- Supporting Information-

$LiGe(SiMe_3)_3$: a new Substituent for the Synthesis of Metalloid Tin Clusters from Metastable Sn^I Halide Solution

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1. Quantum chemical calculations

1.1 $Sn_{10}(Ge(SiMe_3)_3)_6$

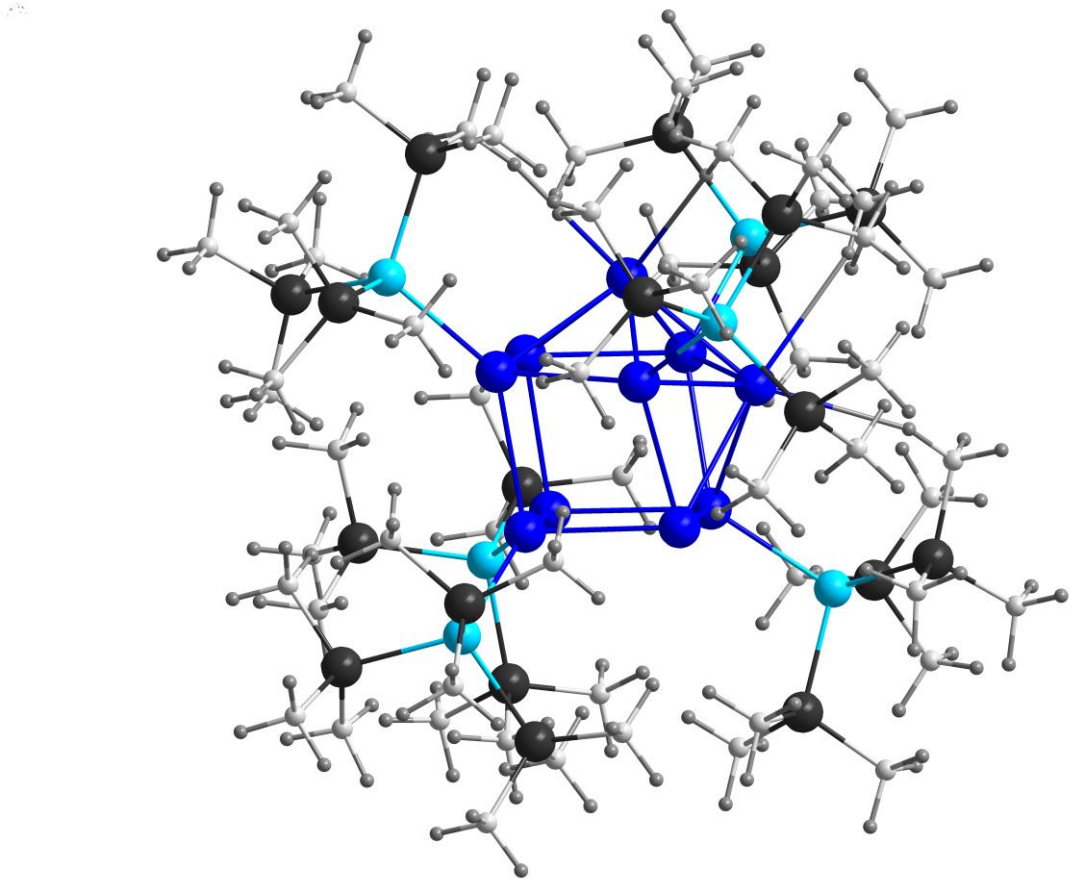

Figure S1: Optimized structure of $Sn_{10}(Ge(SiMe_3)_3)_6$

Point group used:	C_1
Total energy:	-19860.72629796513 H
HOMO-LUMO-gap:	1.065 eV

Atomic coordinates:

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Ge -3.379659 -3.100215 1.366233
Ge 4.327753 -3.075675 -2.346731
Ge -0.291065 1.107265 -5.576807
Ge -2.499995 4.744871 1.541213
Si -0.345671 0.032881 6.735379
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Partial charges:

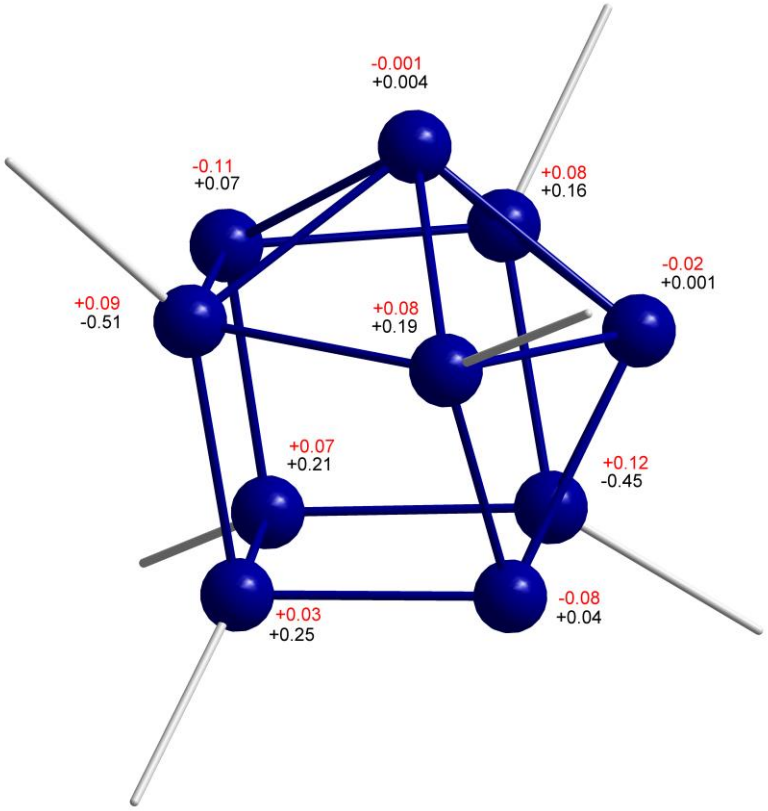

Figure S2: Comparion of the partial charges of the Sn atoms in $Sn_{10}(Si(SiMe_3)_3)_6$ (black) and $Sn_{10}(Ge(SiMe_3)_3)_6$ (red)

atom	charge
1 sn	0.0842
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3 sn	0.1207
4 sn	0.0844
5 sn	0.0775
6 sn	-0.0809
7 sn	-0.0010
8 sn	0.0387
9 sn	-0.0225
10 sn	-0.1138
11 ge	-0.1948
12 ge	-0.1789
13 ge	-0.1839
14 ge	-0.1820
15 ge	-0.1932
16 si	0.4415
17 si	0.4422
18 si	0.4397
19 si	0.4432
20 si	0.4401
21 si	0.4439
22 si	0.4423
23 si	0.4426
24 si	0.4393
25 si	0.4449
26 si	0.4449
27 si	0.4425
28 si	0.4405

29	si	0.4413	85	c	-0.3129
30	si	0.4465	86	c	-0.3234
31	c	-0.3127	87	c	-0.3135
32	c	-0.3293	88	c	-0.3337
33	c	-0.3220	89	h	0.0773
34	c	-0.3245	90	h	0.0506
35	c	-0.3258	91	h	0.0657
36	c	-0.3218	92	h	0.0507
37	c	-0.3217	93	h	0.0631
38	c	-0.3249	94	h	0.0616
39	c	-0.3133	95	h	0.0623
40	c	-0.3209	96	h	0.0517
41	c	-0.3340	97	h	0.0748
42	c	-0.3240	98	h	0.0627
43	c	-0.3246	99	h	0.0612
44	c	-0.3265	100	h	0.0509
45	c	-0.3238	101	h	0.0522
46	c	-0.3247	102	h	0.0847
47	c	-0.3238	103	h	0.0601
48	c	-0.3273	104	h	0.0667
49	c	-0.3257	105	h	0.0497
50	c	-0.3240	106	h	0.0769
51	c	-0.3257	107	h	0.0619
52	c	-0.3242	108	h	0.0634
53	c	-0.3106	109	h	0.0509
54	c	-0.3133	110	h	0.0520
55	c	-0.3134	111	h	0.0737
56	c	-0.3319	112	h	0.0615
57	c	-0.3191	113	h	0.0675
58	c	-0.3141	114	h	0.0845
59	c	-0.3128	115	h	0.0547
60	c	-0.3123	116	h	0.0508
61	c	-0.3288	117	h	0.0624
62	c	-0.3138	118	h	0.0629
63	c	-0.3289	119	h	0.0615
64	c	-0.3250	120	h	0.0516
65	c	-0.3237	121	h	0.0628
66	c	-0.3267	122	h	0.0633
67	c	-0.3248	123	h	0.0516
68	c	-0.3144	124	h	0.0612
69	c	-0.3136	125	h	0.0651
70	c	-0.3128	126	h	0.0506
71	c	-0.3137	127	h	0.0924
72	c	-0.3139	128	h	0.0516
73	c	-0.3219	129	h	0.0847
74	c	-0.3123	130	h	0.0625
75	c	-0.3260	131	h	0.0684
76	ge	-0.1944	132	h	0.0801
77	si	0.4412	133	h	0.0511
78	si	0.4420	134	h	0.0533
79	si	0.4440	135	h	0.0868
80	c	-0.3260	136	h	0.0604
81	c	-0.3138	137	h	0.0787
82	c	-0.3229	138	h	0.0527
83	c	-0.3232	139	h	0.0608
84	c	-0.3249	140	h	0.0628

141 h	0.0520	196 h	0.0617
142 h	0.0626	197 h	0.0797
143 h	0.0517	198 h	0.0504
144 h	0.0621	199 h	0.0651
145 h	0.0626	200 h	0.0631
146 h	0.0772	201 h	0.0513
147 h	0.0517	202 h	0.0629
148 h	0.0610	203 h	0.0801
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151 h	0.0840	206 h	0.0624
152 h	0.0819	207 h	0.0637
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174 h	0.0621	229 h	0.0520
175 h	0.0516	230 h	0.0783
176 h	0.0627	231 h	0.0508
177 h	0.0506	232 h	0.0594
178 h	0.0745	233 h	0.0622
179 h	0.0674	234 h	0.0632
180 h	0.0819	235 h	0.0513
181 h	0.0530	236 h	0.0614
182 h	0.0600	237 h	0.0760
183 h	0.0532	238 h	0.0509
184 h	0.0839	239 h	0.0581
185 h	0.0620	240 h	0.0901
186 h	0.0615	241 h	0.0516
187 h	0.0511	242 h	0.0757
188 h	0.0518	243 h	0.0519
189 h	0.0627	244 h	0.0628
190 h	0.0618	245 h	0.0611
191 h	0.0841	246 h	0.0516
192 h	0.0504	247 h	0.0634
193 h	0.0661	248 h	0.0645
194 h	0.0516	249 h	0.0494
195 h	0.0754	250 h	0.0790

1.2. $Sn_{10}(Ge(SiMe_3)_3)_4^{2-}$

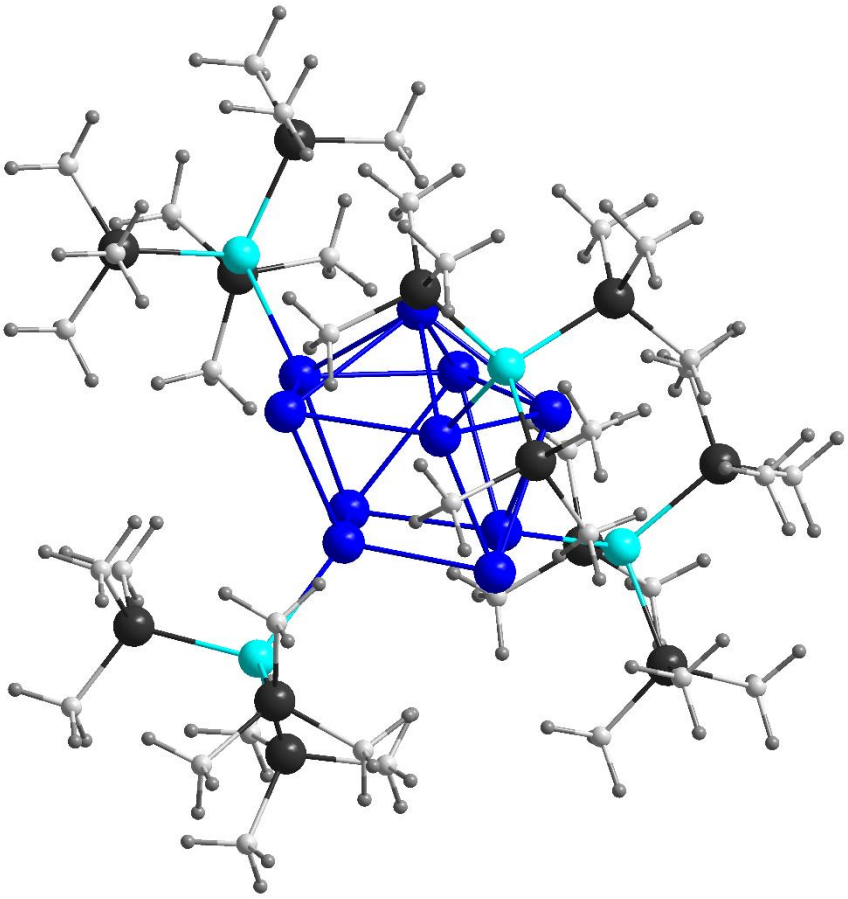

Figure S3: Optimized structure of $Sn_{10}(Ge(SiMe_3)_3)_4^{2-}$

Point group used:	C_1
Total energy:	-13252.12355283562 Hartree
HOMO-LUMO-gap:	1.657 eV

Atomic coordinates:

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Si 3.452065 -5.106277 0.883333
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C -2.298042 4.463307 -3.777521
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Partial charges:

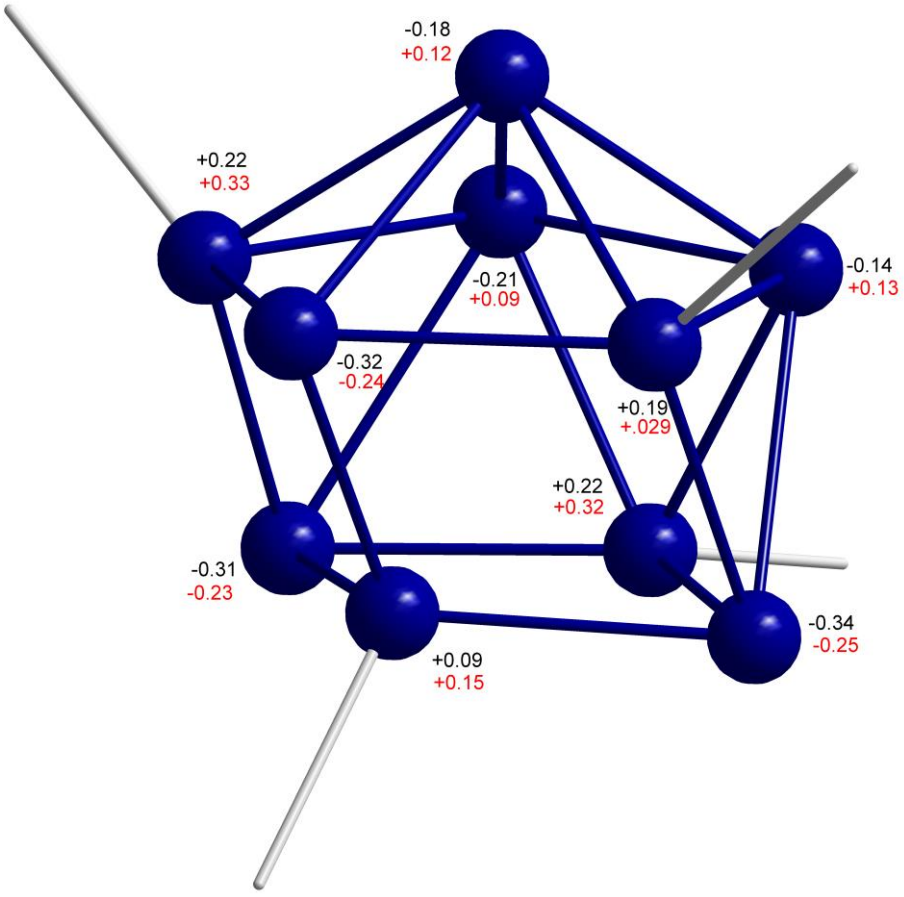


Figure S4: Comparion of the partial charges of the Sn atoms in $Sn_{10}(Si(SiMe_3)_3)_4^{2-}$ (black) and $Sn_{10}(Ge(SiMe_3)_3)_4^{2-}$ (red)

atom	charge
1 sn	-0.1316
2 sn	-0.1869
3 sn	0.1974
4 sn	-0.3370
5 sn	0.1784
6 sn	-0.1537
7 sn	-0.3175
8 sn	0.2027
9 sn	0.1180
10 ge	-0.2592
11 sn	-0.3268
12 ge	-0.2620
13 ge	-0.2569
14 ge	-0.1682
15 si	0.4335
16 si	0.4377
17 si	0.4314
18 si	0.4320
19 si	0.4339
20 si	0.4373
21 si	0.4315
22 si	0.4374
23 si	0.4338
24 si	0.4383
25 si	0.4386
26 si	0.4389
27 c	-0.3165
28 c	-0.3104
29 c	-0.3219
30 c	-0.3167
31 c	-0.3223
32 c	-0.3105
33 c	-0.3103
34 c	-0.3092
35 c	-0.3165
36 c	-0.3105
37 c	-0.3179
38 c	-0.3169
39 c	-0.3171
40 c	-0.3181
41 c	-0.3106
42 c	-0.3173
43 c	-0.3105
44 h	0.0311
45 c	-0.3092
46 c	-0.3105
47 c	-0.3160
48 c	-0.3100
49 c	-0.3173
50 c	-0.3185
51 c	-0.3173
52 c	-0.3100
53 c	-0.3183
54 c	-0.3103
55 c	-0.3167
56 c	-0.3219
57 c	-0.3105
58 c	-0.3165
59 c	-0.3091
60 c	-0.3178
61 c	-0.3099
62 c	-0.3177
63 h	0.0520
64 h	0.0311
65 h	0.0519
66 h	0.0495
67 h	0.0761
68 h	0.0319
69 h	0.0549
70 h	0.0300
71 h	0.0915
72 h	0.0318
73 h	0.0519
74 h	0.0512
75 h	0.0482
76 h	0.0330
77 h	0.0912
78 h	0.0523
79 h	0.0310
80 h	0.0954
81 h	0.0513
82 h	0.0521
83 h	0.0319
84 h	0.0547
85 h	0.0957
86 h	0.0320
87 h	0.0472
88 h	0.0904
89 h	0.0339
90 c	-0.3171
91 h	0.0520
92 h	0.0949
93 h	0.0330
94 h	0.0482
95 h	0.0902
96 h	0.0519
97 h	0.0511
98 h	0.0317
99 h	0.0905
100 h	0.0474
101 h	0.0336
102 h	0.0551
103 h	0.0942
104 h	0.0317

105 h	0.0319	138 h	0.0494
106 h	0.0513	139 h	0.0758
107 h	0.0521	140 h	0.0319
108 h	0.0518	141 h	0.0299
109 h	0.0312	142 h	0.0919
110 h	0.0520	143 h	0.0548
111 h	0.0920	144 h	0.0483
112 h	0.0299	145 h	0.0345
113 h	0.0545	146 h	0.0883
114 h	0.0321	147 h	0.0966
115 h	0.0760	148 h	0.0341
116 h	0.0493	149 h	0.0569
117 h	0.0549	150 h	0.0501
118 h	0.0936	151 h	0.0329
119 h	0.0318	152 h	0.0526
120 h	0.0336	153 h	0.0884
121 h	0.0474	154 h	0.0484
122 h	0.0906	155 h	0.0345
123 h	0.0319	156 h	0.0329
124 h	0.0513	157 h	0.0501
125 h	0.0520	158 h	0.0526
126 h	0.0910	159 h	0.0955
127 h	0.0330	160 h	0.0569
128 h	0.0480	161 h	0.0343
129 h	0.0519	162 h	0.0525
130 h	0.0317	163 h	0.0329
131 h	0.0510	164 h	0.0501
132 h	0.0951	165 h	0.0345
133 h	0.0519	166 h	0.0883
134 h	0.0310	167 h	0.0484
135 h	0.0518	168 h	0.0341
136 h	0.0312	169 h	0.0567
137 h	0.0521	170 h	0.0958

2. NMR

2.1 $Sn_{10}(Ge(SiMe_3)_3)_6$ 1

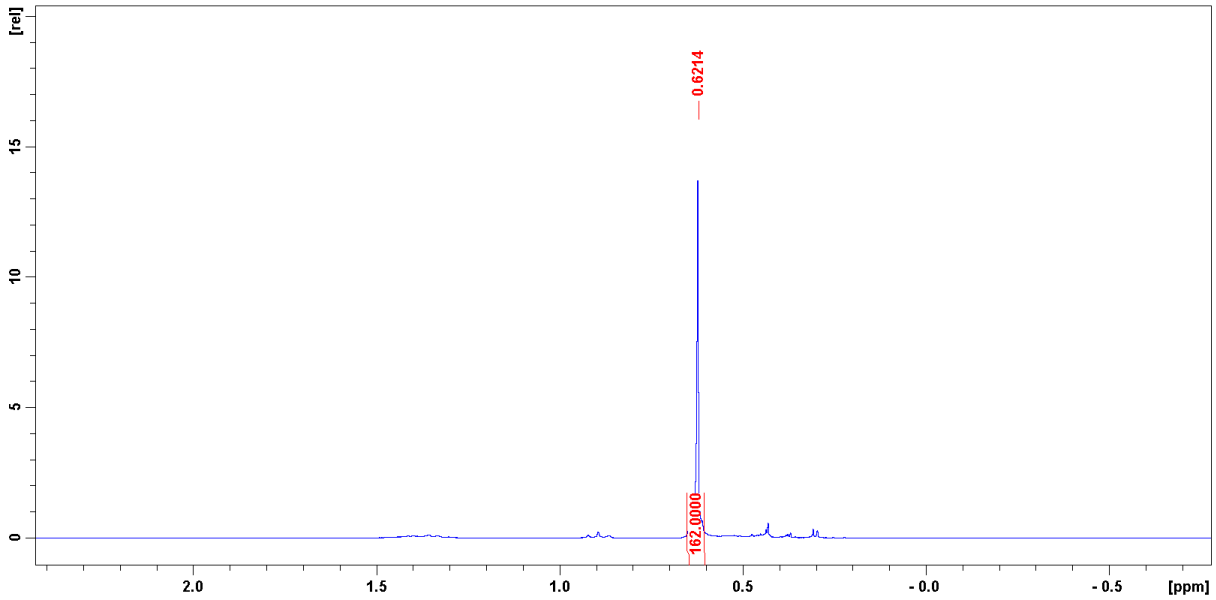


Figure S5: ^{1}H-NMR of **1** dissolved in C_6D_6. The signal at δ = 0.62 ppm shows the Ge(Si*Me*$_3$)$_3$ ligand.

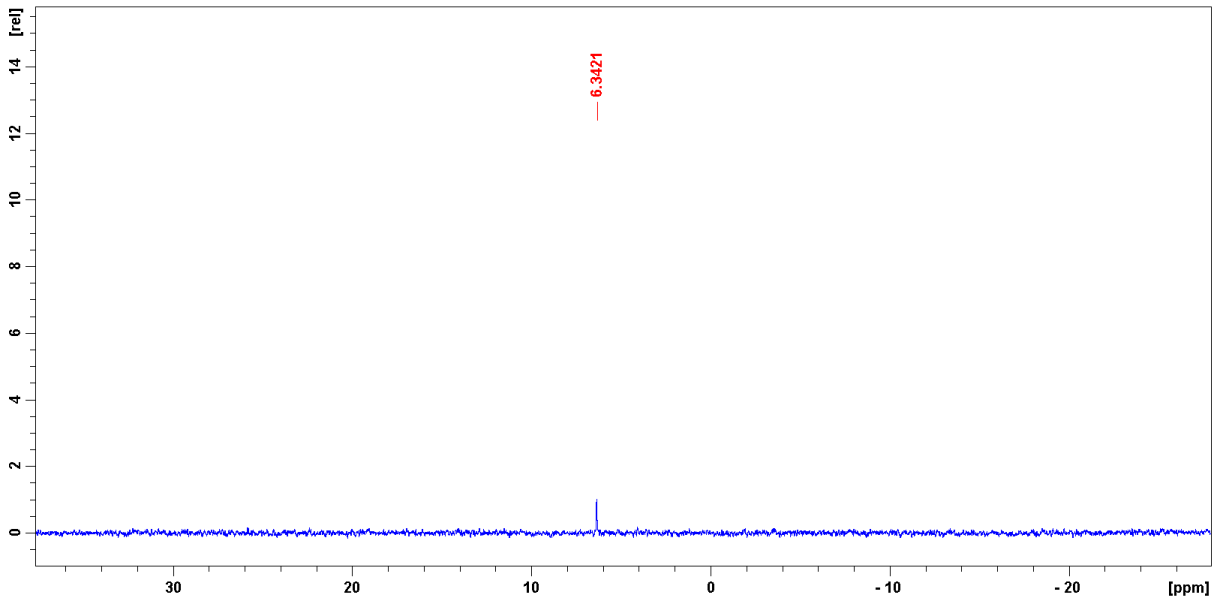


Figure S6: ^{13}C-NMR of **1** dissolved in C_6D_6. The spectra shows one signal at δ = 6.34 ppm for Ge(Si*Me*$_3$)$_3$.

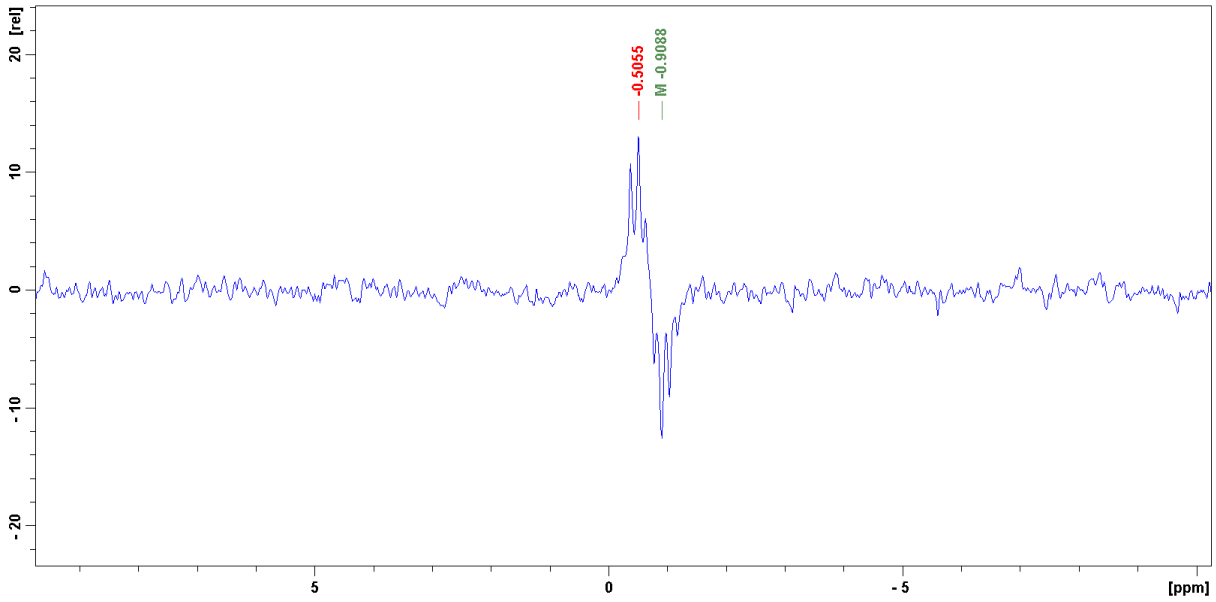


Figure S7: ^{29}Si-IneptND-NMR spectra of **1** dissolved in C_6D_6. The spectra shows a decet at δ = -0.13– -1.29 ppm for Ge(*Si*Me$_3$)$_3$ with $^2J_{Si-H}$ = 6.5 Hz.

2.2. $Sn_{10}(Ge(SiMe_3)_3)_4^{2-}$ 3

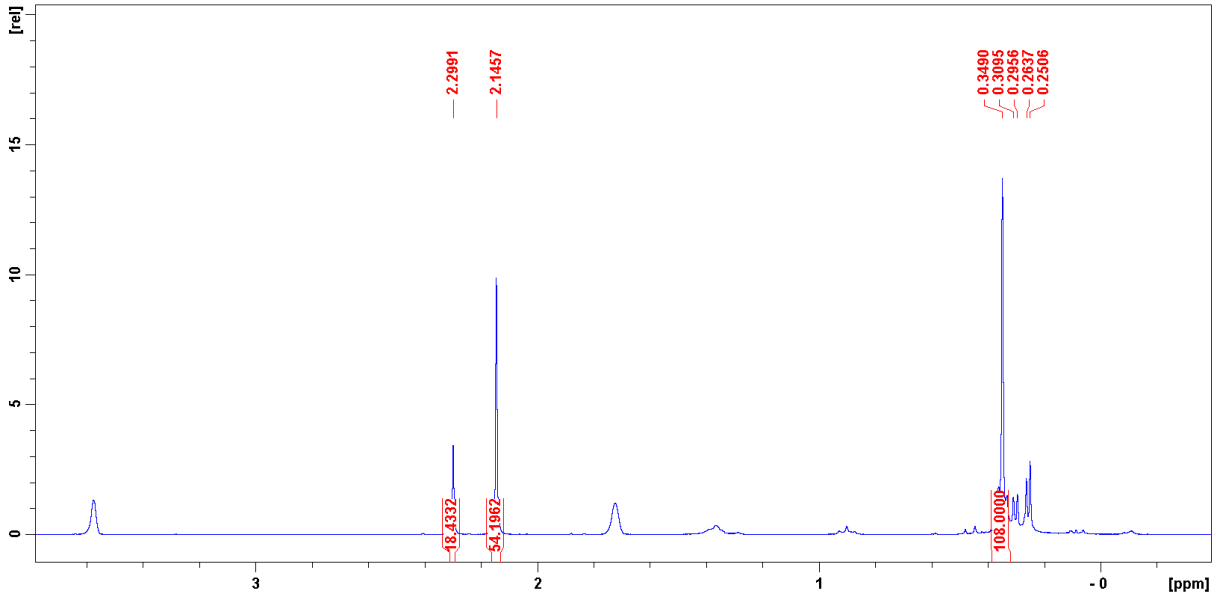


Figure S8: ^{1}H NMR spectra of the concentrated sample of **3**•2[Li(TMEDA)$_2$] in THF-d$_8$ directly after preparation. The signal at δ = 0.35 ppm represents the Ge(Si*Me*$_3$)$_3$, whereby the signals for tmeda can be found at 2.15 ppm and 2.30 ppm An impurity of Si(SiMe$_3$)$_4$ can be observed at 0.25/0.26 ppm.

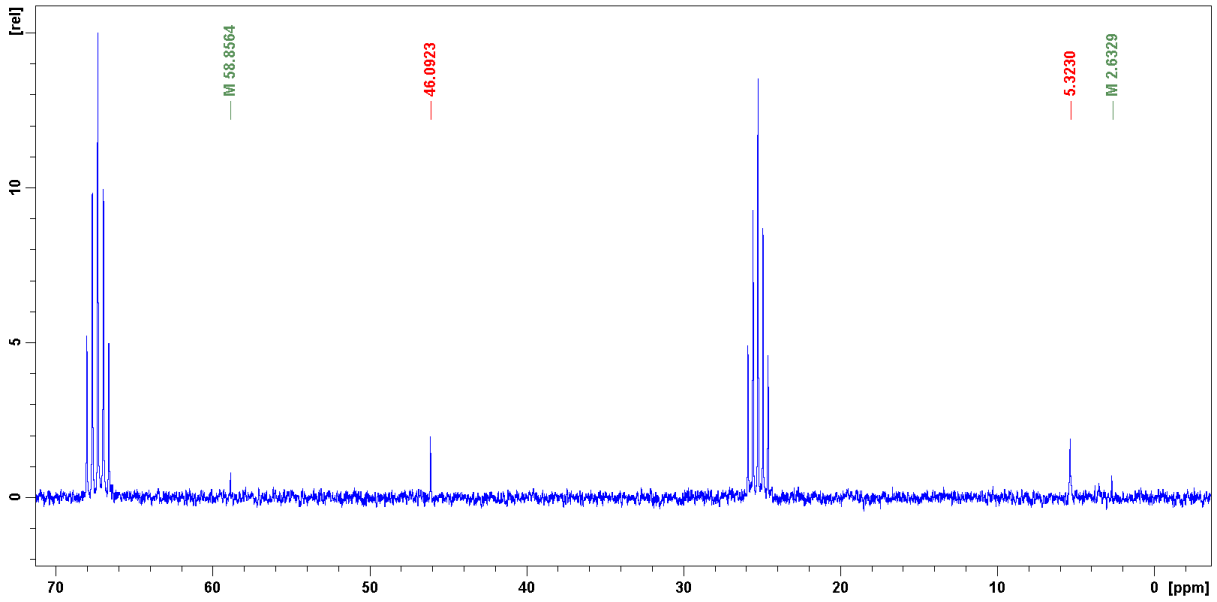


Figure S9: ^{13}C-NMR spectra of **3**•2[Li(TMEDA)$_2$] in THF-d$_8$. The signal at δ = 5.32 ppm represents the Ge(Si*Me*$_3$)$_3$ ligand. The signals for tmeda can be found at 2.15 ppm and 2.30 ppm. An impurity of Si(SiMe$_3$)$_4$ can be observed at 2.63 ppm.

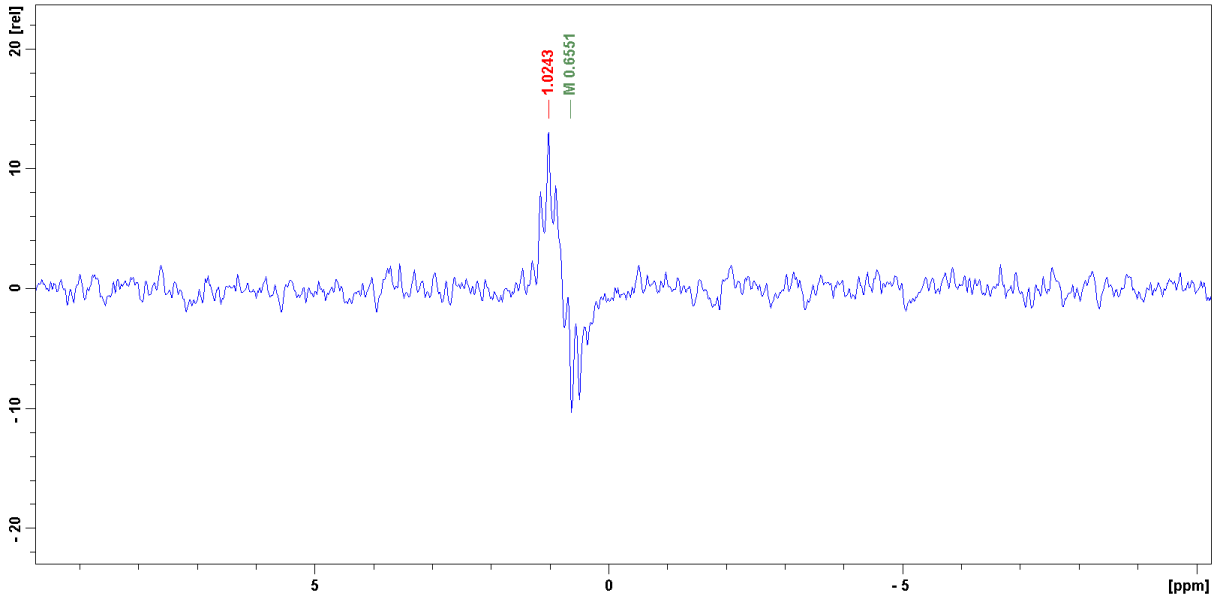
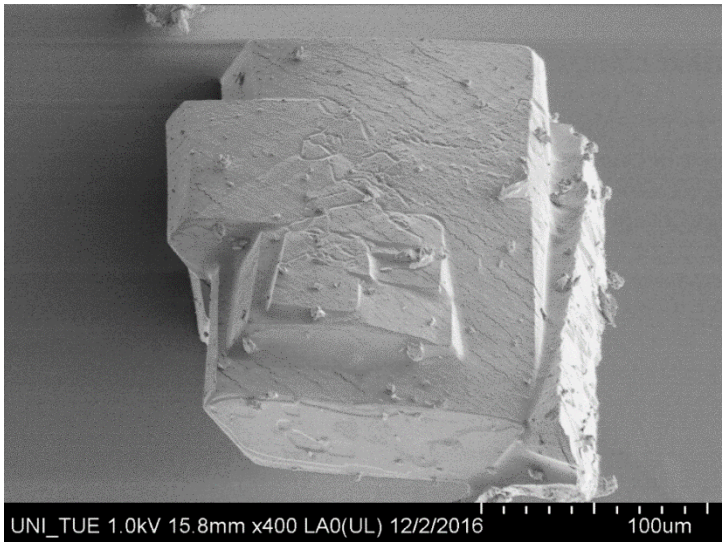


Figure S10: ^{29}Si-IneptND-NMR spectra of **3**•2[Li(TMEDA)$_2$] dissolved in THF-d$_8$. The spectra shows a decet at δ = 0.27 – 1.37 ppm for Ge(*Si*Me$_3$)$_3$ with ^{2}J $_{Si-H}$ = 6.5 Hz.

3. Energy dispersive X-ray spectroscopy (EDX)

3.1. $Sn_{10}(Ge(SiMe_3)_3)_5^-$ 2



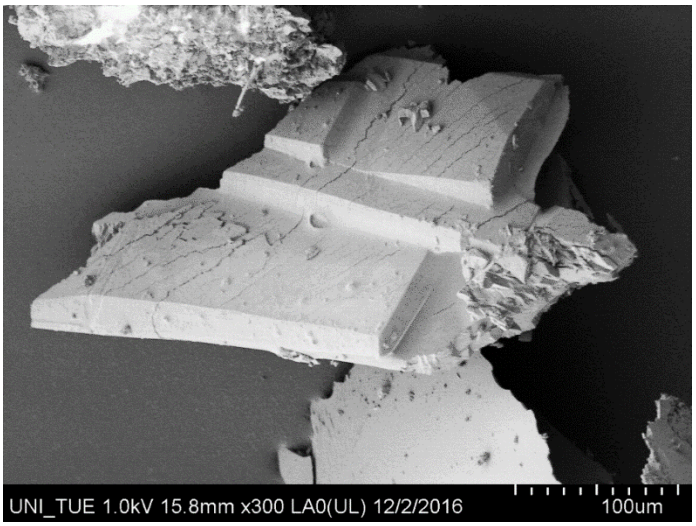


Figure S11**:** SEM-Image of a block shaped single crystal of **2** consisting of layers. The EDX measurements were performed at 7 different areas. Device: HITACHI SU8030 scanning electron microscope with Bruker-EDX

Table S1: Results of the EDX measurements of the crystallite at 7 different areas:

Element	Norm.Wt.%	Atoms calculated	Setpoint
Sn	56.89%	9,44	10
Ge	20.81%	5,65	5
Si	22.30%	15,65	15

4. Bond lenght comparison of $Sn_{10}[Ge(SiMe_3)_3]_4\}^{2-}$ 3 and $\{Sn_{10}[Si(SiMe_3)_3]_4\}^{2-}$.

Table S2: Comparison of the bond lengths in pm of the metalloid clusters $\{Sn_{10}[Ge(SiMe_3)_3]_4\}^{2-}$ **3** and $\{Sn_{10}[Si(SiMe_3)_3]_4\}^{2-}$.

$\{Sn_{10}[Ge(SiMe_3)_3]_4\}2-$ 3		**$[Sn_{10}(Hyp)_4]2-$**	
Sn1-Sn2	293.3	Sn1-Sn2	293.4
Sn3-Sn4	293.8	Sn3-Sn4	292.8
Sn6-Sn8	290.8	Sn6-Sn8	294.9
Sn3-Sn8	293.2	Sn3-Sn8	294.8
Sn5–Sn10	302.3	Sn5-Sn10	302.9
Sn4-Sn7	292.4	Sn4-Sn7	290.3
Sn9-Sn10	302.3	Sn9-Sn10	302.0
Sn8-Sn10	327.4	Sn8-Sn10	326.5
Sn6-Ge4	266.5	Sn6-Si4	263.1