

Electronic supplementary information (ESI)

Mixed guanidinato-amido Ge(IV) and Sn(IV) complexes with Ge=E (E = S, Se) double bond and SnS₄, Sn₂Se₂ rings

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- Fig. S1 ¹H NMR Spectrum of [ArNC(N^{*i*}Pr₂)NAr]GeN(SiMe₃)₂S (**3**)
- Fig. S2 ¹³C NMR Spectrum of [ArNC(N^{*i*}Pr₂)NAr]GeN(SiMe₃)₂S (**3**)
- Fig. S3 ²⁹Si NMR Spectrum of [ArNC(N^{*i*}Pr₂)NAr]GeN(SiMe₃)₂S (**3**)
- Fig. S4 ¹H NMR Spectrum of [ArNC(N^{*i*}Pr₂)NAr]GeN(SiMe₃)₂Se (**4**)
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- Fig. S6 ²⁹Si NMR Spectrum of [ArNC(N^{*i*}Pr₂)NAr]GeN(SiMe₃)₂Se (**4**)
- Fig. S7 ¹H NMR Spectrum of {[ArNC(N^{*i*}Pr₂)NAr]SnN(SiMe₃)₂}S₄ (**5**)
- Fig. S8 ¹³C NMR Spectrum of {[ArNC(N^{*i*}Pr₂)NAr]SnN(SiMe₃)₂}S₄ (**5**)
- Fig. S9 ²⁹Si NMR Spectrum of {[ArNC(N^{*i*}Pr₂)NAr]SnN(SiMe₃)₂}S₄ (**5**)
- Fig. S10 ¹H NMR Spectrum of {[ArNC(N^{*i*}Pr₂)NAr] N(SiMe₃)₂Sn(μ-Se)}₂ (**6**)
- Fig. S11 ¹³C NMR Spectrum of {[ArNC(N^{*i*}Pr₂)NAr] N(SiMe₃)₂Sn(μ-Se)}₂ (**6**)
- Fig. S12 ²⁹Si NMR Spectrum of {[ArNC(N^{*i*}Pr₂)NAr] N(SiMe₃)₂Sn(μ-Se)}₂ (**6**)
- Fig S13 and Fig S14 Computational studies

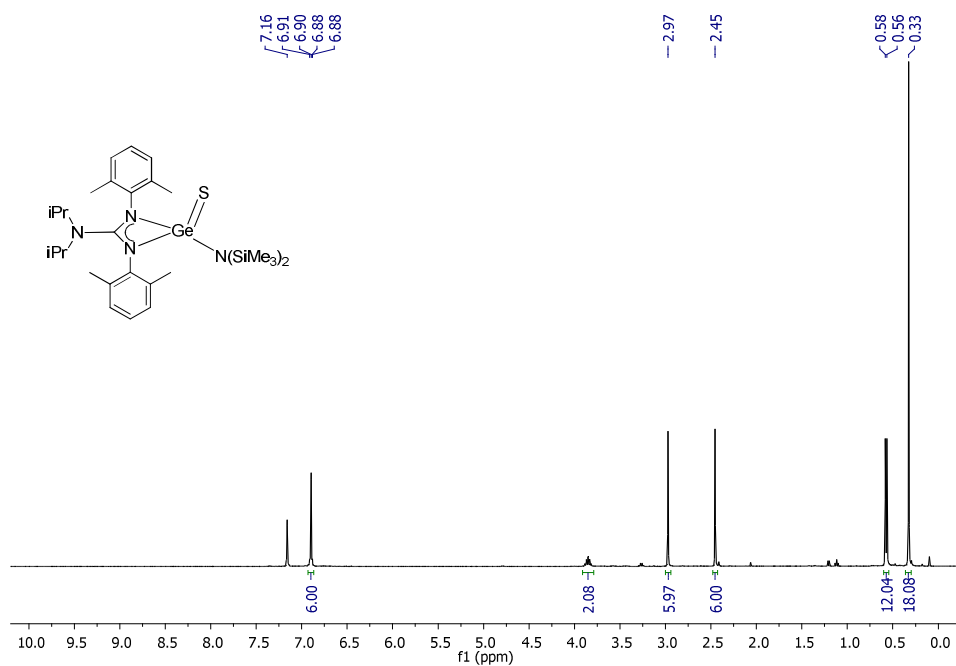


Fig. S1: ^1H NMR Spectrum of $[\{\text{ArNC}(\text{N}^i\text{Pr}_2)\text{NAr}\}\text{GeN}(\text{SiMe}_3)_2(\text{S})]$ (**3**) in C_6D_6

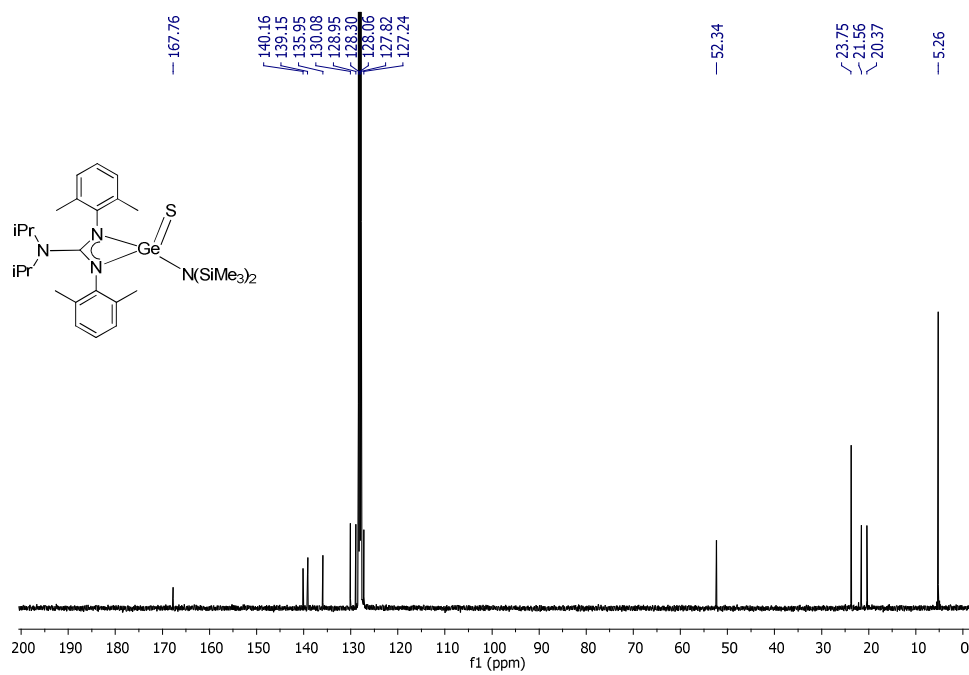


Fig. S2: ^{13}C NMR Spectrum of $[\{\text{ArNC}(\text{N}^i\text{Pr}_2)\text{NAr}\}\text{GeN}(\text{SiMe}_3)_2(\text{S})]$ (**3**) in C_6D_6

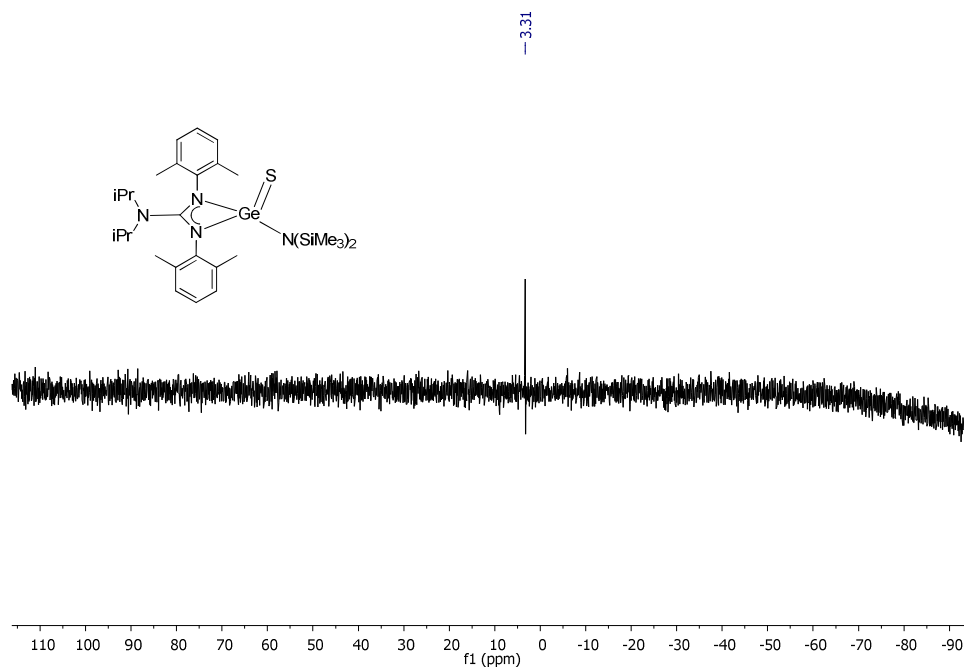


Fig. S3: ^{29}Si NMR Spectrum of [$\{\text{ArNC}(\text{N}^i\text{Pr}_2)\text{NAr}\}\text{GeN}(\text{SiMe}_3)_2(\text{S})$] (**3**) in C_6D_6

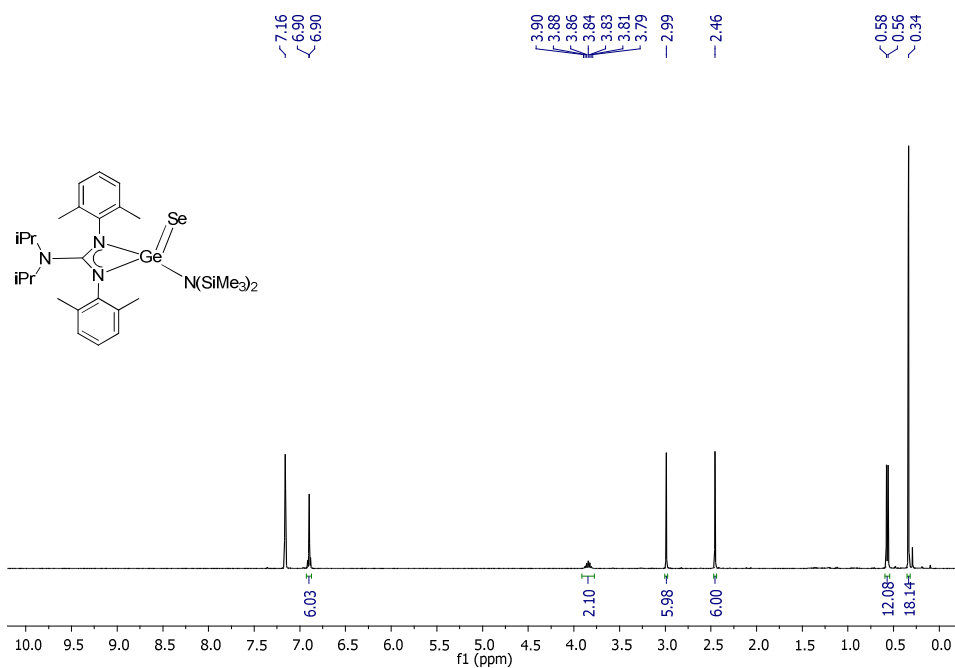


Fig. S4: ¹H NMR Spectrum of [**ArNC(NⁱPr₂)NAr**]**GeN(SiMe₃)₂(Se)** (**4**) in C₆D₆

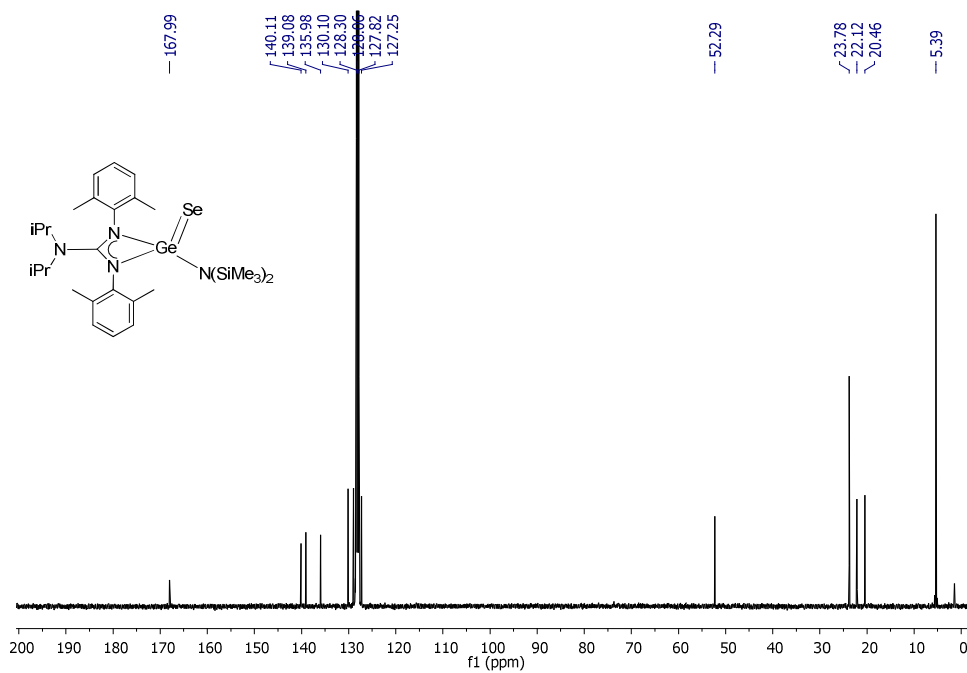


Fig. S5: ¹³C NMR Spectrum of [**ArNC(NⁱPr₂)NAr**]**GeN(SiMe₃)₂(Se)** (**4**) in C₆D₆

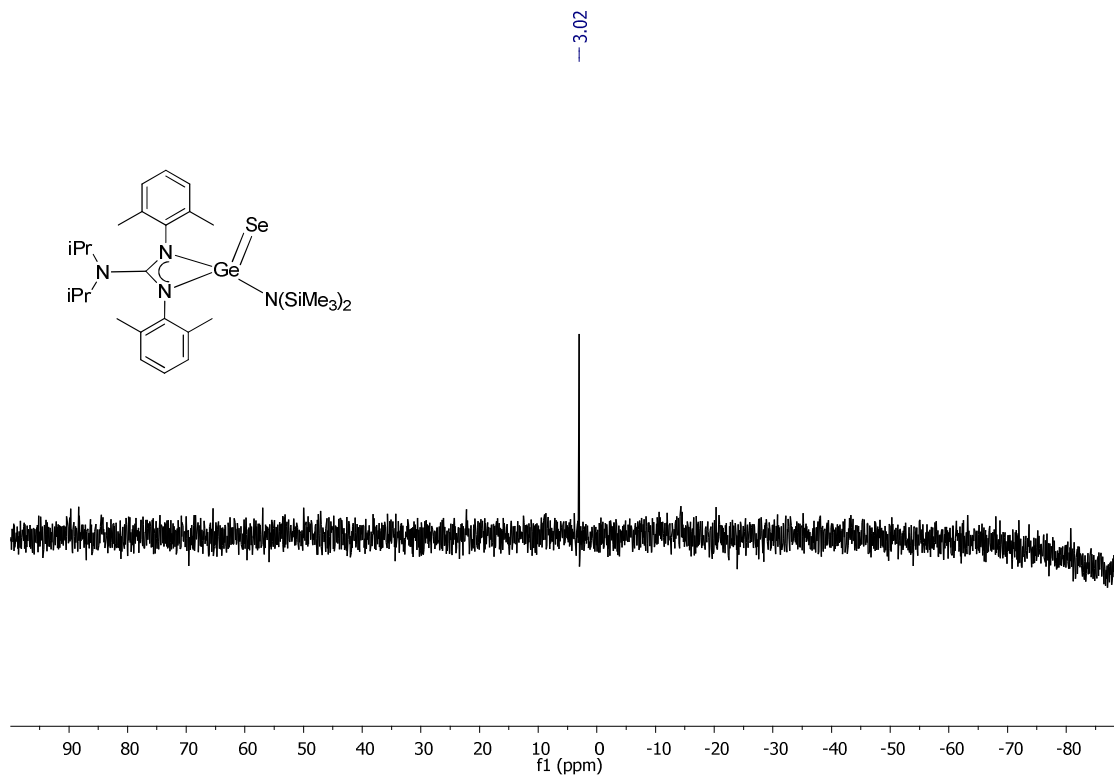
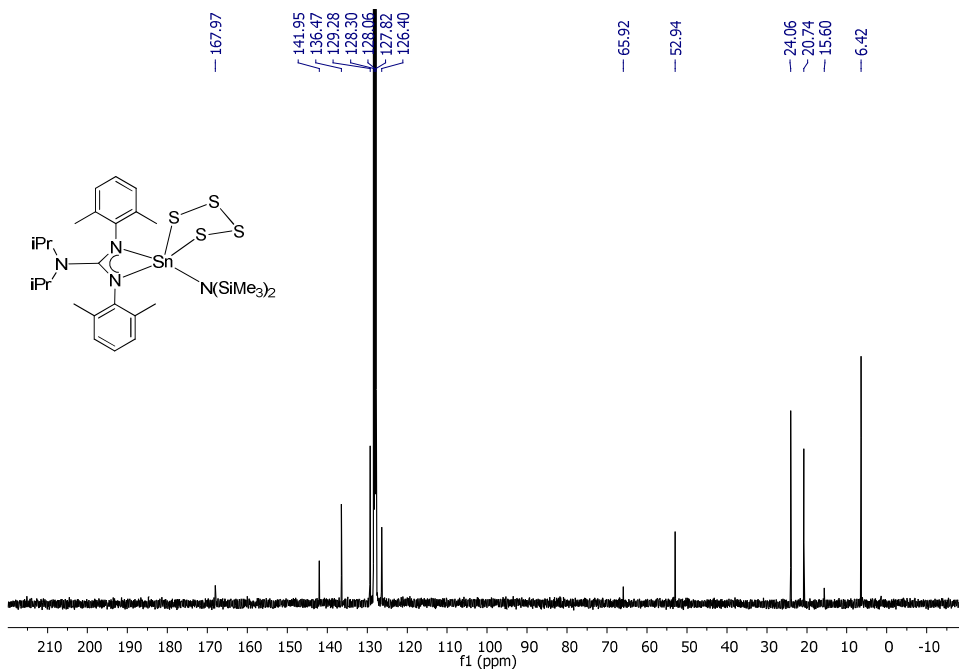
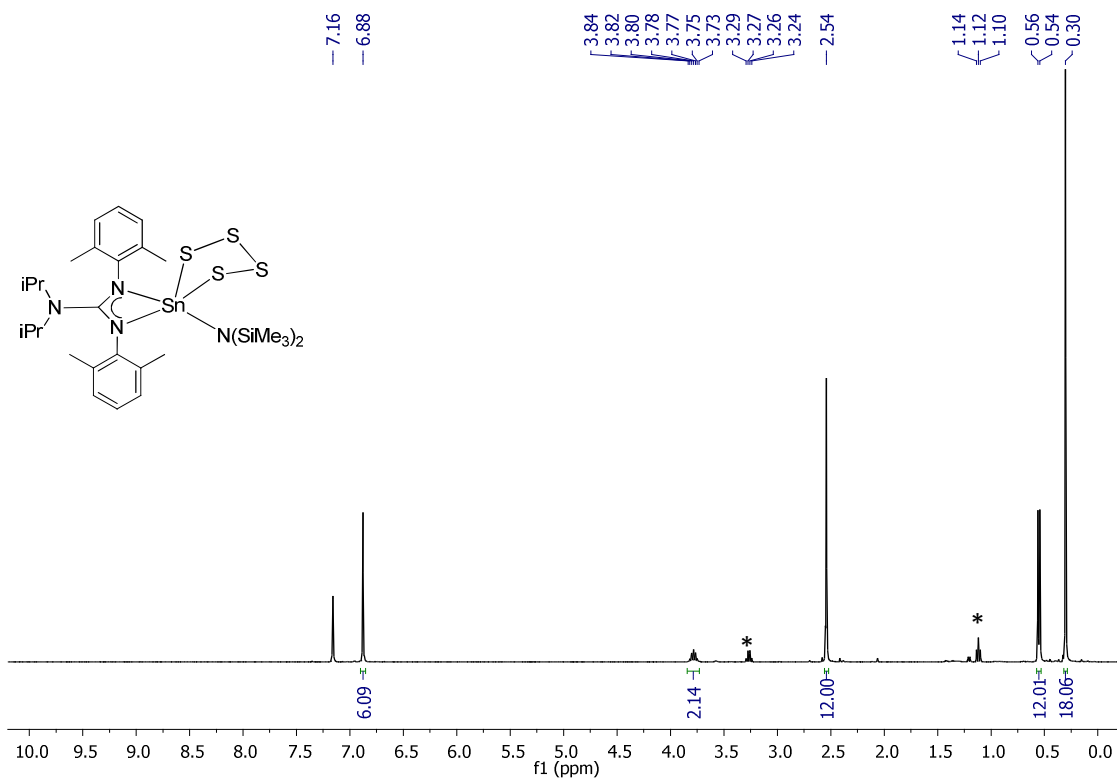


Fig. S6: ^{29}Si NMR Spectrum of [$\{\text{ArNC}(\text{N}^i\text{Pr}_2)\text{NAr}\}\text{GeN}(\text{SiMe}_3)_2(\text{Se})$] (**4**) in C_6D_6



- 5.54

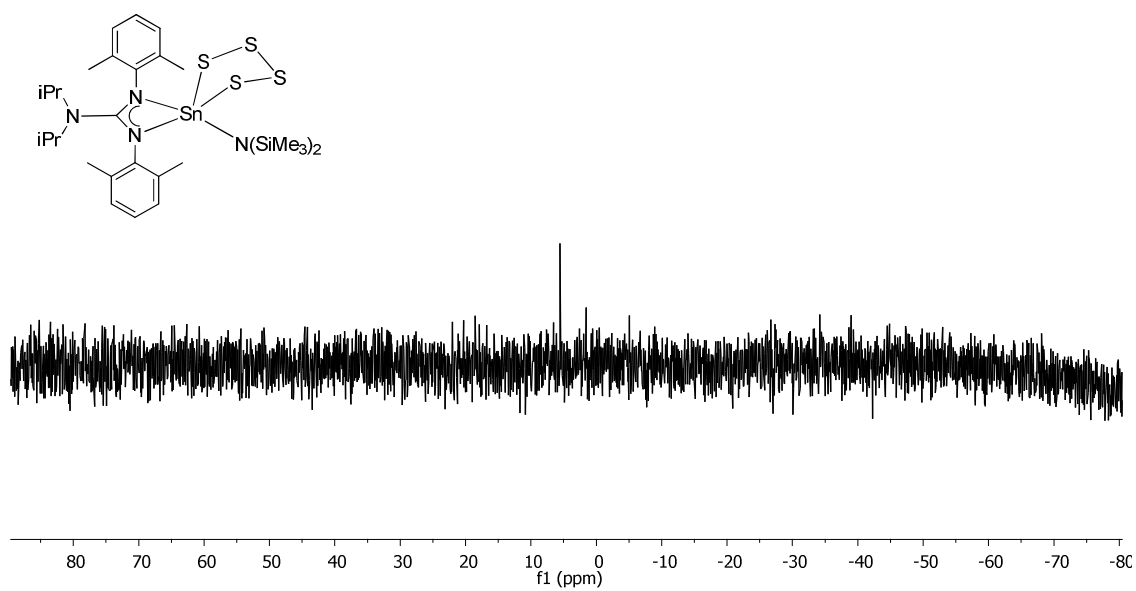


Fig. S9: ^{29}Si NMR Spectrum of [$\{\text{ArNC}(\text{N}^i\text{Pr}_2)\text{NAr}\}\text{SnN}(\text{SiMe}_3)_2(\text{S}_4)$] (**5**) in C_6D_6

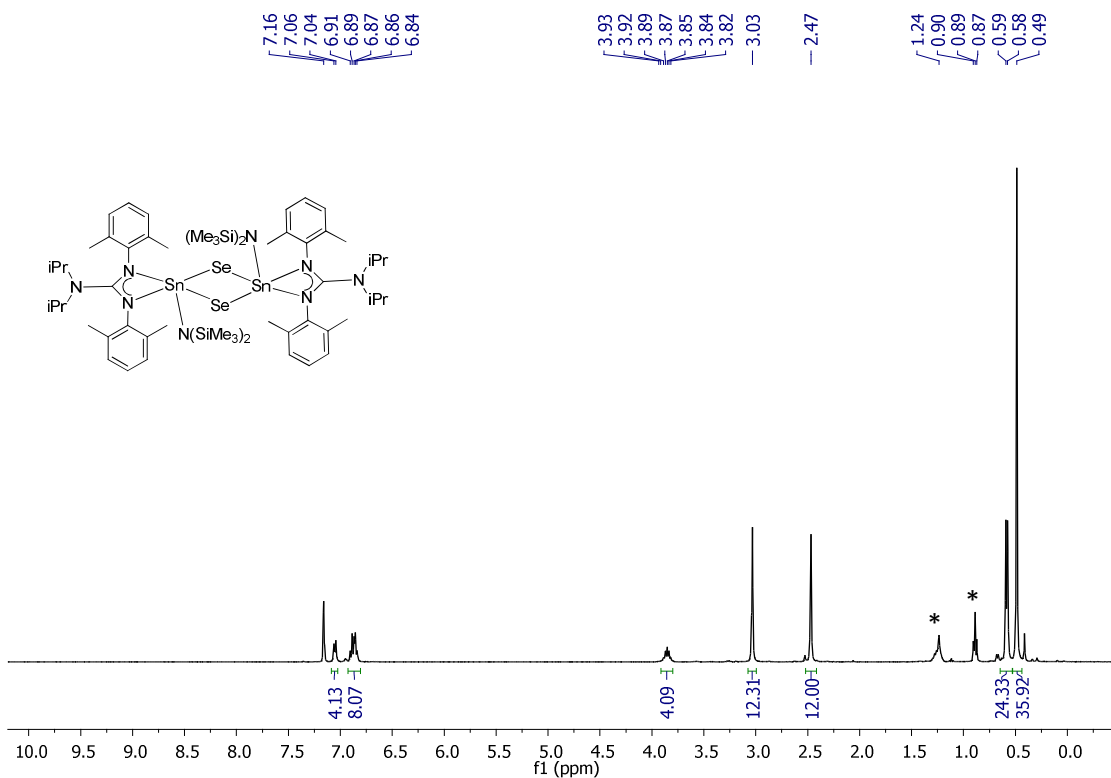


Fig. S10: ^1H NMR Spectrum of $[\{\text{ArNC}(\text{N}^i\text{Pr}_2)\text{NArN}(\text{SiMe}_3)_2\text{Sn}(\mu\text{-Se})\}_2]$ (**6**) in C_6D_6 (* = hexane impurities)

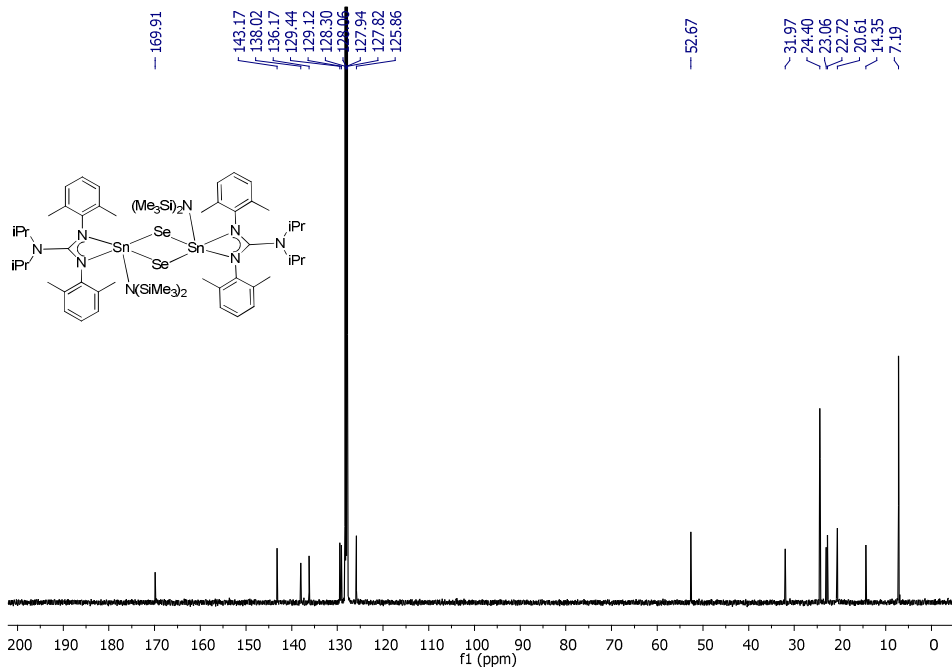


Fig. S11: ^{13}C NMR Spectrum of $[\{\text{ArNC}(\text{N}^i\text{Pr}_2)\text{NArN}(\text{SiMe}_3)_2\text{Sn}(\mu\text{-Se})\}_2]$ (**6**) in C_6D_6

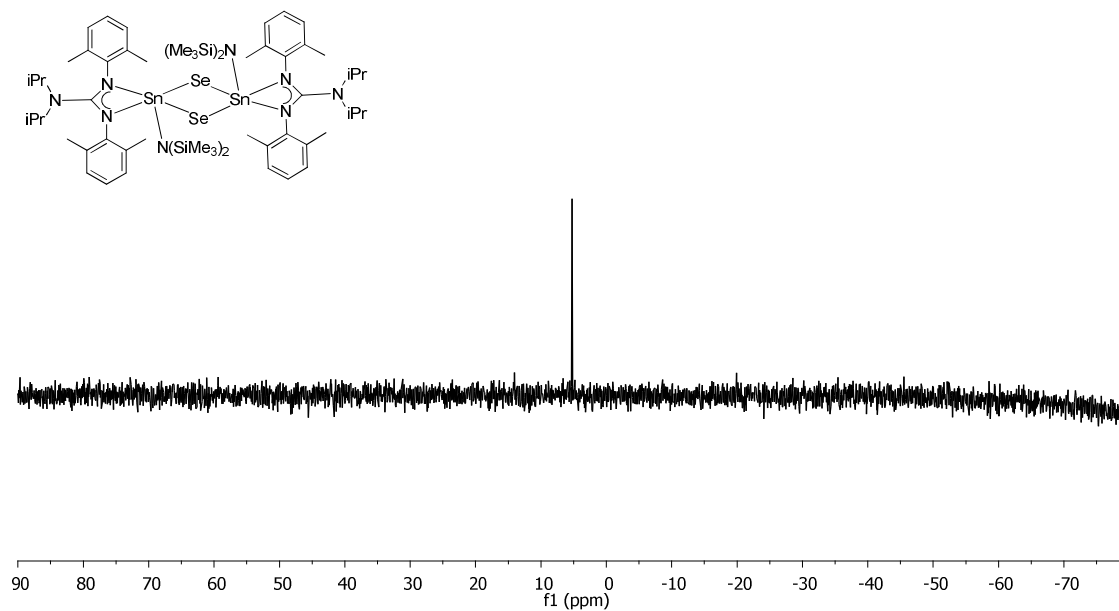
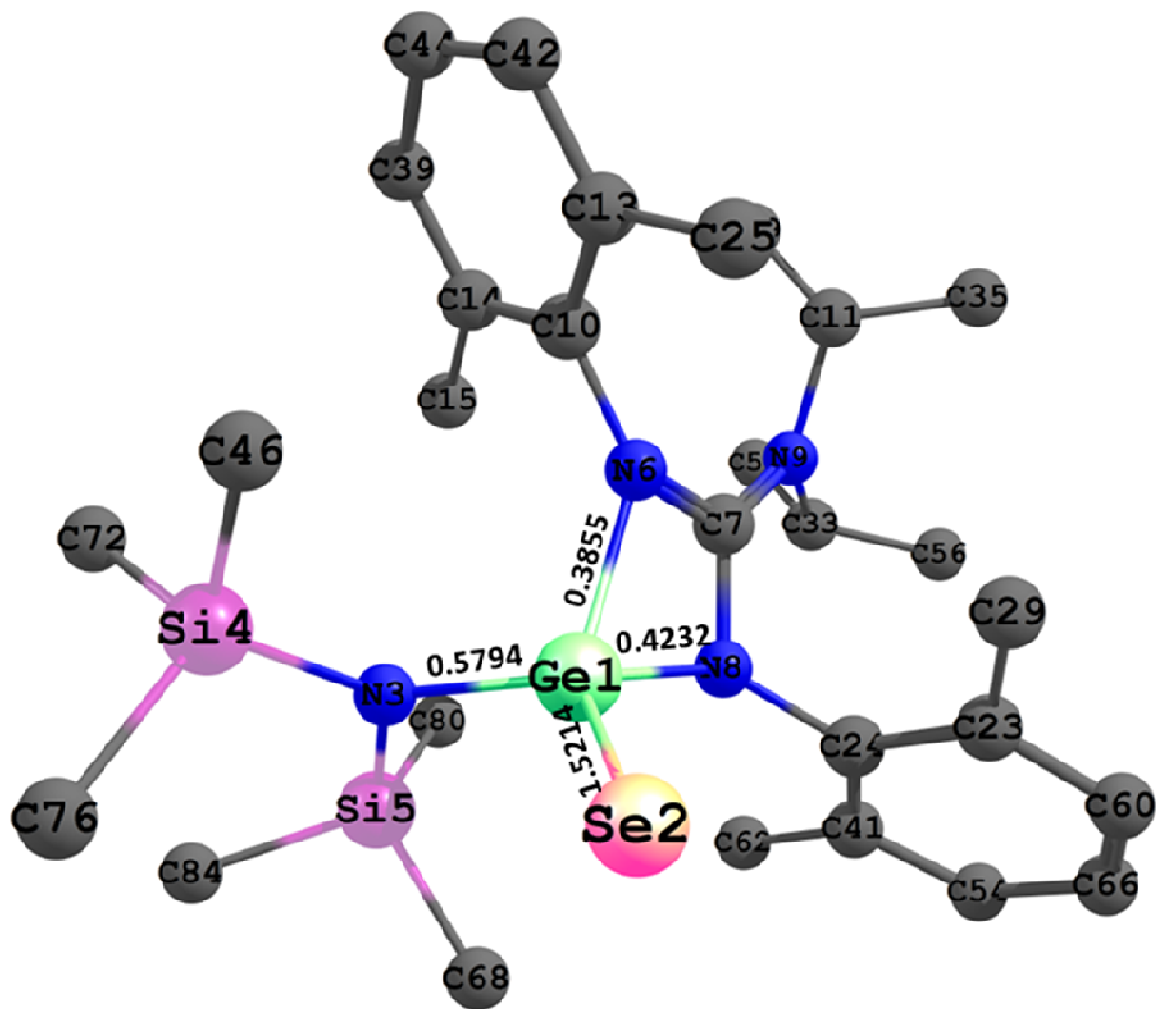


Fig. S12: ^{29}Si NMR Spectrum of $[\{\text{ArNC}(\text{N}^i\text{Pr}_2)\text{NArN}(\text{SiMe}_3)_2\text{Sn}(\mu\text{-Se})\}_2]$ (**6**) in C_6D_6

Computational studies

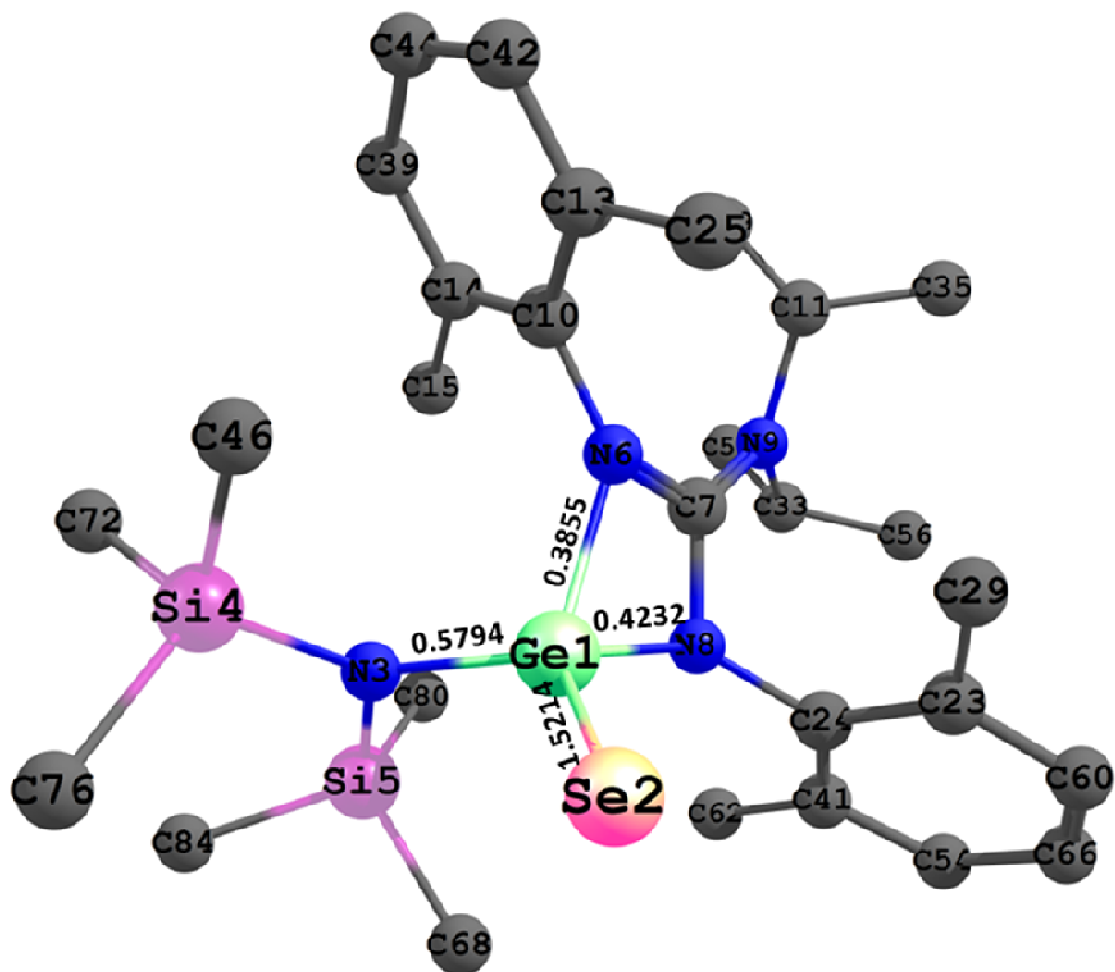
The Wiberg Bond Index (WBI) was computed at B3LYP/6-31+G(d) level of theory. The atomic coordinates were taken from the .cif files of compounds **3** & **4** and no further geometry optimization was carried out. The Wiberg Bond Index (WBI) of Ge–S in compound **3** and Ge–Se in compound **4** are 1.49 and 1.52, respectively, indicating the the existence of double bond between germanium and sulfur or selenium atoms.



(40.48%) 0.6362*Ge 1 s(54.66%)p 0.82(45.01%)d 0.01(0.33%)

(59.52%) 0.7715*S 2 s(16.57%)p 5.02(83.16%)d 0.02(0.27%)

Fig S13: Wiberg Bond Index (WBI) was computed at B3LYP/6-31+G(d) level of theory for compound **3**



(44.79%) 0.6693*Ge 1 s(55.41%)p 0.80(44.22%)d 0.01(0.37%)

(55.21%) 0.7430*Se 2 s(13.36%)p 6.47(86.53%)d 0.01(0.11%)

Fig S14: Wiberg Bond Index (WBI) was computed at B3LYP/6-31+G(d) level of theory for compound **4**