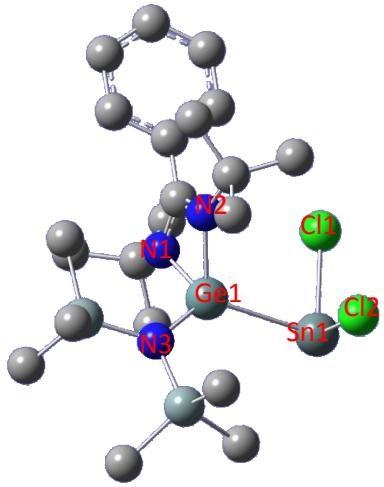


Figure S6. Molecular structure of calculated compound **6**. Hydrogen atoms are omitted for clarity. Selected bond lengths (Å) and angles (°): Ge1–Sn1 2.828, Ge1–N1 1.980, Ge1–N2 1.976, Ge1–N3 1.854; Cl1-Sn1-Cl2 97.95, Cl1-Sn1-Ge1 84.00, Cl2-Sn1-Ge1 85.80, N1-Ge1-N2 66.41, N1-Ge1-N3 110.62, N2-Ge1-N3 110.46, N1-Ge1-Sn1 110.60, N2-Ge1-Sn1 112.95, N3-Ge1-Sn1 128.85.

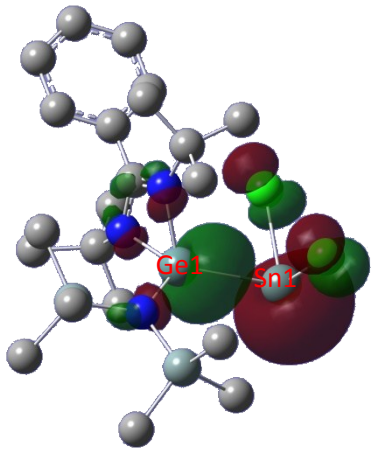


Figure S7. HOMO of calculated compound **6** showing the donor−acceptor interaction between the Ge(II) and Sn(II) centres (isovalue = 0.04)

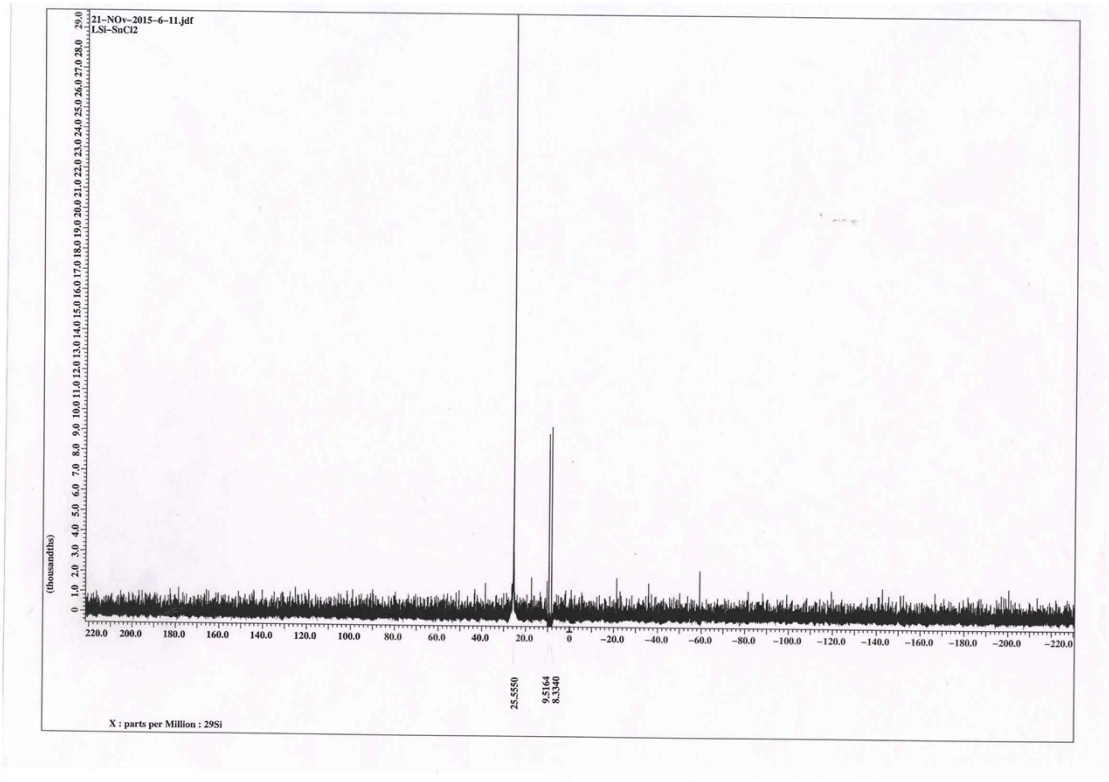
Table S1. NBO analysis of the donor−acceptor Si→E: (E = Sn, Pb) interactions in calculated compounds **2** and **3** and the donor−acceptor Ge→E: (E = Ge, Sn) interactions in calculated compounds **5** and **6**

Bond	Atom	NPA charge	Polarization (%)	s-character (%)	p-character (%)	d-character (%)	Wiberg bond index
Si—Sn: in **2**	Si	1.494	74.17	31.87	67.96	0.17	0.699
	Sn	0.902	25.83	5.76	93.60	0.65	
Si—Pb: in **3**	Si	1.486	74.87	31.87	67.99	0.13	0.678
	Pb	0.869	25.13	4.30	95.50	0.20	
Ge—Ge: in **5**	Ge_{donor}	1.706	61.76	30.86	68.89	0.25	0.849
	$Ge_{acceptor}$	0.529	38.24	6.34	92.19	1.47	
Ge—Sn: in **6**	Ge	1.533	73.12	31.22	68.45	0.33	0.698
	Sn	0.929	26.88	5.11	94.04	0.85	

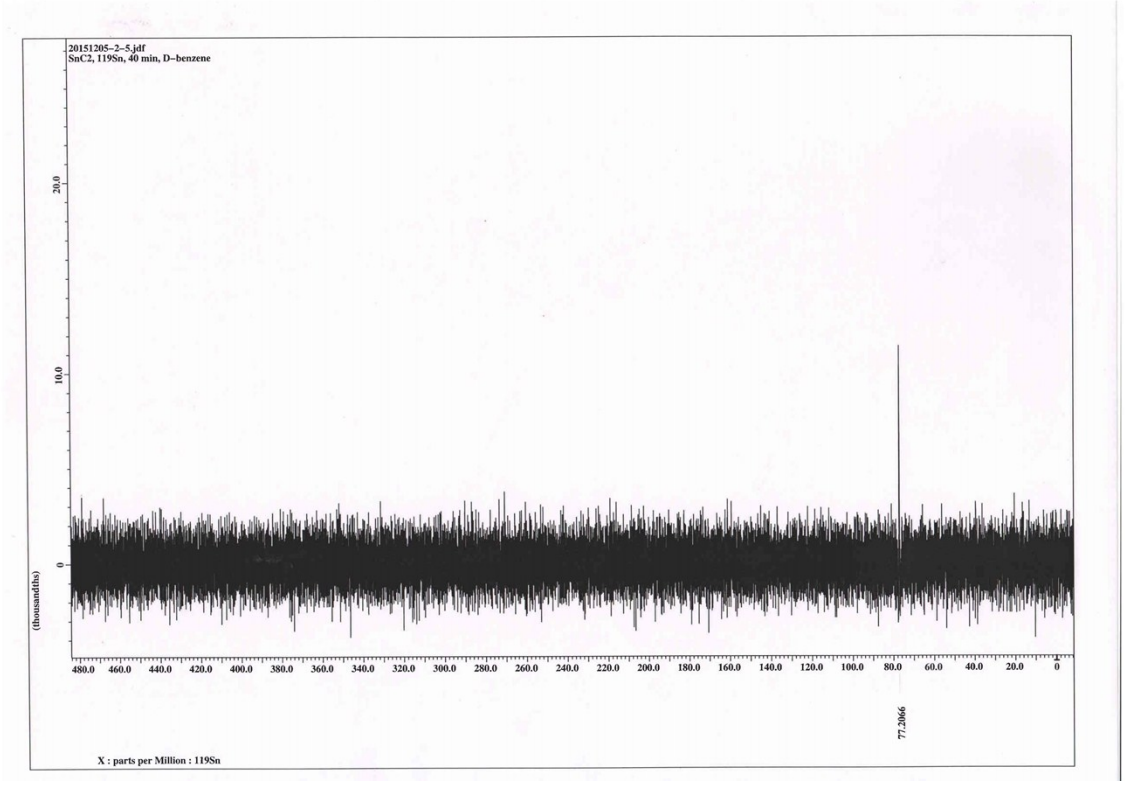
Table S2. The bond dissociation energies (BDEs) of [L{$(Me_3Si)_2N$}$SiEX_2$] (**2**: E = Sn, X = Cl; **3**: E = Pb, X = Br) into [L{$(Me_3Si)_2N$}Si:] and EX_2; the bond dissociation energies of [L{$(Me_3Si)_2N$}$GeECl_2$] (**5**: E = Ge; **6**: E = Sn) into [L{$(Me_3Si)_2N$}Ge:] and ECl_2; the bond dissociation energies of H_3Si-EH_3 into $H_3Si^{\bullet}$ and $H_3E^{\bullet}$ (E = Sn, Pb) and the bond dissociation energies of H_3Ge-EH_3 into $H_3Ge^{\bullet}$ and $H_3E^{\bullet}$ (E = Ge, Sn)

Compound	**2**	**3**	**5**	**6**
BDE	43.94	41.95	34.67	35.93
Compound	SiH_3-SnH_3	SiH_3-PbH_3	GeH_3-GeH_3	GeH_3-SnH_3
BDE	68.34	62.03	64.30	64.57

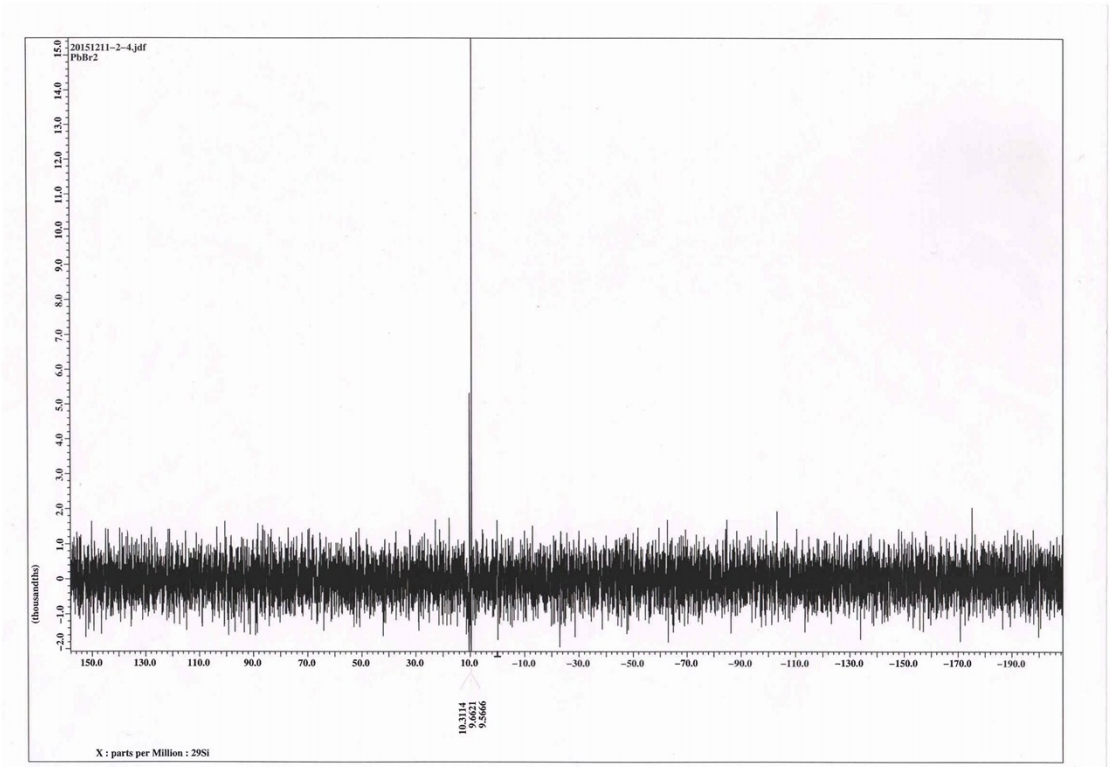
3. Selected NMR spectra of **2**, **3** and **6**



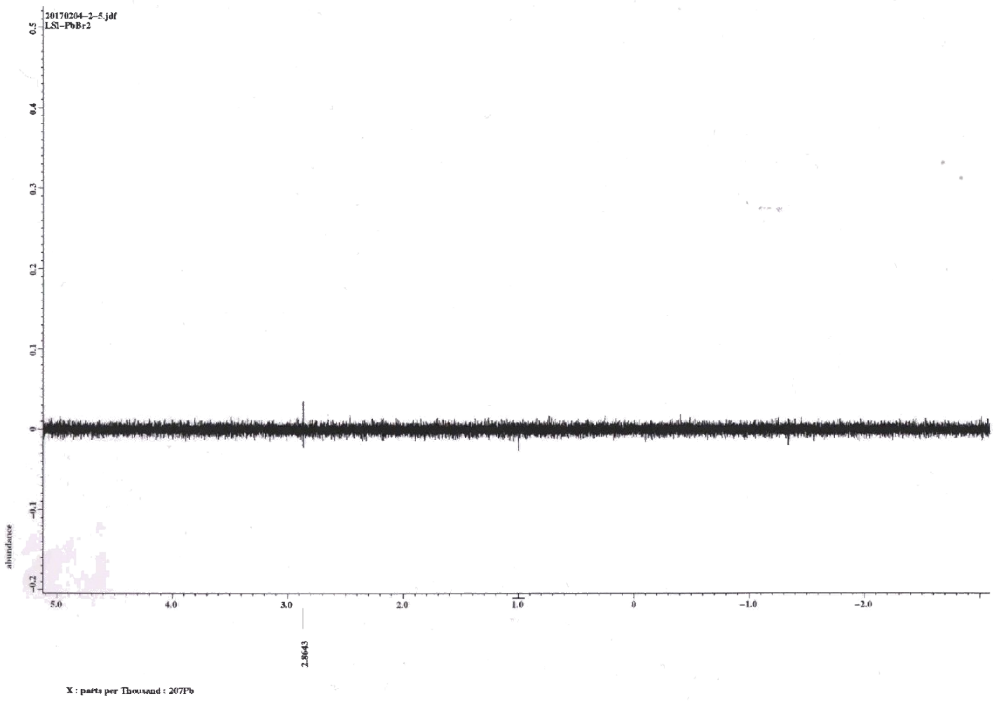
(a) ^{29}Si NMR spectrum of compound **2**



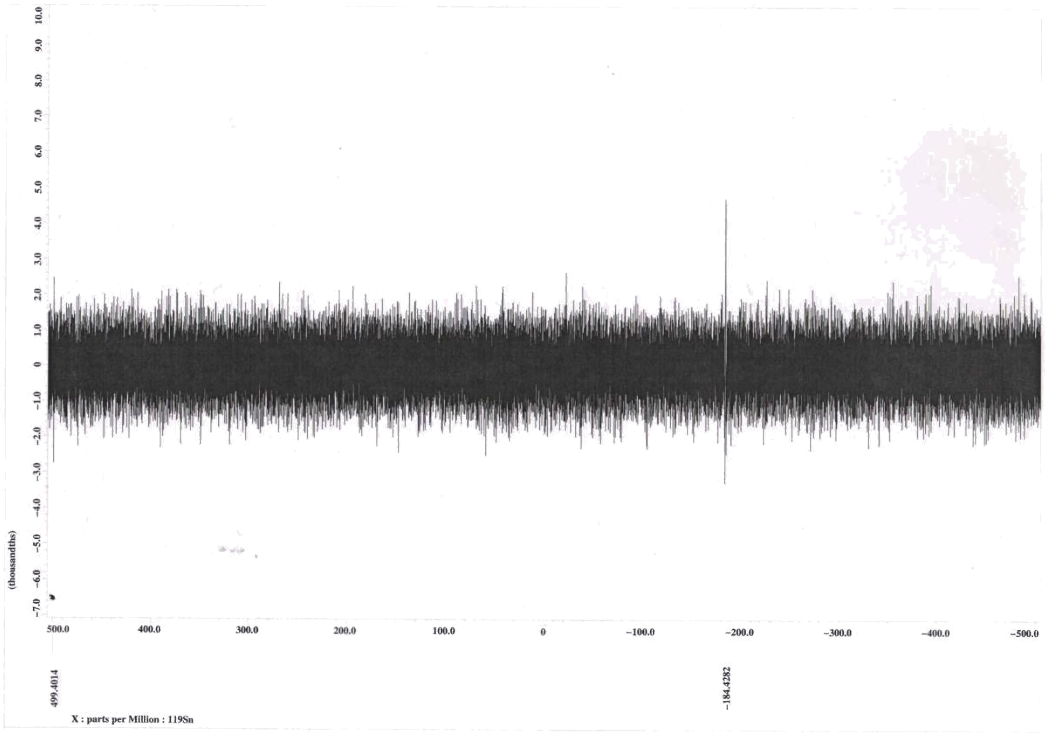
(b) ^{119}Sn NMR spectrum of compound **2**



(c) ^{29}Si NMR spectrum of compound **3**



(d) ^{207}Pb NMR spectrum of compound **3**



(e) ^{119}Sn NMR spectrum of compound **6**

4. Selected crystallographic data of **2**, **3**, **5**, and **6**.

	2	**3**	**5**	**6**
Formula	$C_{28}H_{49}Cl_2N_3Si_3Sn$	$C_{21}H_{41}Br_2N_3PbSi_3$	$C_{21}H_{41}Cl_2Ge_2N_3Si_2$	$C_{23}H_{45}Cl_2GeN_3O_{0.5}Si_2Sn$
M	701.56	786.85	607.83	689.98
Color	colorless	yellow	colorless	colorless
Crystal System	triclinic	monoclinic	monoclinic	triclinic
Space group	P -1	P 1 21/c 1	P 1 21/c 1	P -1
a/Å	10.4822(13)	11.0430(8)	8.7099(14)	9.0571(5)
b/Å	12.7267(14)	17.9127(12)	8.9827 (7)	11.1854(6)
c/Å	26.832(3)	15.2372(10)	18.1042(12)	16.8300(10)
α/deg	90.404(3)	90	90	107.251(2)
ß/deg	90.567(3)	91.423(3)	106.594(2)	98.186(2)
γ/deg	102.754(3)	90	90	104.147(2)
V/Å^3	3490.9(7)	3013.1(4)	2916.0(4)	1570.91(15)
Z	4	4	4	2
d_{calcd}/g cm^{-3}	1.335	1.735	1.385	1.459
μ/ mm^{-1}	1.009	8.384	2.340	2.016
F(000)	1455	1528	1256	704
Crystal size/ mm	0.140 x 0.180 x 0.280	0.180 x 0.260 x 0.340	0.280 x 0.300 x 0.420	0.240 x 0.260 x 0.420
Index range	-13 ≤ *h* ≤ 13	-14 ≤ *h* ≤ 14	-27 ≤ *h* ≤ 26	-14 ≤ *h* ≤ 14

	-17 ≤ *k* ≤ 16 -35 ≤ *l* ≤ 35	-24 ≤ *k* ≤ 24 -15 ≤ *l* ≤ 20	-12 ≤ *k* ≤ 12 -26 ≤ *l* ≤ 26	-17 ≤ *k* ≤ 17 -26 ≤ *l* ≤ 26
No. of reflections collected	17417	43279	56180	70764
R1, wR2 [I > 2σ(I)]	0.0773, 0.1410	0.0404, 0.0690	0.0360, 0.0712	0.0442, 0.0874
R1, wR2 (all data)	0.1434, 0.1655	0.0715, 0.0760	0.0645, 0.0807	0.0708, 0.0976
GOF, F^2	1.053	1.007	1.003	1.081
no. of data/ restraints/ param	17417 / 670 / 774	7806/ 36/ 283	9295/ 0/ 283	12678 / 60 / 328

5. The optimized geometries of compounds **2**, **3**, **5** and **6**

(a) Compound **2**

Standard orientation:

Atom	Coordinates (Angstroms) X	Y	Z
C	-0.985742	0.033630	2.515174
C	0.404558	0.213477	3.126121
H	0.363221	0.049214	4.204431
H	0.787294	1.221034	2.941499
H	1.107456	-0.511794	2.709019
C	-1.949356	1.051936	3.132798
H	-1.897191	0.967089	4.220502
H	-2.983053	0.870776	2.838074
H	-1.680754	2.076754	2.864540
C	-1.488985	-1.385103	2.785068
H	-0.786839	-2.131373	2.413655
H	-2.456256	-1.556910	2.308219
H	-1.608145	-1.528117	3.862549
C	-1.689345	0.461137	0.085079
C	-3.167159	0.558481	0.213991
C	-3.737261	1.817056	0.413190
H	-3.100424	2.692071	0.489648
C	-5.115754	1.943361	0.510115
H	-5.557444	2.921167	0.664462
C	-5.927505	0.816704	0.406885
H	-7.004506	0.916846	0.480659
C	-5.357062	-0.435659	0.212912
H	-5.985607	-1.315463	0.138618
C	-3.975101	-0.571867	0.116362
H	-3.522610	-1.545215	-0.032080
C	-1.396137	0.667767	-2.457461
C	-0.198960	1.274918	-3.193306
H	-0.005748	2.292029	-2.842548
H	-0.389440	1.308920	-4.267611
H	0.707153	0.682220	-3.030223
C	-2.618753	1.566981	-2.665667
H	-3.537434	1.109019	-2.298977
H	-2.740519	1.745178	-3.736578
H	-2.495405	2.535564	-2.175893
C	-1.695375	-0.730594	-3.001333
H	-0.814079	-1.374802	-2.944590
H	-2.000670	-0.668851	-4.049145
H	-2.493404	-1.210042	-2.431775
C	-0.355719	3.419220	0.196734
H	-0.932795	3.194406	-0.700380
H	-0.409087	4.499533	0.366071
H	-0.824318	2.927022	1.049287
C	2.277283	3.691200	1.567467
H	1.813987	3.287113	2.471897
H	2.130080	4.775678	1.587058
H	3.350354	3.509606	1.643713
C	2.085601	3.867164	-1.520466
H	3.031476	4.387142	-1.357262
H	1.356009	4.612805	-1.849841
H	2.235328	3.168119	-2.346481
C	3.909666	0.376304	1.837167
H	3.615514	1.187933	2.507577
H	4.987208	0.223322	1.950226
H	3.416387	-0.538823	2.176646
C	4.619341	2.074762	-0.624857
H	4.452763	2.243440	-1.691454
H	5.645367	1.710555	-0.512383
H	4.569184	3.039952	-0.120937
C	3.860086	-0.785436	-0.985561

H	3.676962	-1.720019	-0.450929
H	4.927993	-0.776428	-1.224997
H	3.323137	-0.806295	-1.937975
Cl	-1.413973	-3.013808	-0.254269
Cl	1.833490	-2.958436	1.512690
N	-0.807229	0.268734	1.064975
N	-0.981860	0.591531	-1.044122
N	1.773865	1.237983	-0.091273
Si	0.546775	0.013178	-0.170809
Si	1.461326	2.982331	0.026210
Si	3.480867	0.735933	0.050489
Sn	0.977363	-2.668456	-0.789829

Rotational constants (GHZ): 0.1252833 0.0994310 0.0784091

(b) Compound **3**

Standard orientation:

Atom	Coordinates (Angstroms) X	Y	Z
Pb	1.605576	-1.768448	-0.813386
Br	-0.749211	-3.052397	-0.411590
Br	2.667939	-1.752483	1.680465
Si	0.224646	0.632386	-0.167738
Si	0.096372	3.742173	0.038960
Si	2.748778	2.326537	-0.112952
C	-1.913357	0.615913	-2.402905
C	-2.609233	1.933678	-2.756622
H	-1.935632	2.783496	-2.620652
H	-3.494084	2.082903	-2.133264
H	-2.934775	1.917592	-3.799641
C	-0.663720	0.457456	-3.274142
H	0.077906	1.228503	-3.039469
H	-0.925938	0.550423	-4.329581
H	-0.211287	-0.527809	-3.129334
C	-2.856571	-0.562219	-2.664597
H	-2.439295	-1.489610	-2.266874
H	-2.988281	-0.676456	-3.743690
H	-3.843286	-0.404937	-2.227568
C	-2.037048	0.350684	0.140885
C	-3.470036	-0.000715	0.321433
C	-4.416858	1.023019	0.334802
H	-4.103188	2.054833	0.226852
C	-5.760876	0.721362	0.521479
H	-6.492883	1.520517	0.540164
C	-6.161430	-0.599741	0.688970
H	-7.210079	-0.833793	0.832805
C	-5.214868	-1.619284	0.673646
H	-5.523115	-2.650583	0.799633
C	-3.868509	-1.325471	0.494245
H	-3.128585	-2.115865	0.461752
C	-1.172885	0.187881	2.552171
C	0.035974	0.923164	3.135635
H	0.073165	0.782504	4.217460
H	-0.017751	1.995261	2.925350
H	0.967746	0.528951	2.720299
C	-1.052641	-1.309412	2.838282
H	-0.137720	-1.718717	2.409622
H	-1.900730	-1.856401	2.423657
H	-1.030673	-1.475413	3.918600
C	-2.458552	0.733588	3.182425
H	-2.361307	0.673407	4.268713
H	-3.337924	0.155196	2.898473
H	-2.632522	1.779480	2.920884
C	-1.718429	3.557838	0.468991
H	-2.287218	3.093712	-0.335040
H	-2.116617	4.567195	0.615097
H	-1.887144	3.000829	1.389938
C	0.161742	4.691913	-1.590099
H	0.994496	5.394875	-1.644284
H	-0.759621	5.264829	-1.730594
H	0.256453	4.009704	-2.439670
C	0.813833	4.770758	1.442881
H	0.629908	4.284645	2.405272
H	0.303374	5.738753	1.469691
H	1.883595	4.971472	1.379475
C	3.298766	3.918158	-0.956238
H	2.995437	3.929753	-2.006933
H	4.392956	3.936437	-0.937406
H	2.958131	4.847348	-0.500099
C	3.402624	2.238955	1.637557
H	2.921370	2.960937	2.301553

H	4.479731	2.429872	1.658675
H	3.242721	1.239027	2.051662
C	3.568341	0.969276	-1.126405
H	3.763310	0.068895	-0.539079
H	4.546810	1.334517	-1.452907
H	3.014705	0.709655	-2.033602
N	-1.430510	0.674075	-1.009431
N	-1.115312	0.440182	1.096128
N	0.970165	2.203087	-0.119412

Rotational constants (GHZ): 0.0977260 0.0846458 0.0630661

(c) Compound **5**

Standard orientation:

Atom	Coordinates (Angstroms) X	Y	Z
Ge	-0.618987	-0.257258	-0.224324
Ge	-0.861705	-2.759928	-0.937261
C	1.417506	0.723587	-2.466138
C	0.282895	0.166446	-3.331207
H	0.196230	-0.917487	-3.208889
H	0.472704	0.370863	-4.386439
H	-0.673366	0.630720	-3.065370
C	2.713227	-0.020030	-2.807529
H	3.589411	0.451435	-2.361187
H	2.850439	-0.012933	-3.891686
H	2.663361	-1.058706	-2.473817
C	1.579344	2.220701	-2.746470
H	0.645861	2.756526	-2.556354
H	1.860138	2.381714	-3.790303
H	2.363365	2.649828	-2.118249
C	1.683629	0.395945	0.056589
C	3.149320	0.597127	0.195027
C	3.656047	1.891984	0.286860
H	2.980014	2.740113	0.265223
C	5.023829	2.088484	0.440663
H	5.417734	3.095036	0.521260
C	5.882307	0.995522	0.496627
H	6.948678	1.150607	0.615181
C	5.373146	-0.296269	0.399532
H	6.041010	-1.149057	0.435979
C	4.006851	-0.500767	0.251706
H	3.601885	-1.502013	0.157196
C	1.084188	-0.206492	2.473846
C	1.579291	-1.640095	2.679074
H	0.876522	-2.364449	2.266861
H	1.692564	-1.838081	3.748444
H	2.548562	-1.791200	2.201129
C	2.076916	0.777022	3.105636
H	3.103510	0.585602	2.792306
H	2.037347	0.662061	4.191164
H	1.831502	1.814465	2.868476
C	-0.288095	-0.041403	3.133632
H	-0.673917	0.971745	2.988335
H	-0.218641	-0.236599	4.205296
H	-1.007123	-0.752221	2.714484
C	-3.843873	-1.132707	-1.070514
H	-3.301741	-1.067033	-2.018147
H	-4.905334	-1.232016	-1.318114
H	-3.559313	-2.059888	-0.567849
C	-4.827200	1.664780	-0.679779
H	-4.858259	2.618592	-0.152475
H	-5.835113	1.240911	-0.632832
H	-4.611471	1.868086	-1.732177
C	-4.095172	-0.079035	1.770778
H	-3.506730	-0.943651	2.094076
H	-5.149647	-0.361326	1.842163
H	-3.915243	0.731978	2.480335
C	-2.193360	3.687521	-1.314213
H	-1.888294	3.148795	-2.216295
H	-1.694462	4.660996	-1.328187
H	-3.266633	3.868021	-1.391139
C	-2.697528	3.312600	1.719880
H	-3.761818	3.075710	1.688474
H	-2.609541	4.400064	1.808022
H	-2.294415	2.880493	2.640543
C	0.069036	3.186454	0.610268
H	0.463429	2.661630	1.480065
H	0.083831	4.258021	0.833713
H	0.736071	3.015106	-0.234241

Cl	-1.543797	-3.284898	1.208341
Cl	1.426535	-2.966804	-0.646551
N	0.980398	0.530661	-1.071512
N	0.854816	0.069220	1.041697
N	-1.964311	0.993267	-0.031242
Si	-3.633292	0.385834	0.015146
Si	-1.708682	2.723176	0.229648

Rotational constants (GHZ): 0.1375700 0.0986256 0.0818144

(d) Compound **6**

Standard orientation:

Atom	Coordinates (Angstroms)		
	X	Y	Z
C	1.525603	0.629064	-2.480904
C	0.342380	0.139604	-3.322020
H	0.151492	-0.923412	-3.146345
H	0.550943	0.269865	-4.385388
H	-0.564778	0.705814	-3.084152
C	2.737676	-0.266460	-2.759784
H	3.658649	0.147188	-2.347629
H	2.871844	-0.358653	-3.840657
H	2.585705	-1.265182	-2.344446
C	1.843165	2.078444	-2.862906
H	0.968292	2.719549	-2.727956
H	2.148959	2.132616	-3.910800
H	2.662062	2.470121	-2.255388
C	1.759874	0.456391	0.057138
C	3.236715	0.566209	0.188303
C	4.021414	-0.577812	0.326172
H	3.553501	-1.555240	0.298916
C	5.397972	-0.452119	0.467281
H	6.008489	-1.342200	0.566162
C	5.990399	0.807145	0.477331
H	7.064570	0.900249	0.590948
C	5.204643	1.946626	0.341756
H	5.661953	2.929202	0.356218
C	3.827392	1.828434	0.194148
H	3.208300	2.715655	0.114799
C	1.117981	0.062313	2.506085
C	2.180131	1.012295	3.072289
H	3.188722	0.736130	2.763875
H	2.143383	0.963520	4.162919
H	1.999537	2.048169	2.776820
C	1.504119	-1.385461	2.817586
H	0.750225	-2.083605	2.453282
H	1.598639	-1.514131	3.899412
H	2.459821	-1.642537	2.358023
C	-0.238862	0.376534	3.143138
H	-0.548436	1.402427	2.922858
H	-0.186188	0.253568	4.226569
H	-1.007118	-0.308049	2.770704
C	0.390065	3.395031	0.384929
H	0.756404	2.886861	1.276718
H	0.486920	4.472512	0.551955
H	1.029417	3.129970	-0.456503
C	-2.341897	3.838857	1.485784
H	-3.424792	3.708727	1.474331
H	-2.144183	4.915250	1.491810
H	-1.975264	3.438224	2.435659
C	-1.834523	3.920050	-1.567860
H	-1.499433	3.327226	-2.424314
H	-1.321786	4.885374	-1.617186
H	-2.900953	4.107606	-1.700884
C	-4.638655	2.158647	-0.738797
H	-4.572683	3.164398	-0.322569
H	-5.676666	1.831442	-0.623844
H	-4.438752	2.225721	-1.811761
C	-3.995871	0.615320	1.865070
H	-3.466589	-0.253649	2.268988
H	-5.066807	0.419074	1.971773
H	-3.749357	1.477232	2.489559
C	-3.895385	-0.733607	-0.848838
H	-3.382163	-0.809196	-1.812176
H	-4.968847	-0.770554	-1.058922
H	-3.672806	-1.620554	-0.250265
Cl	1.389777	-3.000568	-0.345488
Cl	-1.778871	-2.948150	1.610839
Ge	-0.589911	-0.051424	-0.193177
N	1.066597	0.572086	-1.080872
N	0.911541	0.249235	1.056004

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     N         -1.822774    1.327654   -0.068645
     Si        -1.422151    3.044281    0.046405
     Si        -3.530310    0.868956    0.067764
     Sn        -1.040151   -2.789682   -0.736992
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 Rotational constants (GHZ):      0.1213311      0.0966199      0.0754789
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