

Supporting Information

for

Synthesis and exploration of a 1*H*-germol-1-ide/pyridine bidentate ligand

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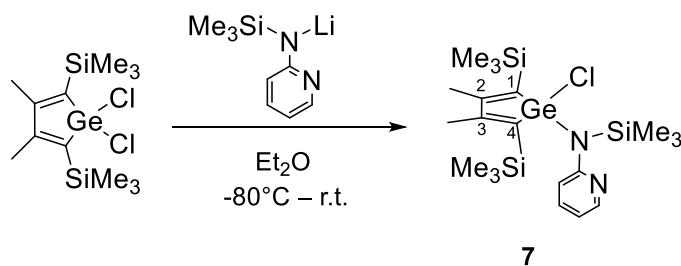
Experimental Part

General. All manipulations of air- and moisture-sensitive compounds were carried out under an argon 5.0 or nitrogen 5.0 atmosphere using Schlenk techniques or a standard glove box (Braun Unilab). Glassware was dried in an oven at $T = 120\text{ }^{\circ}\text{C}$ and evacuated prior to use. The solvents THF, diethylether and *n*-hexane were dried over sodium and distilled under a nitrogen atmosphere. Benzene- d_6 was stored over molecular sieves (4 Å) after drying over potassium. All used standard chemicals were obtained from commercial suppliers and used as delivered if not mentioned otherwise. Dichlorogermole^[S1] and $\text{PyN}(\text{SiMe}_3)\text{Li}$ ^[S2] were prepared according to modified literature procedures.

NMR spectroscopy. NMR spectra were recorded on Bruker Avance DRX 500 and Bruker Avance III 500 spectrometers. ^1H NMR spectra were calibrated against the residual proton signal of the solvent as internal reference (Benzene- d_6 : $\delta\ ^1\text{H}(\text{C}_6\text{D}_5\text{H}) = 7.15$; and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra by using the central line of the solvent signal (Benzene- d_6 : $\delta\ ^{13}\text{C}(\text{C}_6\text{D}_6) = 128.06$. $^{29}\text{Si}\{^1\text{H}\}$ NMR spectra were calibrated against an external standard ($\delta\ ^{29}\text{Si}(\text{Me}_2\text{SiHCl}) = 11.1$ versus tetramethylsilane (TMS). $^{119}\text{Sn}\{^1\text{H}\}$ NMR were referenced to an external standard tetramethyltin(IV) ($\delta\ ^{119}\text{Sn}(\text{Me}_4\text{Sn in C}_6\text{D}_6) = 0$). The $^{29}\text{Si}\{^1\text{H}\}$ NMR inverse gated spectra were recorded with a relaxation delay $D1 = 10\text{ s}$.

Mass spectrometry: Mass spectra were recorded on a Waters Q-ToF Premier (ESI-MS) and Thermo Scientific DFS (CI-/EI-MS). The used method for each compound is given in the experimental part.

Synthesis of 7:



Scheme S1

7. A solution of Germole-Cl₂ (258 mg, 0.7 mmol, 1 eq.) in Et₂O (6 mL) was slowly added to a solution of PyN(SiMe₃)Li (137 mg, 0.7 mmol) in Et₂O (10 mL) at -80 °C. The reaction mixture was allowed to warm to room temperature and reacted for overnight. The solvent was removed under vacuum. The residue was re-dissolved in n-hexane (15 mL) and the filtrate was removed solvent to get brown solid **7**. Yellow single crystals suitable for XRD investigations were obtained from the evaporation of n-hexane solvent of compound **7**. Yield: 250mg (0.50 mmol, 71%).

NMR spectra for **7** recorded in C₆D₆ at 305 K.

¹H NMR (499.9 MHz, 305.0 K, C₆D₆): δ = 0.24 (s, 18 H, C-Si(CH₃)₃), 0.56 (s, 9 H, N-Si(CH₃)₃), 1.96 (s, 6H, CH₃), 6.21 (m, 1H, Py), 6.57 (d, 1H, Py), 6.94 (m, 1H, Py), 7.49 (m, 1H, Py).

¹³C{¹H} NMR (125.8 MHz, 305.0 K, C₆D₆): δ = 0.70 (C-SiMe₃), 3.41 (N-SiMe₃), 19.83 (CH₃), 112.65, 114.74, 137.80 (Py), 139.38(C^{1/4}), 145.61 (Py), 154.71 (C^{2/3}), 161.96 (Py).

²⁹Si{¹H} NMR (99.4 MHz, 305.0 K, C₆D₆): δ = -8.54 (C-SiMe₃), 7.15 (N-SiMe₃).

EA: C/H/N [%] calculated for C₂₀H₃₇ClGeN₂Si₃: 48.25/7.49/5.63;

found:48.34/7.63/5.46.

HR-MS (ESI): m/z calculated for C₂₀H₃₇ClGeN₂Si₃ +H: 499.1238; found: 499.1233.

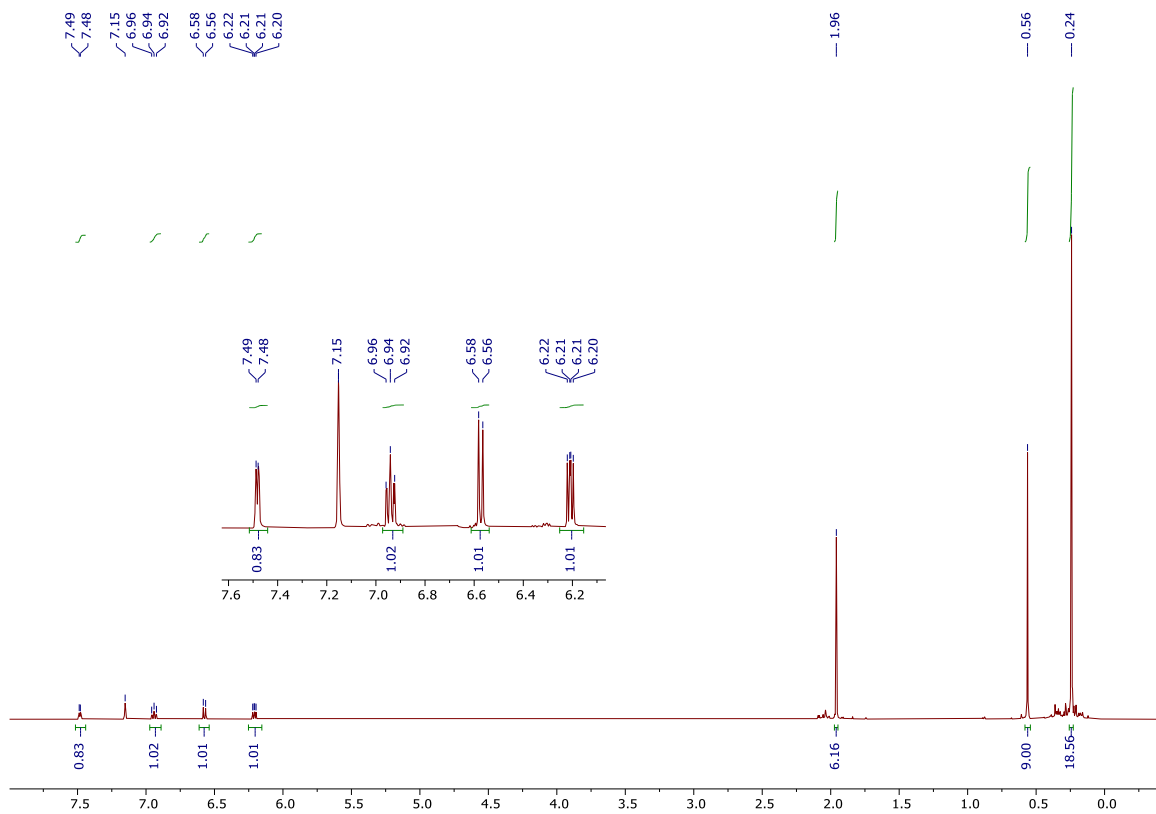


Figure S1a. ^1H NMR (499.9 MHz, 305.0 K, C_6D_6) spectrum of **7**.

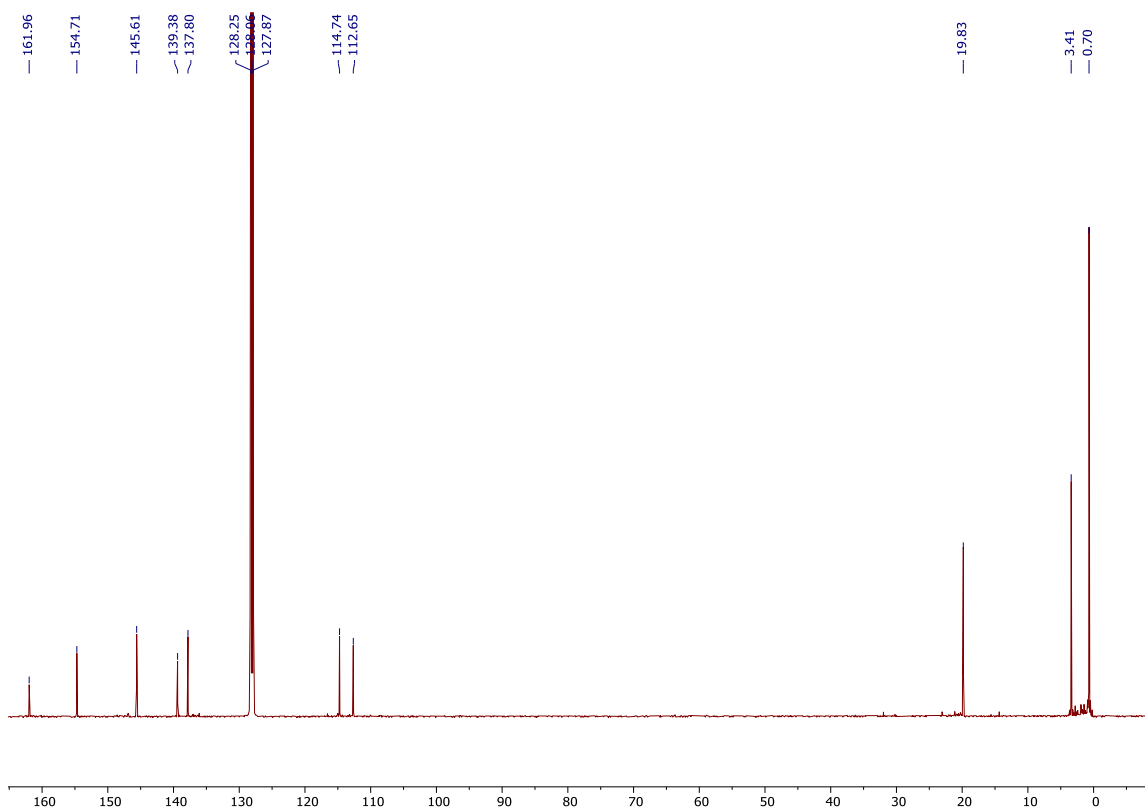


Figure S1b. $^{13}\text{C}\{^1\text{H}\}$ NMR (125.8 MHz, 305.0 K, C_6D_6) spectrum of **7**.

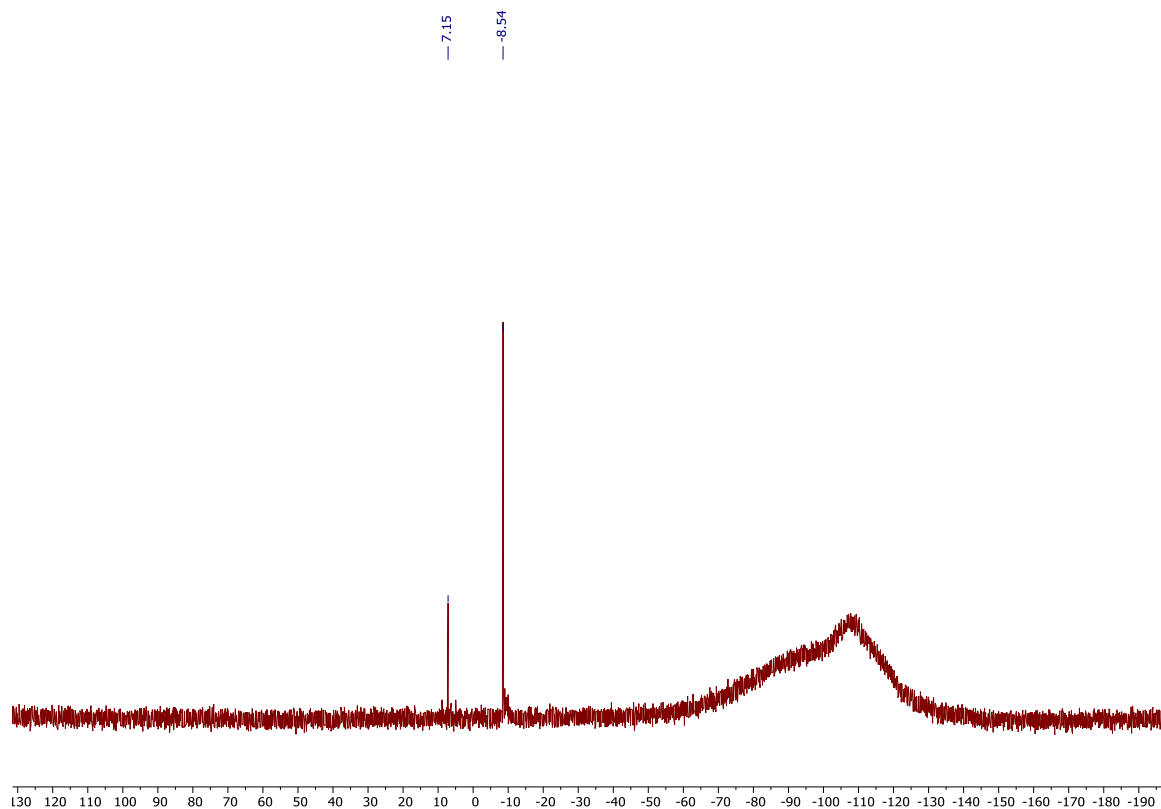
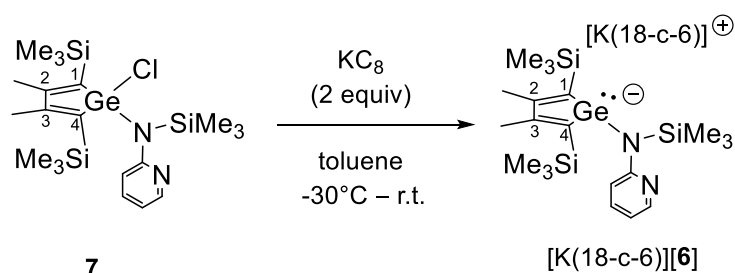


Figure S1c. $^{29}\text{Si}\{^1\text{H}\}$ NMR (99.4 MHz, 305.0 K, C_6D_6) spectrum of **7**.

Synthesis of [K(18-c-6)][6]:



Scheme S2

[K(18-c-6)][6]. KC_8 (81 mg, 0.6 mmol) was added to a toluene solution of compound **7** (150 mg, 0.30 mmol) and 18-c-6 (79 mg, 0.30 mmol) at -30°C . The reaction was kept stirring for overnight at room temperature. After that, the precipitate was removed through PTFE filter. The filtrate was concentrated to about 2 mL at $+5^\circ\text{C}$ to get reddish crystals of [K(18-c-6)][6] after three days. Yield: 117 mg (0.15 mmol, 50 %)

NMR spectra recorded in C_6D_6 at 305 K.

^1H NMR (499.9 MHz, 305.0 K, C_6D_6): δ = 0.46 (s, 18H, C-SiMe₃), 0.89 (s, 9H, N-SiMe₃), 2.46 (s, 6H, CH₃), 3.10 (s, 24H, 18-C-6), 6.29 (m, 1H, Py), 6.42 (m, 1H, Py), 7.12 (m, 1H, Py), 8.20 (m, 1H, Py),

$^{13}\text{C}\{^1\text{H}\}$ NMR (125.8 MHz, 305.0 K, C_6D_6): δ = 2.73 (C-SiMe₃), 5.84 (N-SiMe₃), 22.42 (CH₃), 69.96 (18-c-6), 110.24, 116.33, 135.35 (Py), 145.21 (C^{2/3}), 147.58 (Py), 168.97 (C^{1/4}), 171.23 (Py).

$^{29}\text{Si}\{^1\text{H}\}$ NMR (99.4 MHz, 305.0 K, C_6D_6): δ = -12.87 (C-SiMe₃), -3.10 (N-SiMe₃).

EA: C/H/N [%] calculated for $\text{C}_{32}\text{H}_{61}\text{GeKN}_2\text{O}_6\text{Si}_3$: 50.19/8.03/3.66; found: 50.46/8.44/3.87.

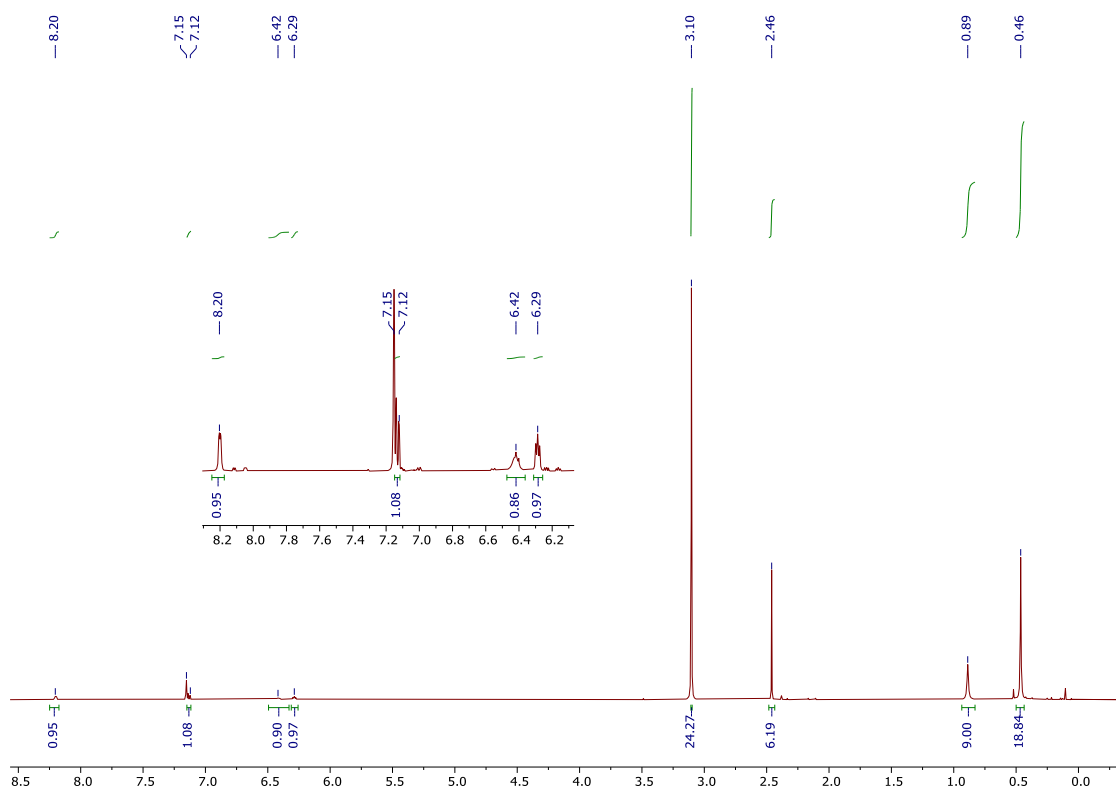


Figure S2a. ^1H NMR (499.0 MHz, 305.0 K, C_6D_6) spectrum of $[\text{K}(18\text{-c-6})][\mathbf{6}]$.

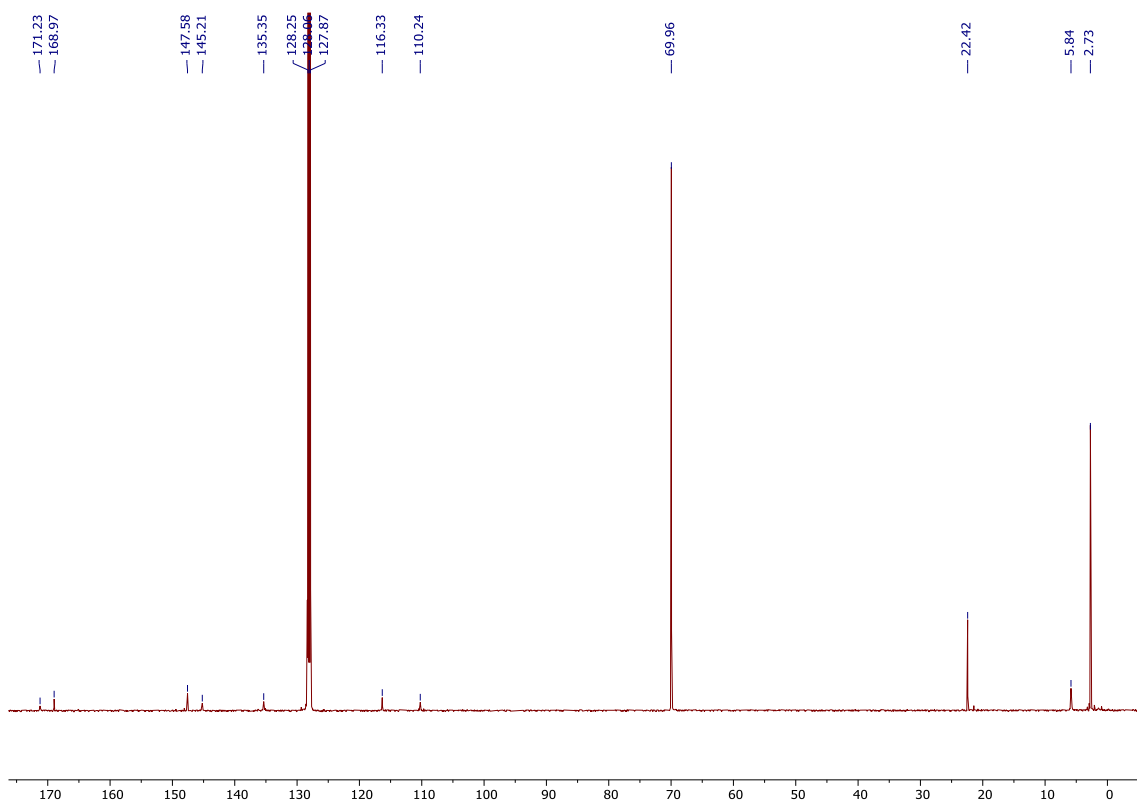


Figure S2b. $^{13}\text{C}\{^1\text{H}\}$ NMR (125.8 MHz, 305.0 K, C_6D_6) spectrum of $[\text{K}(18\text{-c-6})][\mathbf{6}]$.

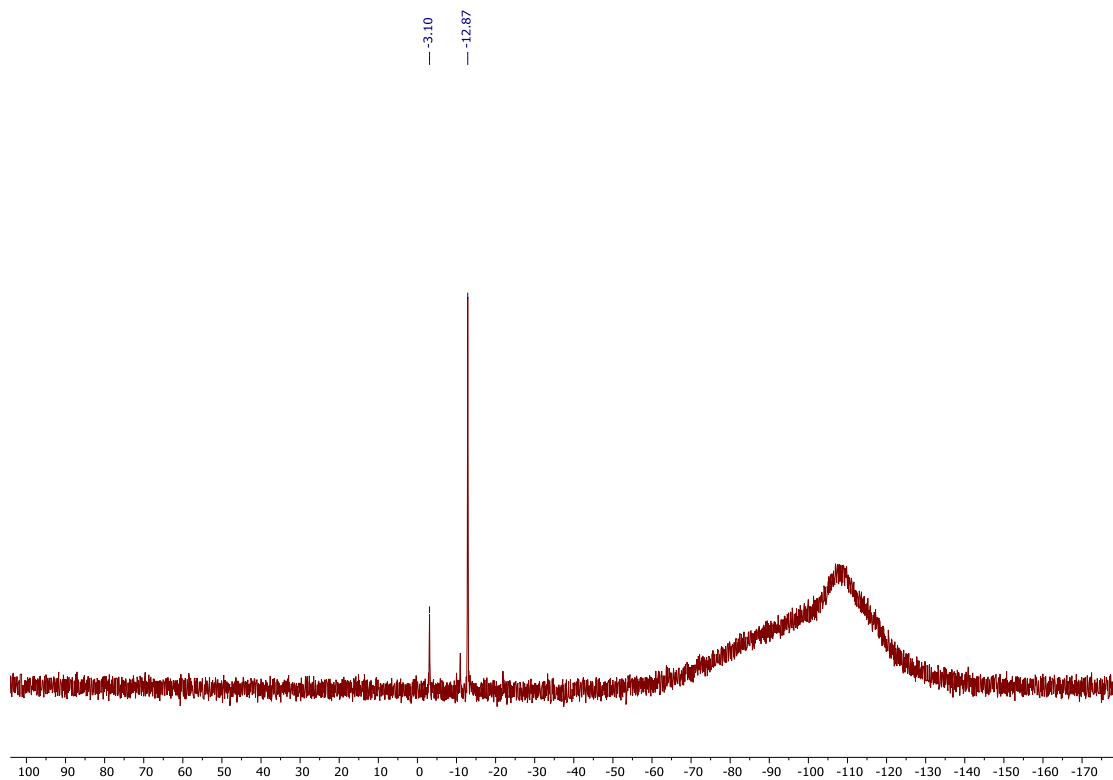
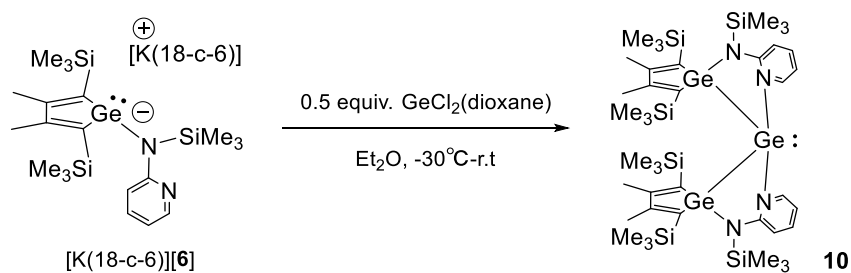


Figure S2c. $^{29}\text{Si}\{^1\text{H}\}$ NMR (99.4 MHz, 305.0 K, C_6D_6) spectrum of $[\text{K}(18\text{-c-}6)][\mathbf{6}]$.

Synthesis of 10:



10. $\text{GeCl}_2(\text{dioxane})$ (46 mg, 0.20 mmol) was added to an Et_2O solution of compound $[\text{K}(18\text{-c-}6)][\mathbf{6}]$ (307 mg, 0.40 mmol) at $-30\text{ }^\circ\text{C}$. The reaction was kept stirring for overnight at room temperature. The solvent was removed under vacuum. The residue was re-dissolved in n-hexane (15 mL) and the filtrate was removed solvent to get yellow solid **10**. Yield: 149 mg raw product contaminated with residual crown ether. From the ^1H NMR (Figure S3a) a yield of 63 mg of **10** is calculated (0.06 mmol) (31%). A small crop of crystal for sc-XRD were collected from diethyl ether.

NMR spectra recorded in C_6D_6 at 305 K.

^1H NMR (499.9 MHz, 305.0 K, C_6D_6): δ = 0.15 (s, 18H, C-SiMe₃), 0.34 (s, 18H, N-SiMe₃), 0.40 (s, 18H, C-SiMe₃), 1.95 (s, 6H, CH₃), 2.17 (s, 6H, CH₃), 5.99-6.02 (m, 2H, Py), 6.31-6.33 (m, 1H, Py), 6.75 (d, 1H, Py), 6.85-6.88 (m, 1H, Py), 6.93-7.05 (m, 1H, Py), 7.88-7.90 (m, 1H, Py), 8.08-8.13 (m, 1H, Py).

$^{13}\text{C}\{^1\text{H}\}$ NMR (125.8 MHz, 305.0 K, C_6D_6): δ = 1.10 (C-SiMe₃), 1.40 (N-SiMe₃), 2.34 (C-SiMe₃), 21.08, 21.14 (CH₃), 110.15, 110.93, 113.18, 115.28, 136.61, 137.10, 146.90 (Py), 148.53, 148.64 ($\text{C}^{1/4}$), 155.43 (Py), 156.82, 157.17 ($\text{C}^{2/3}$), 160.50, 162.19 (Py).

$^{29}\text{Si}\{^1\text{H}\}$ NMR (99.4 MHz, 305.0 K, C_6D_6): δ = -10.02, 9.93 (C-SiMe₃), 8.24 (N-SiMe₃).

HR-MS (ESI): m/z calculated for $\text{C}_{40}\text{H}_{74}\text{Ge}_3\text{N}_4\text{Si}_6 + \text{H}$: 1001.2237; found: 1001.2239.

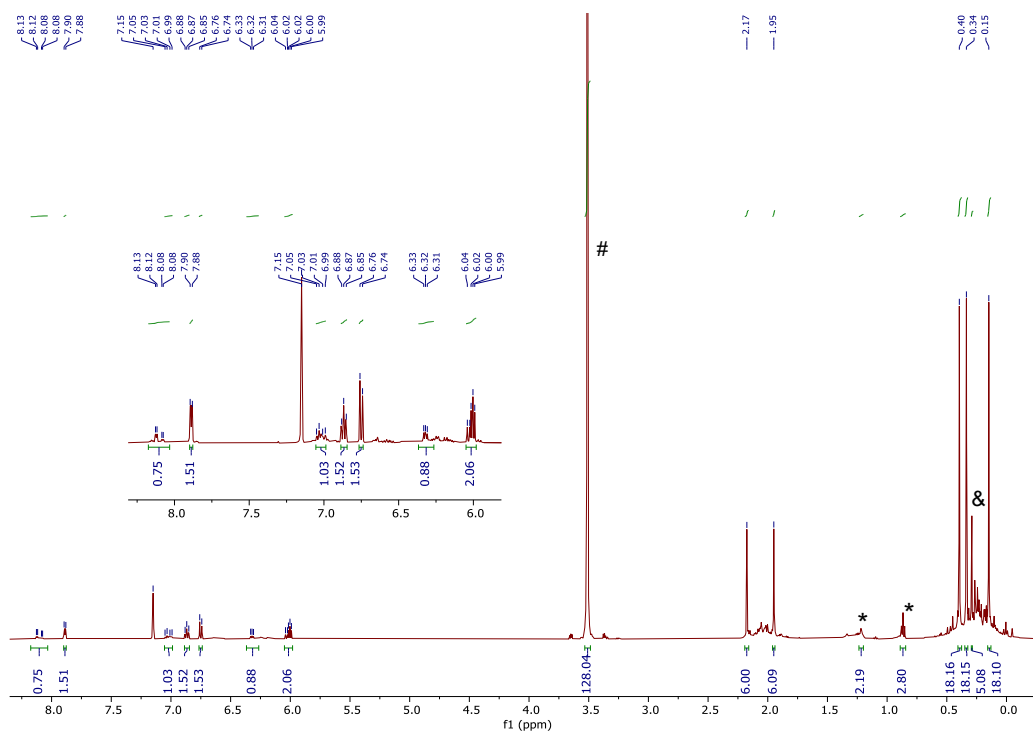


Figure S3a. ^1H NMR (499.0 MHz, 305.0 K, C_6D_6) spectrum of **10** (*n-hexane, #free 18-c-6, &unknown impurities).

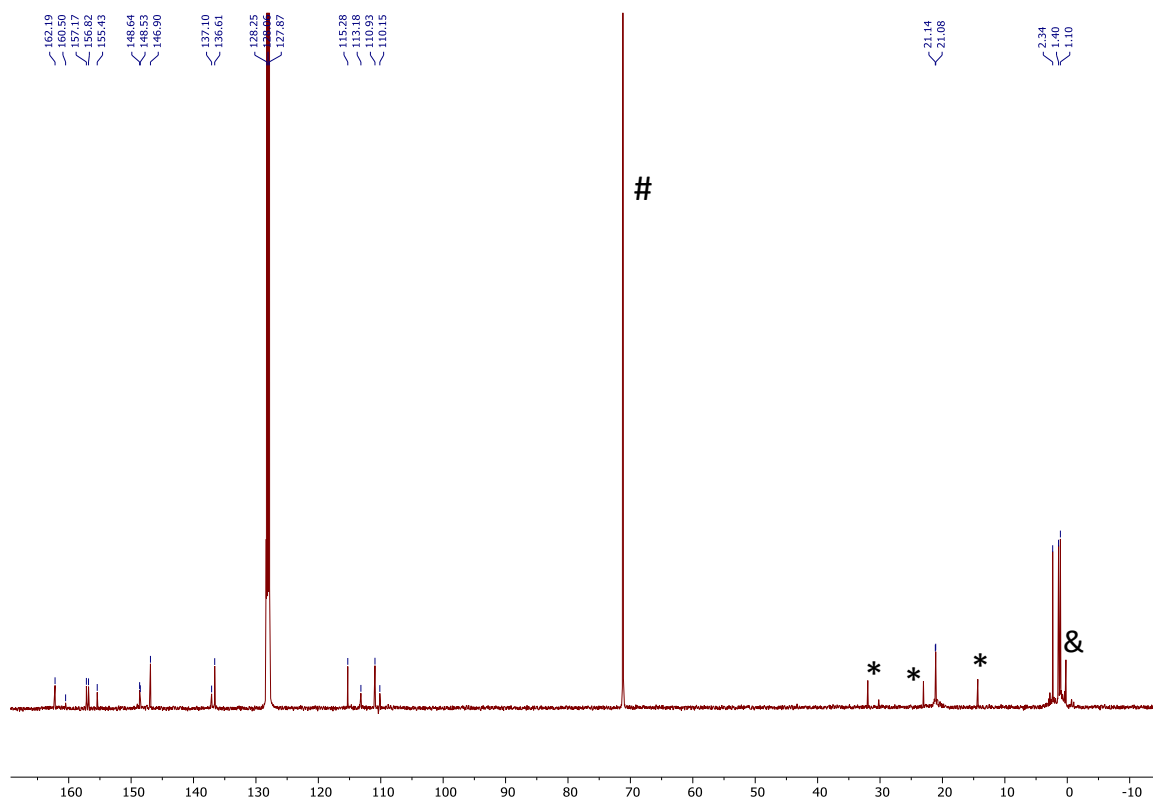


Figure S3b. $^{13}\text{C}\{^1\text{H}\}$ NMR (125.8 MHz, 305.0 K, C_6D_6) spectrum of **10** (*n-hexane, #free 18-c-6, &unknown impurities).

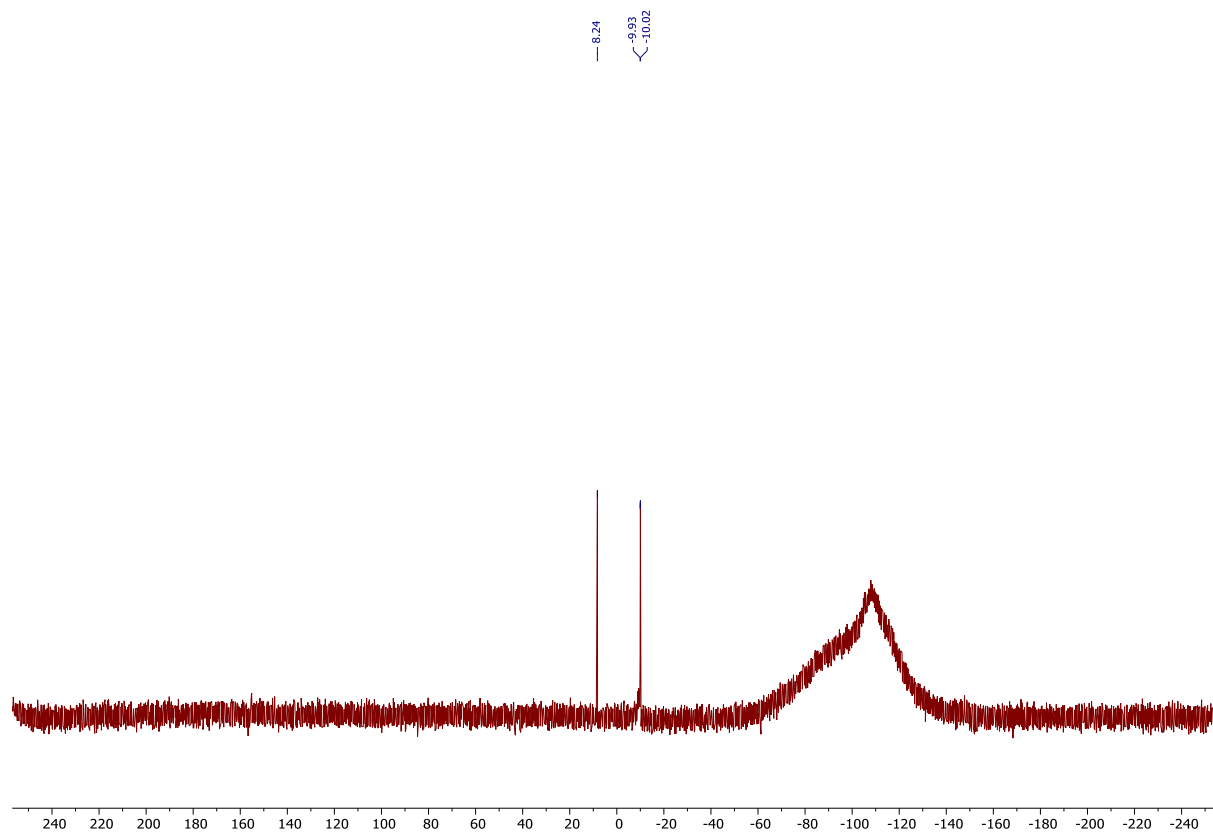
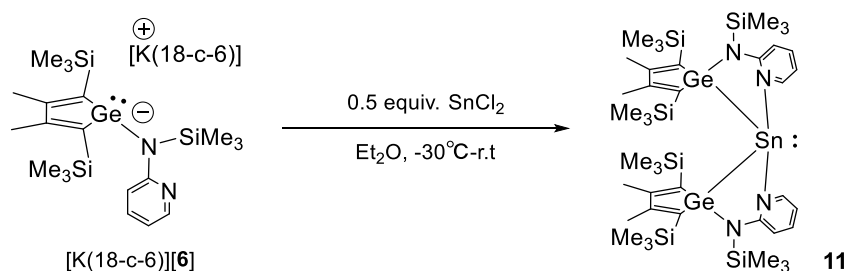


Figure S3c. $^{29}\text{Si}\{^1\text{H}\}$ NMR (99.4 MHz, 305.0 K, C_6D_6) spectrum of **10**.

Synthesis of 11:



11. SnCl₂ (27 mg, 0.15 mmol) was added to an Et₂O solution of compound [K(18-c-6)][**6**] (223 mg, 0.29 mmol) at -30 °C. The reaction was kept stirring for overnight at room temperature. The solvent was removed under vacuum. The residue was re-dissolved in n-hexane (15 mL) and the filtrate was removed solvent to get yellow solid **11**. Yield: 117 mg raw product contaminated with residual crown ether. From the ¹H NMR (Figure S4a) a yield of 93 mg of **11** is calculated (0.09 mmol) (60%). A small crop of crystal for sc-XRD were collected from diethyl ether.

NMR spectra recorded in C₆D₆ at 305 K.

¹H NMR (499.9 MHz, 305.0 K, C₆D₆): δ = 0.16 (s, 18H, C-SiMe₃), 0.34 (s, 18H, N-SiMe₃), 0.49 (s, 18H, C-SiMe₃), 2.05 (s, 6H, CH₃), 2.21 (s, 6H, CH₃), 5.94-5.97(m, 2H, Py), 6.79-6.86 (m, 4H, Py), 7.67-7.68 (m, 2H, Py).

¹³C{¹H} NMR (125.8 MHz, 305.0 K, C₆D₆): δ = 1.41 (C-SiMe₃), 1.55 (N-SiMe₃), 2.06 (C-SiMe₃), 21.15 (CH₃), 110.07, 111.50, 113.19, 115.87, 137.11, 147.65, 148.57, 151.05 (Py), 155.55 (C^{1/4}), 156.60 (Py), 157.54 (C^{2/3}), 163.42 (Py).

²⁹Si{¹H} NMR (99.4 MHz, 305.0 K, C₆D₆): δ = -10.31 (C-SiMe₃), 9.10 (N-SiMe₃).

¹¹⁹Sn{¹H} NMR (186.4 MHz, 305.0 K, C₆D₆): δ = -263.3.

HR-MS (ESI): m/z calculated for C₄₀H₇₄Ge₂N₄Si₆Sn+H: 1047.2047; found: 1047.2053.

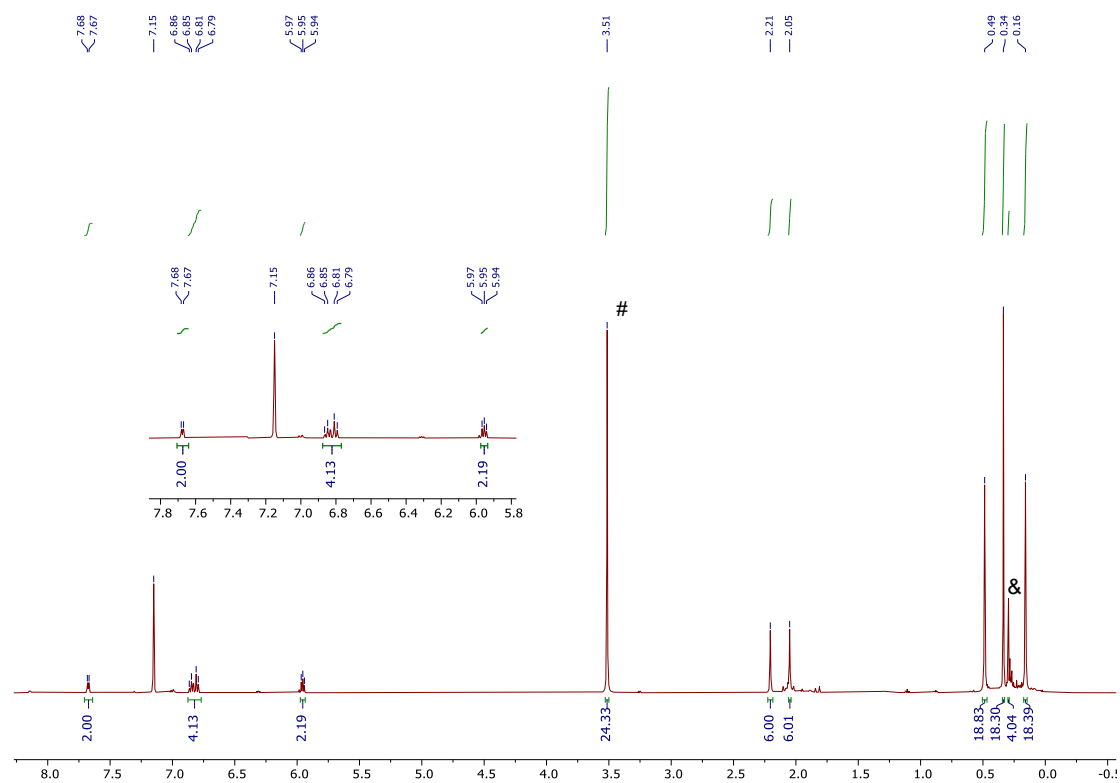


Figure S4a. ^1H NMR (499.0 MHz, 305.0 K, C_6D_6) spectrum of **11** (#free 18-c-6, &unknown impurities).

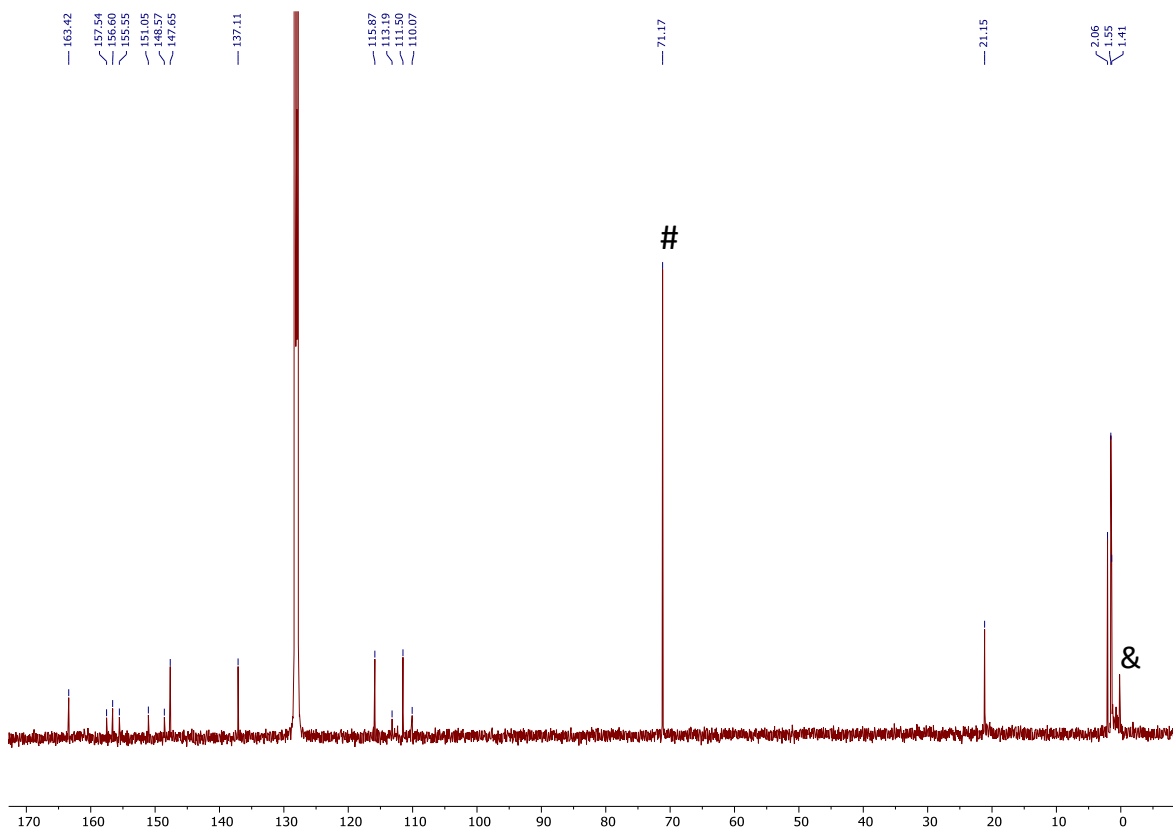
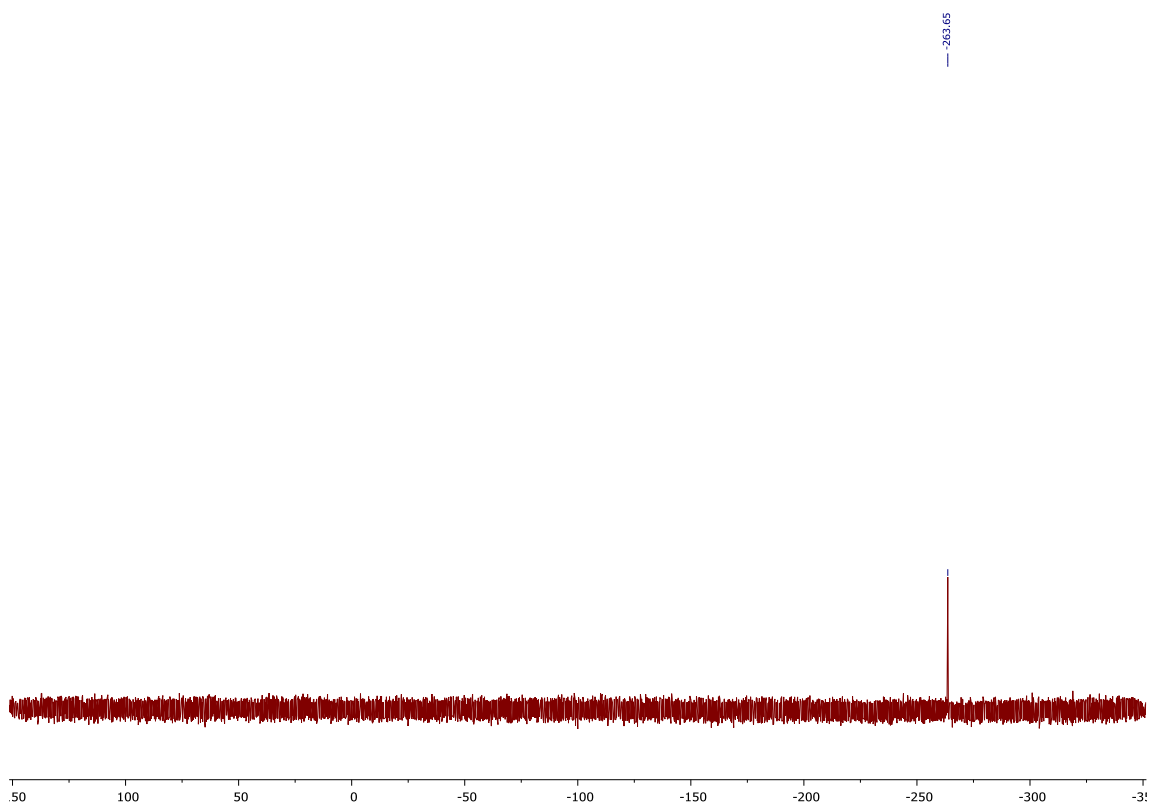
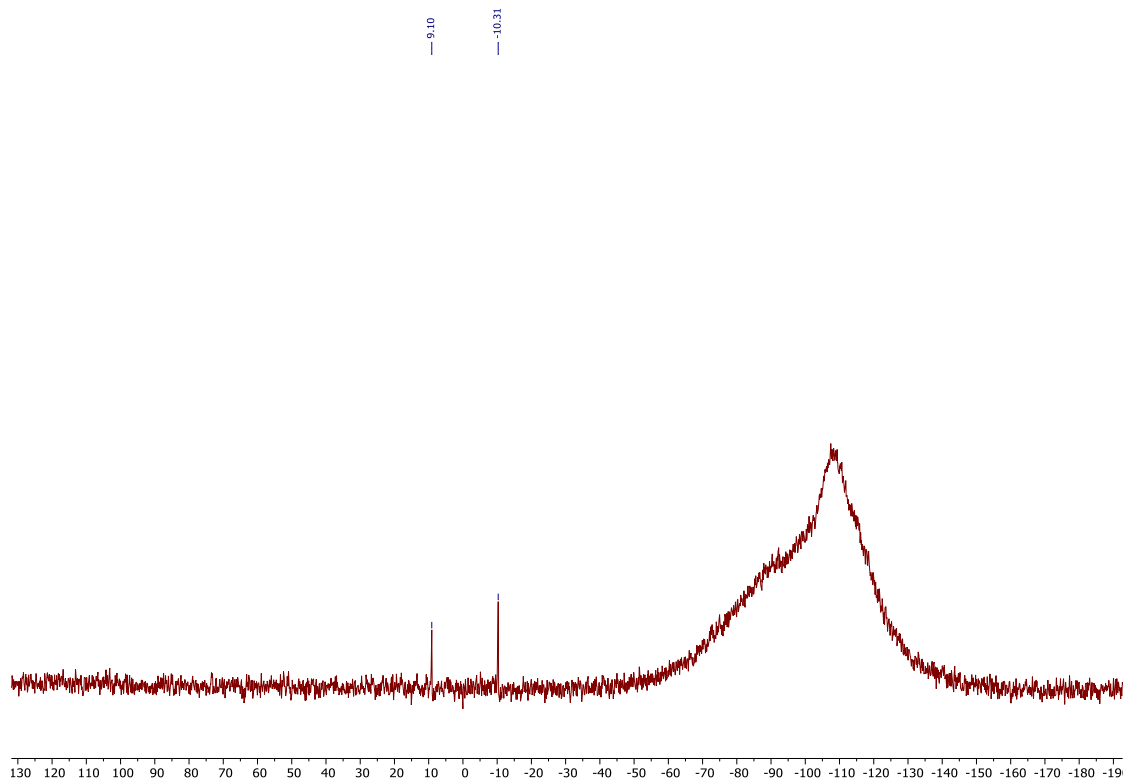


Figure S4b. $^{13}\text{C}\{^1\text{H}\}$ NMR (125.8 MHz, 305.0 K, C_6D_6) spectrum of **11** (#free 18-c-6, &unknown impurities).



Details of X-ray Analysis

Single crystal X-ray data were measured on a Bruker AXS Apex II diffractometer (Mo-K α radiation, $\lambda = 0.71073\text{\AA}$, Kappa 4 circle goniometer, Bruker Apex II detector). The crystal was kept at 100.0 K during data collection. Absorption corrections based on symmetry-related measurements (multi-scan) were performed with the program SADABS.^[S3] The structures were solved with the program SHELXS and refined with SHELXL.^[S4] Pertinent data are summarized in Table S1-S5. CCDC-2392569 (**7**), CCDC-2392567 ([K(18-c-6)]**[6]**), CCDC-2392568 (**10**), CCDC-2392570 (**11**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre. The Director, CCDC, 12 Union Road, Cambridge CB2 1EZ, UK [Fax: (internat.) +44-1223/336-033; E-mail: deposit@ccdc.cam.ac.uk].

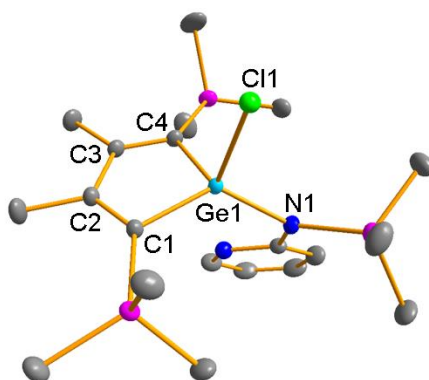
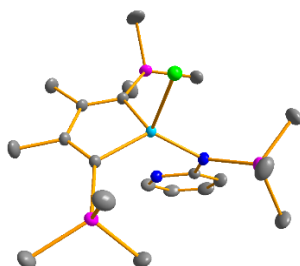
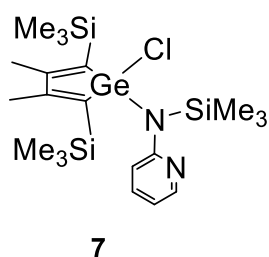
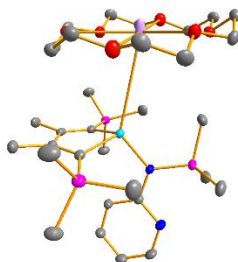
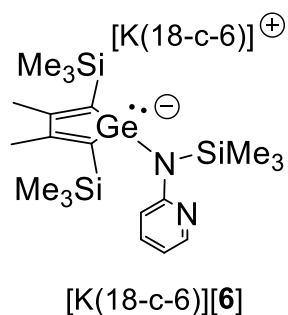


Figure S6. Molecular structure of **7** in the crystal. (Hydrogen atoms are omitted for clarity. Thermal ellipsoids are shown at the 50 % probability level.) Selected bond lengths [pm] and angles [°]: Ge1–Cl1 223.6(4), Ge1–C1 194.0(6), Ge1–C4 193.0(8), Ge1–N1 187.1(6), C1–C2 135.8(8), C2–C3 152.0(9), C3–C4 135.6(9).

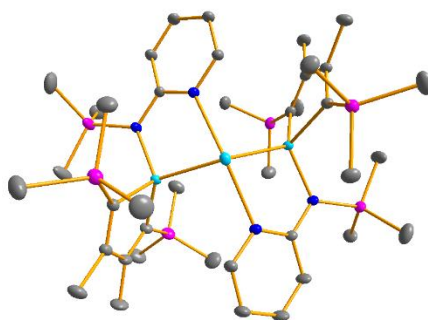
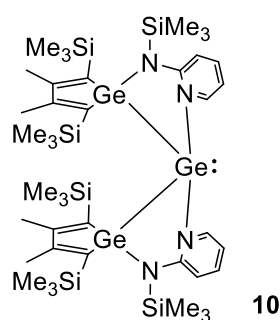
Table S1.

Name	7	
CCDC	2392569	
Empirical formula	C ₂₀ H ₃₇ Cl Ge N ₂ Si ₃	
Formula weight	497.82	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 ₁ /c	
Unit cell dimensions	a = 10.2981(5) Å	a = 90°.
	b = 15.1609(7) Å	b = 99.0183(19)°.
	c = 17.3330(8) Å	g = 90°.
Volume	2672.7(2) Å ³	
Z	4	
Density (calculated)	1.237 Mg/m ³	
Absorption coefficient	1.389 mm ⁻¹	
F(000)	1048	
Crystal size	0.110 x 0.100 x 0.080 mm ³	
Theta range for data collection	1.794 to 40.248°	
Index ranges	-18 ≤ h ≤ 18, -27 ≤ k ≤ 27, -31 ≤ l ≤ 31	
Reflections collected	202917	
Independent reflections	16828 (R(int) = 0.0394)	
Observed reflections (I > 2(I))	14550	
Completeness to theta = 40.248°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.0000 and 0.9290	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	16828 / 0 / 255	
Goodness-of-fit on F ²	1.048	
Final R indices (I > 2σ(I))	R1 = 0.0222, wR2 = 0.0560	
R indices (all data)	R1 = 0.0291, wR2 = 0.0586	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.734 and -0.425 e.Å ⁻³	

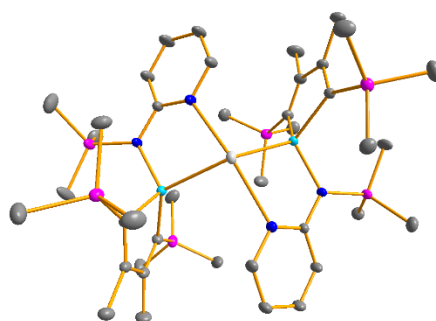
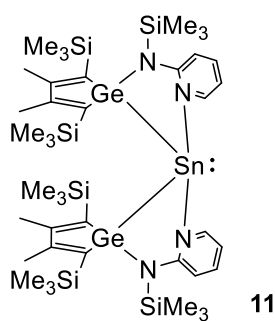
Table S2.



Name	[K(18-c-6)][6]	
CCDC	2392567	
Empirical formula	C ₃₂ H ₆₁ Ge K N ₂ O ₆ Si ₃	
Formula weight	765.78	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 ₁ /c	
Unit cell dimensions	a = 19.6032(9) Å	a = 90°.
	b = 10.9806(5) Å	b = 110.1445(14)°.
	c = 20.4878(8) Å	g = 90°.
Volume	4140.3(3) Å ³	
Z	4	
Density (calculated)	1.229 Mg/m ³	
Absorption coefficient	0.966 mm ⁻¹	
F(000)	1632	
Crystal size	0.140 x 0.080 x 0.060 mm ³	
Theta range for data collection	2.024 to 32.031°	
Index ranges	?<=h<=?, ?<=k<=?, ?<=l<=?	
Reflections collected	14418	
Independent reflections	14418 (R(int) = ?)	
Observed reflections (I > 2(I))	12216	
Completeness to theta = 32.031°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.000000 and 0.844277	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	14418 / 0 / 420	
Goodness-of-fit on F ²	1.033	
Final R indices (I>2sigma(I))	R1 = 0.0410, wR2 = 0.0817	
R indices (all data)	R1 = 0.0546, wR2 = 0.0867	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.638 and -0.623 e.Å ⁻³	

Table S3.

Name	10	
CCDC	2392568	
Empirical formula	C ₄₀ H ₇₄ Ge ₃ N ₄ Si ₆	
Formula weight	997.34	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.8498(5) Å	a = 76.534(2)°.
	b = 14.8521(7) Å	b = 82.7769(19)°.
	c = 16.7213(8) Å	g = 88.1701(19)°.
Volume	2599.6(2) Å ³	
Z	2	
Density (calculated)	1.274 Mg/m ³	
Absorption coefficient	1.891 mm ⁻¹	
F(000)	1044	
Crystal size	0.110 x 0.100 x 0.030 mm ³	
Theta range for data collection	1.262 to 36.318°	
Index ranges	-18<=h<=18, -24<=k<=24, -27<=l<=27	
Reflections collected	208606	
Independent reflections	25206 (R(int) = 0.0468)	
Observed reflections (I > 2(I))	21572	
Completeness to theta = 36.318°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.0000 and 0.8787	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	25206 / 0 / 500	
Goodness-of-fit on F ²	1.127	
Final R indices (I > 2sigma(I))	R1 = 0.0300, wR2 = 0.0741	
R indices (all data)	R1 = 0.0390, wR2 = 0.0771	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.931 and -0.719 e.Å ⁻³	

Table S4.

Name	11	
CCDC	2392570	
Empirical formula	C ₄₀ H ₇₄ Ge ₂ N ₄ Si ₆ Sn	
Formula weight	1043.44	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 11.9907(7) Å	a = 79.3746(19)°.
	b = 14.3069(8) Å	b = 84.9106(19)°.
	c = 15.3368(8) Å	g = 89.631(2)°.
Volume	2575.6(2) Å ³	
Z	2	
Density (calculated)	1.345 Mg/m ³	
Absorption coefficient	1.810 mm ⁻¹	
F(000)	1080	
Crystal size	0.140 x 0.120 x 0.100 mm ³	
Theta range for data collection	1.356 to 40.249°	
Index ranges	-21 ≤ h ≤ 21, -26 ≤ k ≤ 26, -27 ≤ l ≤ 27	
Reflections collected	336545	
Independent reflections	32397 (R(int) = 0.0347)	
Observed reflections (I > 2(I))	29390	
Completeness to theta = 40.249°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.0000 and 0.9181	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	32397 / 0 / 500	
Goodness-of-fit on F ²	1.057	
Final R indices (I > 2σ(I))	R1 = 0.0176, wR2 = 0.0452	
R indices (all data)	R1 = 0.0214, wR2 = 0.0466	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.990 and -0.781 e.Å ⁻³	

Computational Details

All quantum chemical calculations were carried out using the Gaussian16 package.^[S5] The natural bond orbital (NBO)^[S6] analysis was done with the program NBO 7.0.^[S7] The molecular structure optimization were performed using the M06-2X functional^[S8] along with the 6-311+G(d,p) basis set. For the element Sn the corresponding pseudo potentials were applied.^[S9] The AIMALL program was used to perform the QTAIM analysis.^[S10] For visualization of the natural bond orbitals the program Jmol was used.^[S11]

For the NBO analysis, the M06-2X functional along with a 6-311+G(d,p) basis set/pseudo potentials was used to generate the density to be analysed. For the QTAIM analysis single point calculations using an all-electron basis set for Sn (def2-mTZVP) and for Ge, Si, N, C, H the 6-311+G(d,p) basis set.^[S12]

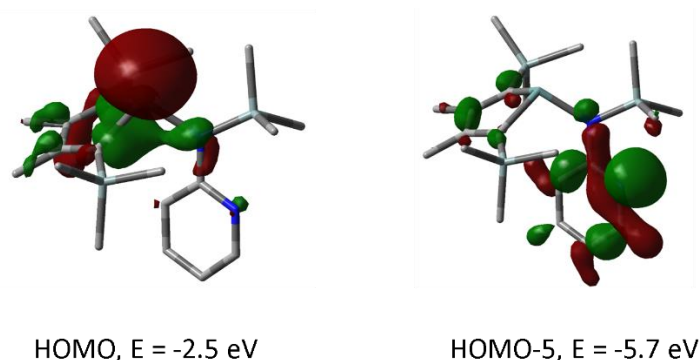


Figure S7. Surface diagrams of selected molecular orbitals of germolide [6] (M06-2X/6-311+G(d,p), isosurface value: 0.04)

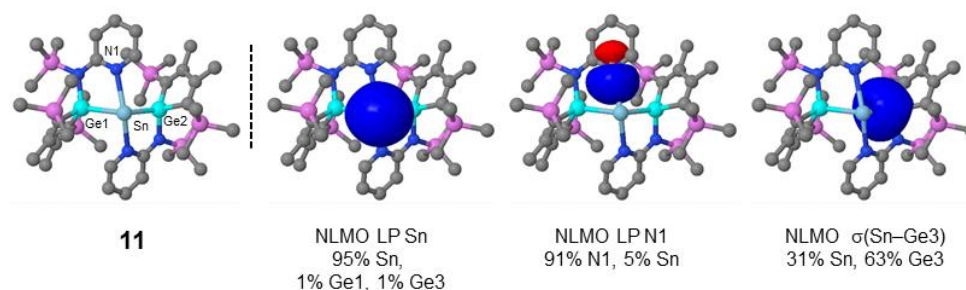


Figure S8. Computed pertinent NLMOs of **11**, showing the interactions between the tin atom Sn1 with the germolyl substituents and the remote pyridine ligand (M06-2X/6-311+G(d,p) (C,H,N,Si,Ge), def2-mTZVP (Sn), isodensity value 0.04 a.u. (Colour code: violet Si, cyan Ge, sky blue Sn, blue N, gray C).

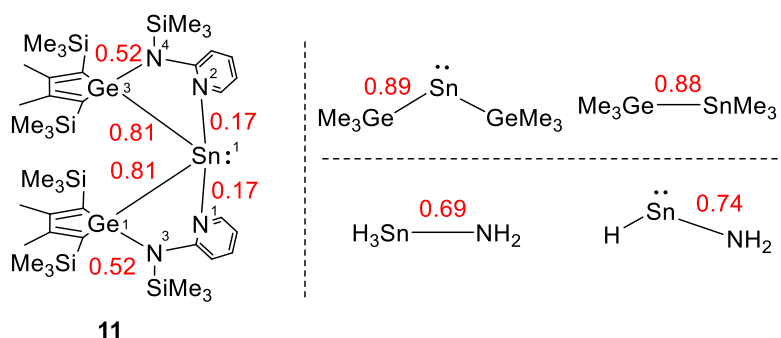


Figure S9. Computed WBIs (red) of *bis*-germylyl stannylene **11**, and related compounds (M06-2X/6-311+G(d,p) (C,H,N,Si,Ge), def2-mTZVP (Sn)).

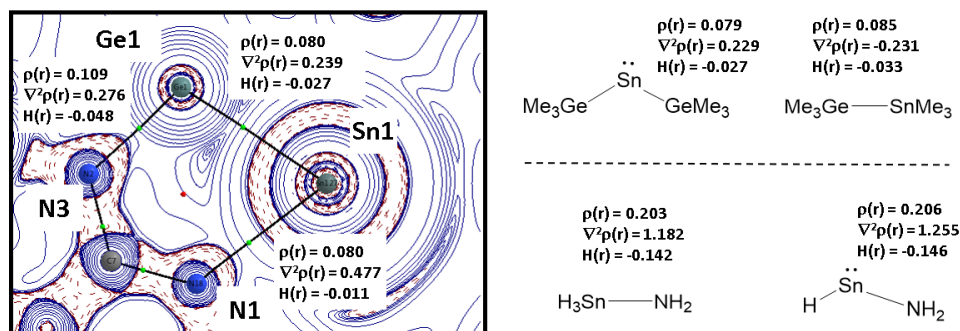


Figure S10. Results of the QTAIM analysis of *bis*-germylyl stannylene **11**, and related compounds. Left side: Part of the molecular graph of stannylene **11** projected on a contour plot of the Laplacian of the electron density in the Ge1Sn1N1 plane. (Green spheres: bond critical points (bcp), red sphere: ring critical point (rcp), electron density at the bcp, $\rho(r)$, in $\text{e}(\text{bohr})^{-3}$; Laplacian at the bcp, $\nabla^2\rho(r)$, in $\text{e}(\text{bohr})^{-5}$; total energy density at the bcp, $H(r)$, in a.u.(bohr) $^{-3}$, calculations at M06-2X/6-311+G(d,p) (C,H,N,Si,Ge), def2-mTZVP (Sn)).

Table S5. Selected NBO parameters of **10** and **11** (M062X/6-311+G(d,p) (C, H, N, Si, Ge,) def2-mTZVP (Sn)).

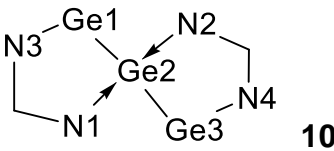
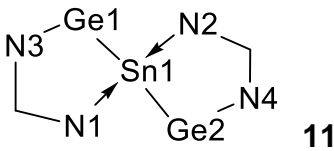
					
	WBI	Charge		WBI	Charge
Ge1		1.42	Ge1		1.26
Ge2		0.19	Sn1		0.57
Ge3		1.42	Ge2		1.26
N1		-0.59	N1		-0.61
N2		-0.60	N2		-0.61
N3-Ge1	0.51		N3-Ge1	0.52	
N1-Ge2	0.21		N1-Sn1	0.17	
Ge1-Ge2	0.92		Ge1-Sn1	0.81	
N4-Ge3	0.51		N4-Ge2	0.52	
N2-Ge2	0.23		N2-Sn1	0.17	
Ge2-Ge3	0.92		Sn1-Ge2	0.81	

Table S6. Selected QTAIM parameters of **10** and **11** (M062X/6-311+G(d,p) (C, H, N, Si, Ge,) def2-mTZVP (Sn)).

	10						
	$\rho(r\text{BCP})$ [e(bohr) ⁻³]	$\nabla^2\rho(r\text{BCP})$ [e(bohr) ⁻⁵]	ϵ	H(rBCP) [a.u. (bohr) ⁻³]	$\rho(r\text{RCP})$ [e(bohr) ⁻³]	$\nabla^2\rho(r\text{RCP})$ [e(bohr) ⁻⁵]	H(rRCP) [e(bohr) ⁻³]
Ge1-Ge2	0.076	-0.046	0.178	-0.030			
N1-Ge2	0.043	0.109	0.048	-0.001			
N3-Ge1	0.112	0.278	0.047	-0.050			
CN2Ge2					0.019	0.079	0.002
	11						
Ge1-Sn1	0.080	0.239	0.066	-0.027			
N1-Sn1	0.080	0.477	0.033	-0.011			
N3-Ge1	0.109	0.276	0.023	-0.048			
CN2GeSn					0.021	0.086	0.001

BCP bond critical point; RCP ring critical point; $\rho(r\text{BCP})$ electron density at BCP; $\nabla^2\rho(r\text{BCP})$: Laplacian at BCP; ϵ ellipticity; H(rBCP): total energy density at BCP; $\rho(r\text{RCP})$ electron density at RCP; $\nabla^2\rho(r\text{RCP})$: Laplacian at RCP; H(rRCP): total energy density at BCP.

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