Electronic Supporting Information

For

Bonding analysis in ytterbium(II) distannyl and related tetryls

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Table of Contents

NMR Spectra of Novel Compounds
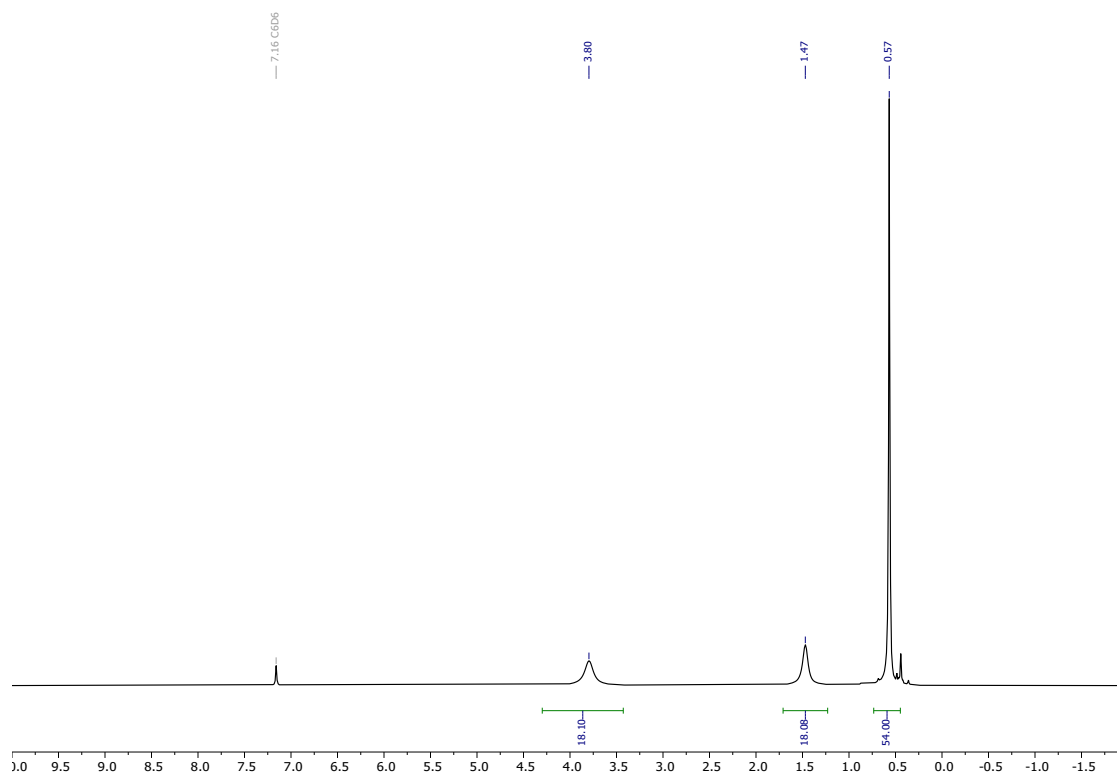
Figure S1. ^{1}H NMR spectrum (500.13 MHz, benzene-d_6, 300 K) of [Yb{Sn(SiMe$_3$)$_3$}$_2$.(thf)$_4$] (**Yb-Sn**).
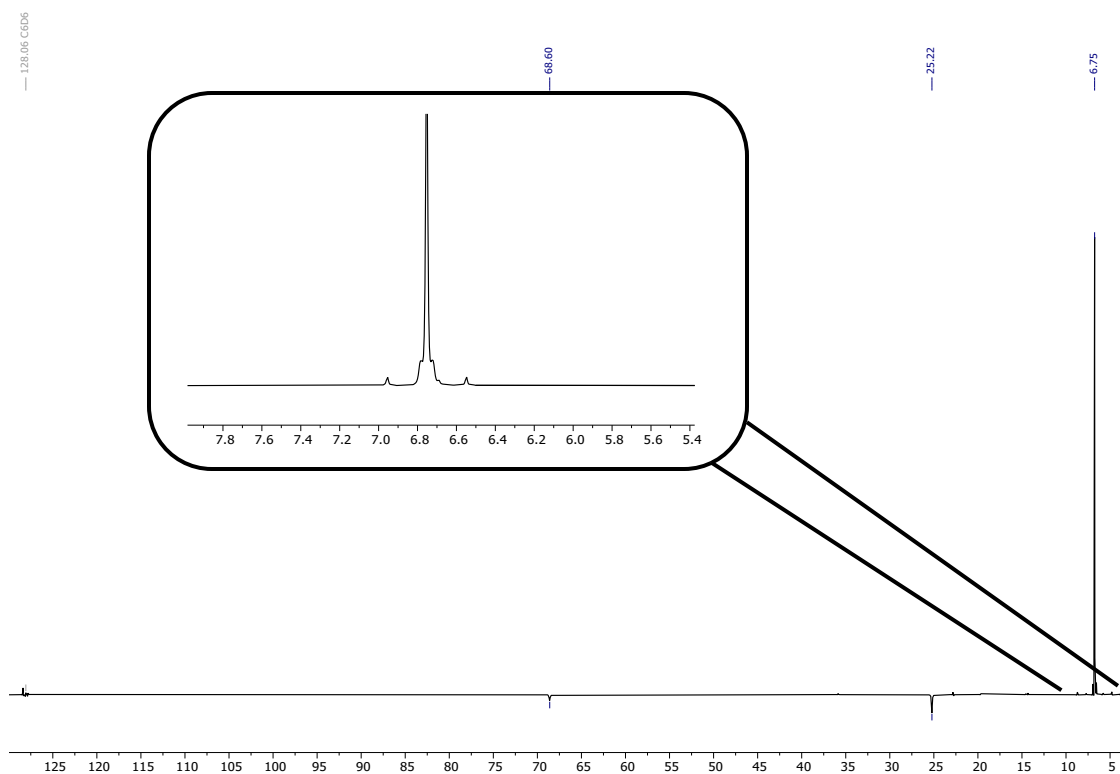
Figure S2. $^{13}C\{^1H\}$ DEPT-135 NMR spectrum (500.13 MHz, benzene-d_6, 300 K) of [Yb{Sn(SiMe$_3$)$_3$}$_2$.(thf)$_4$] (**Yb-Sn**). Inset shows resonance at 6.75 ppm with observable satellites.
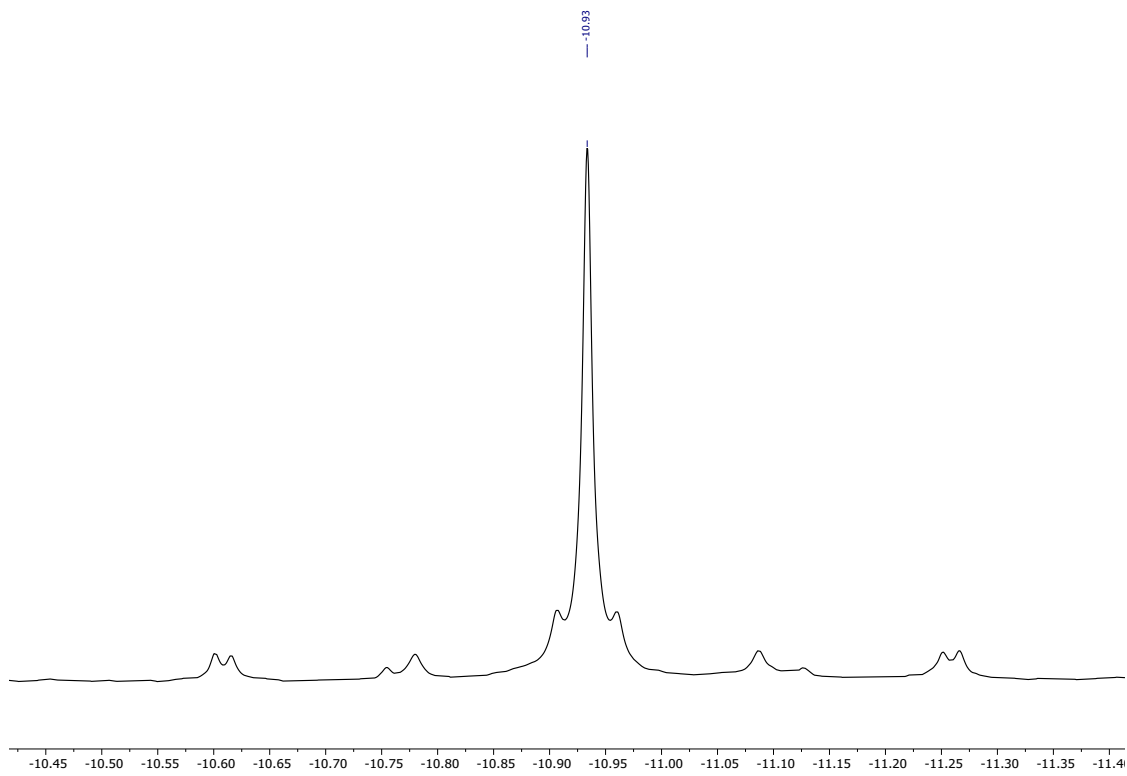
Figure S3. $^{29}Si\{^1H\}$ DEPT NMR spectrum (99.36 MHz, benzene-d_6, 300 K) of [Yb{Sn(SiMe$_3$)$_3$}$_2$.(thf)$_4$] (**Yb-Sn**).

−756.90
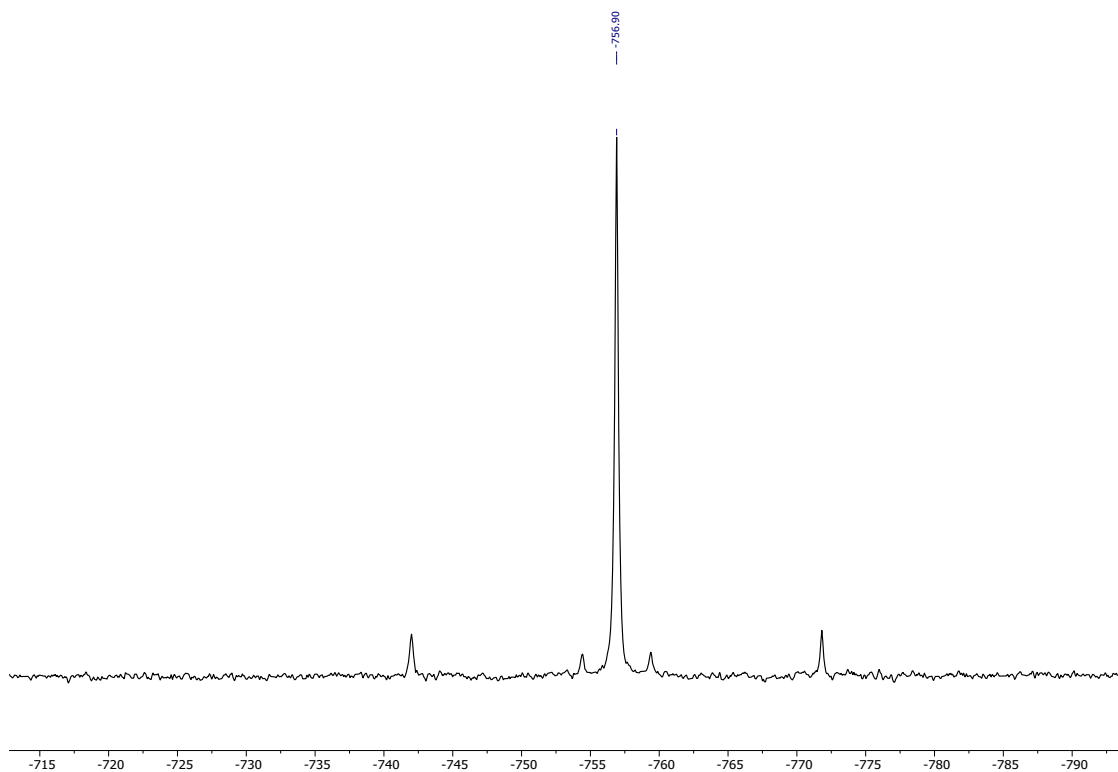
Figure S4. ^{119}Sn NMR spectrum (186.36 MHz, benzene-d_6, 300 K) of [Yb{Sn(SiMe$_3$)$_3$}$_2$.(thf)$_4$] (**Yb-Sn**).

534.64
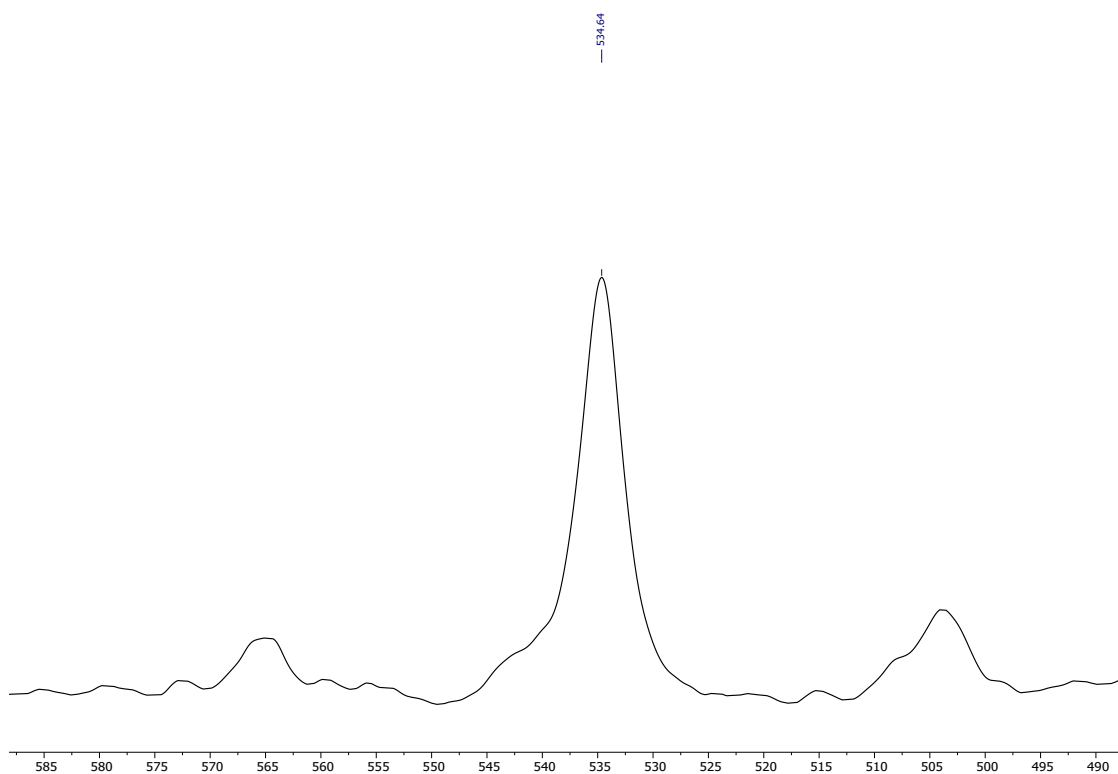
Figure S5. [171]Yb NMR spectrum (87.57 MHz, benzene-d_6, 300 K) of [Yb{Sn(SiMe$_3$)$_3$}$_2$.(thf)$_4$] (**Yb-Sn**).
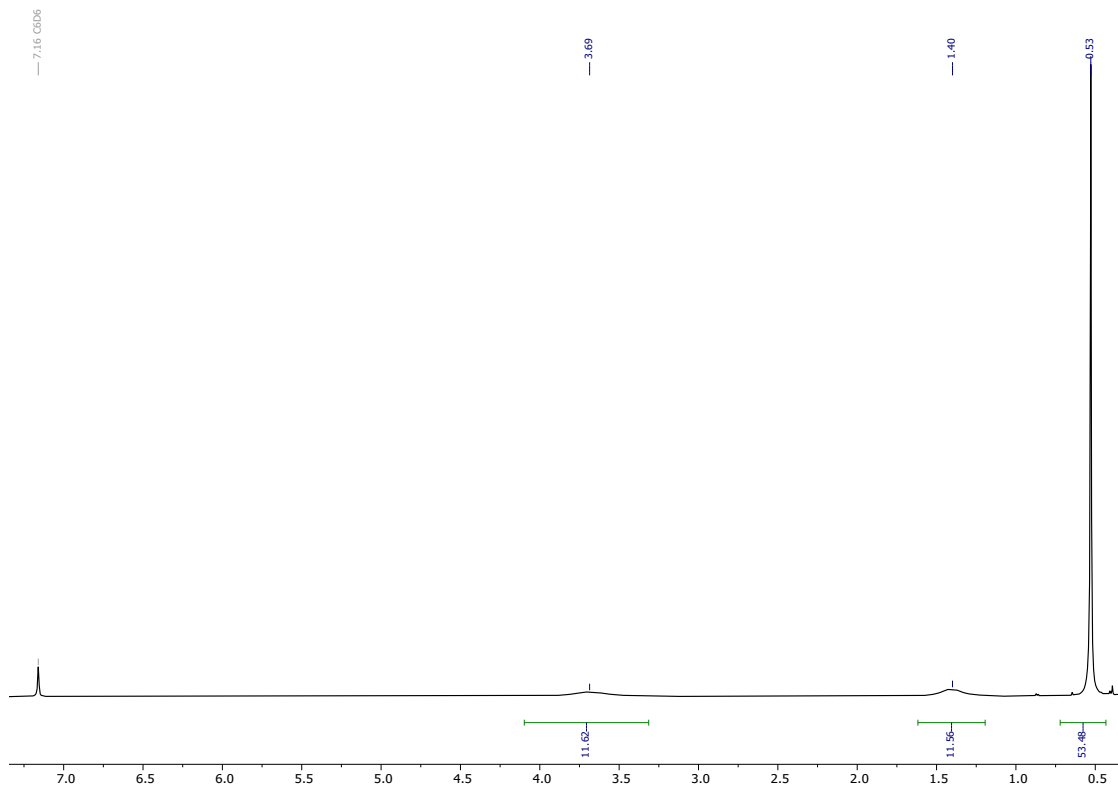
Figure S6. ^{1}H NMR spectrum (500.13 MHz, benzene-d_6, 298 K) of [Yb{Ge(SiMe$_3$)$_3$}$_2$.(thf)$_3$] (**Yb-Ge**).
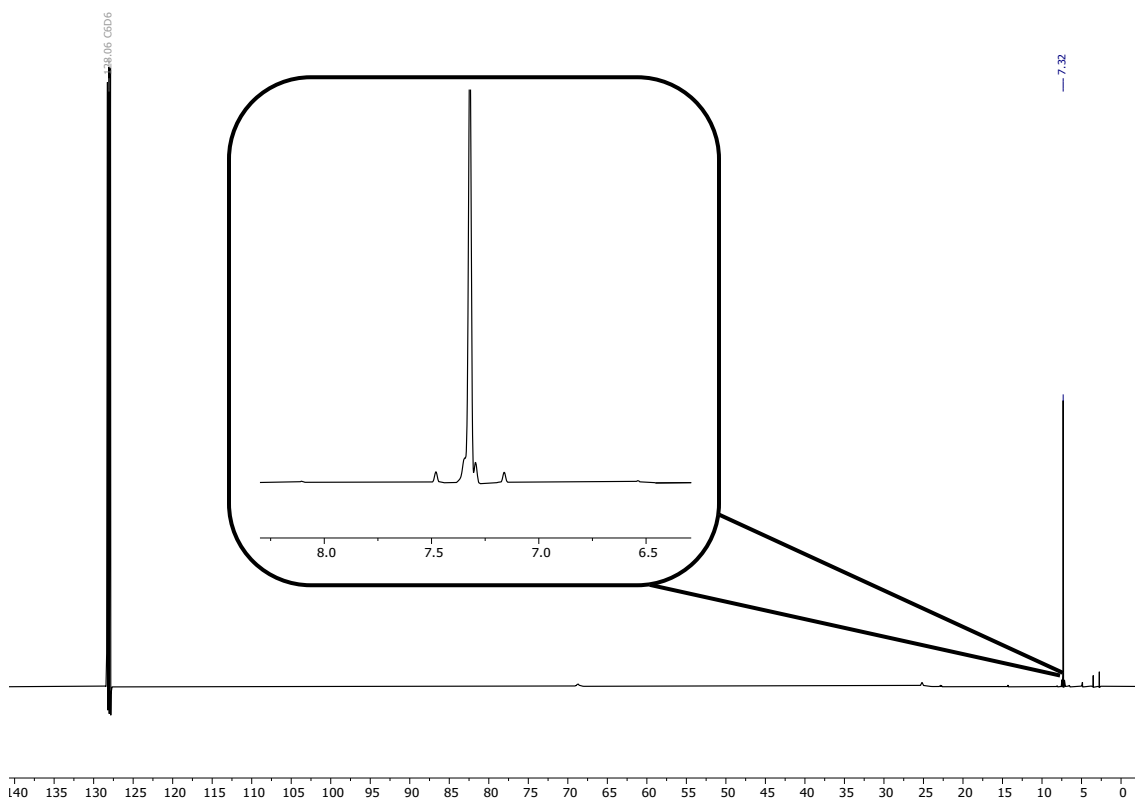
Figure S7. ^{13}C{^{1}H} NMR spectrum (125.13 MHz, benzene-d_6, 298 K) of [Yb{Ge(SiMe$_3$)$_3$}$_2$.(thf)$_3$] (**Yb-Ge**). Inset shows resonance at 7.32 ppm with detectable satellites.
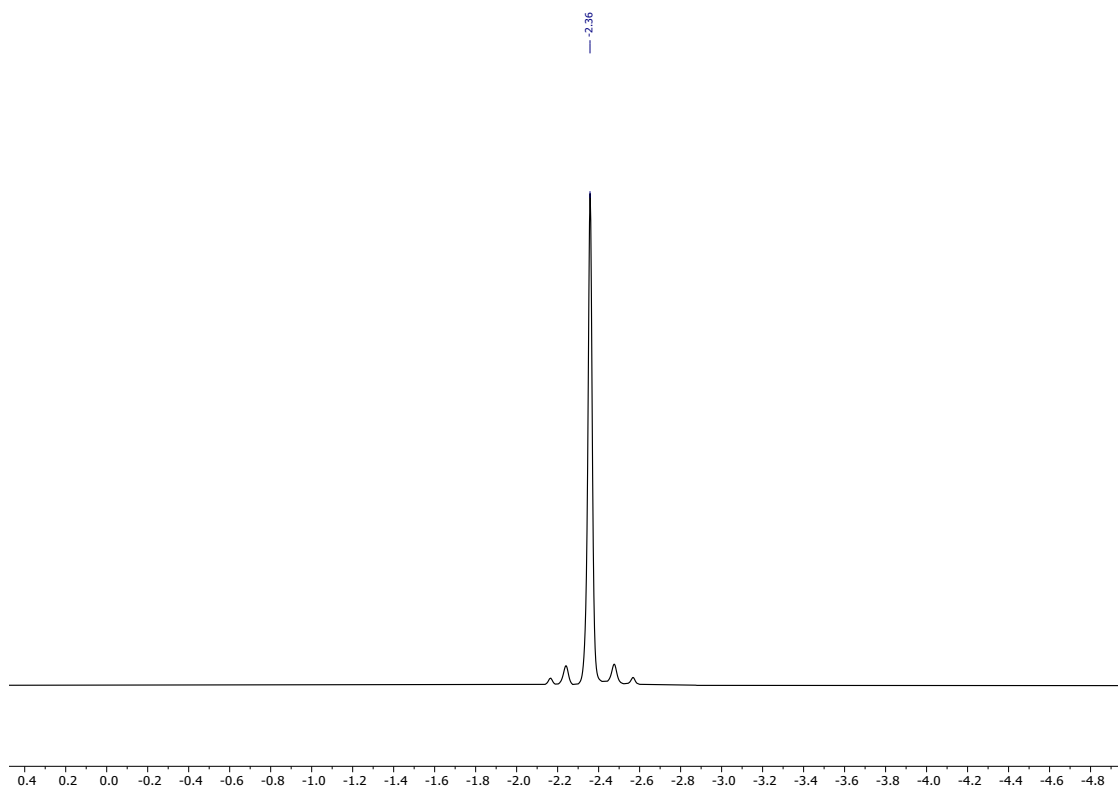
Figure S8. $^{29}Si\{^1H\}$ DEPT NMR spectrum (99.36 MHz, benzene-d_6, 298 K) of [Yb{Ge(SiMe$_3$)$_3$}$_2$.(thf)$_3$] (**Yb-Ge**).
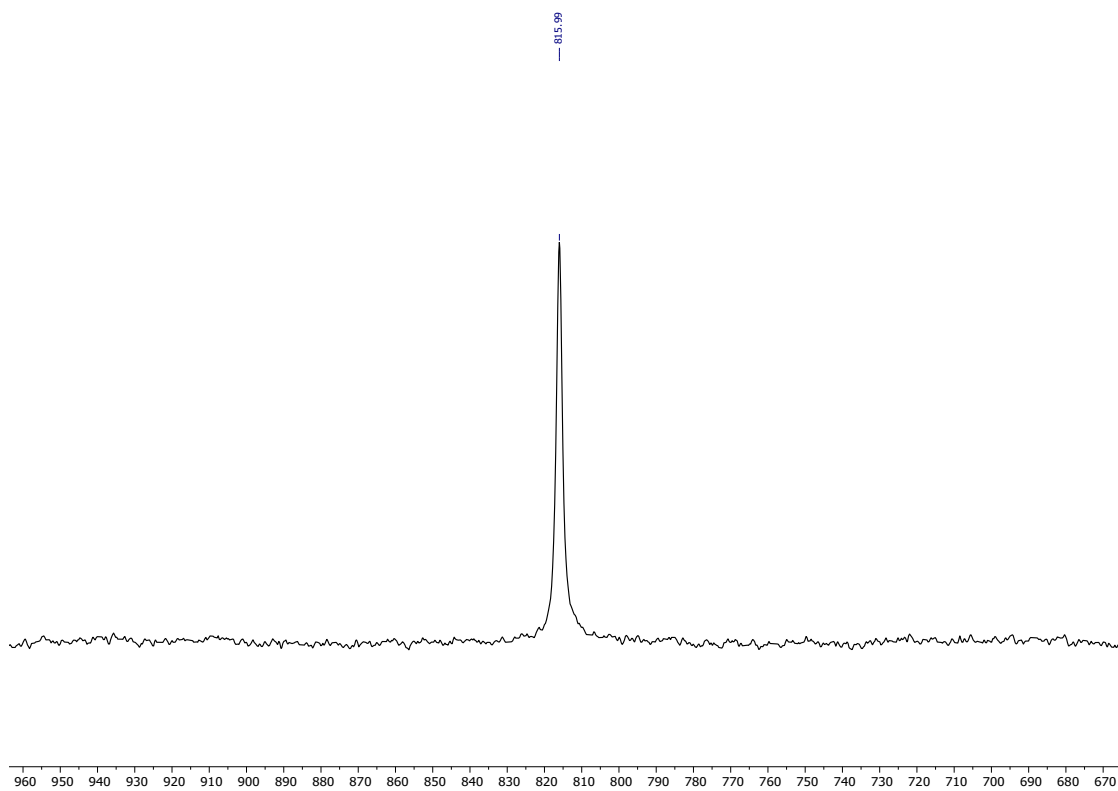
Figure S9. ^{171}Yb NMR spectrum (87.57 MHz, benzene-d_6, 298 K) of [Yb{Ge(SiMe$_3$)$_3$}$_2$.(thf)$_3$] (**Yb-Ge**).

New NMR spectra for previously reported compounds
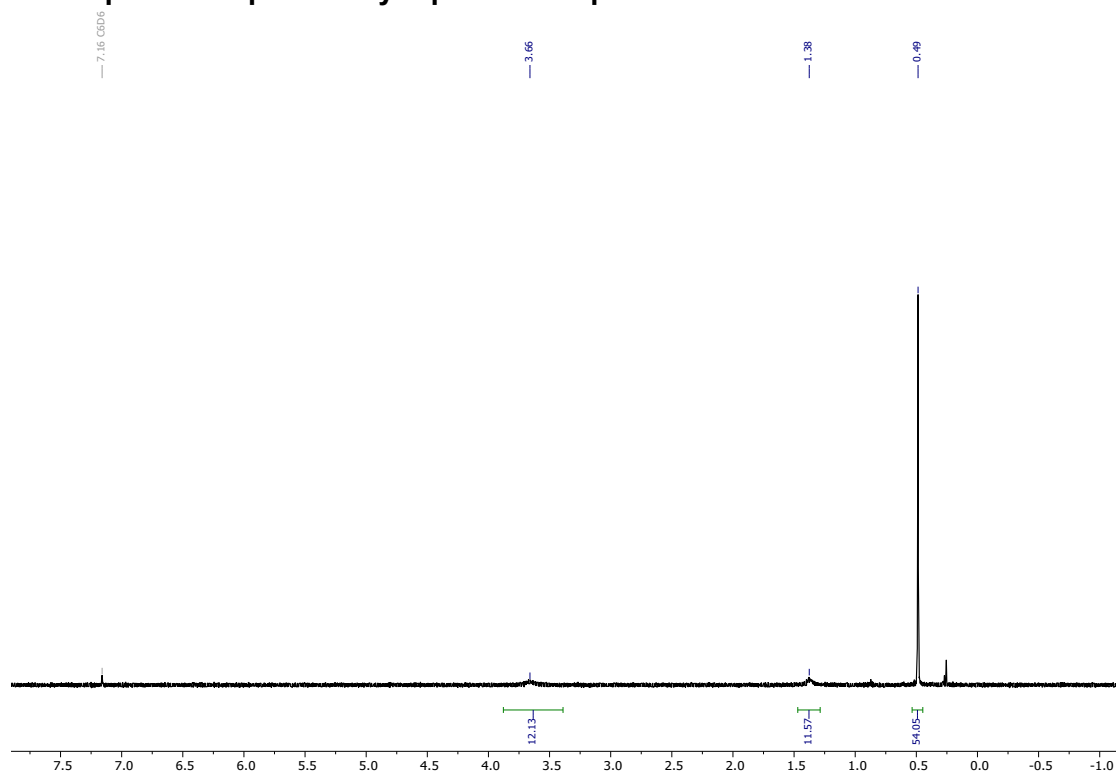
Figure S10. ¹H NMR spectrum (500.13 MHz, benzene-d_6, 300 K) of [Yb{Si(SiMe$_3$)$_3$}$_2$.(thf)$_3$] (**Yb-Si**).
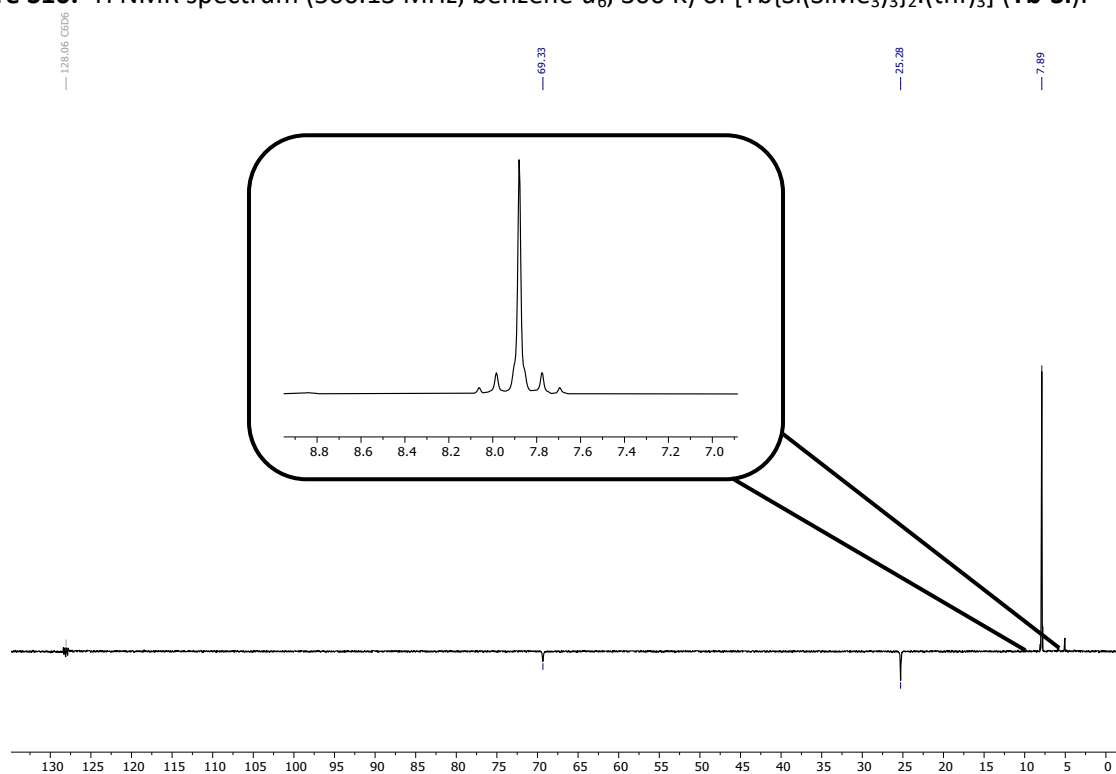
Figure S11. ¹³C{¹H} DEPT-135 NMR spectrum (100.65 MHz, benzene-d_6, 300 K) of [Yb{Si(SiMe$_3$)$_3$}$_2$.(thf)$_3$] (**Yb-Si**). Inset shows resonance at 7.89 ppm with detectable satellites.
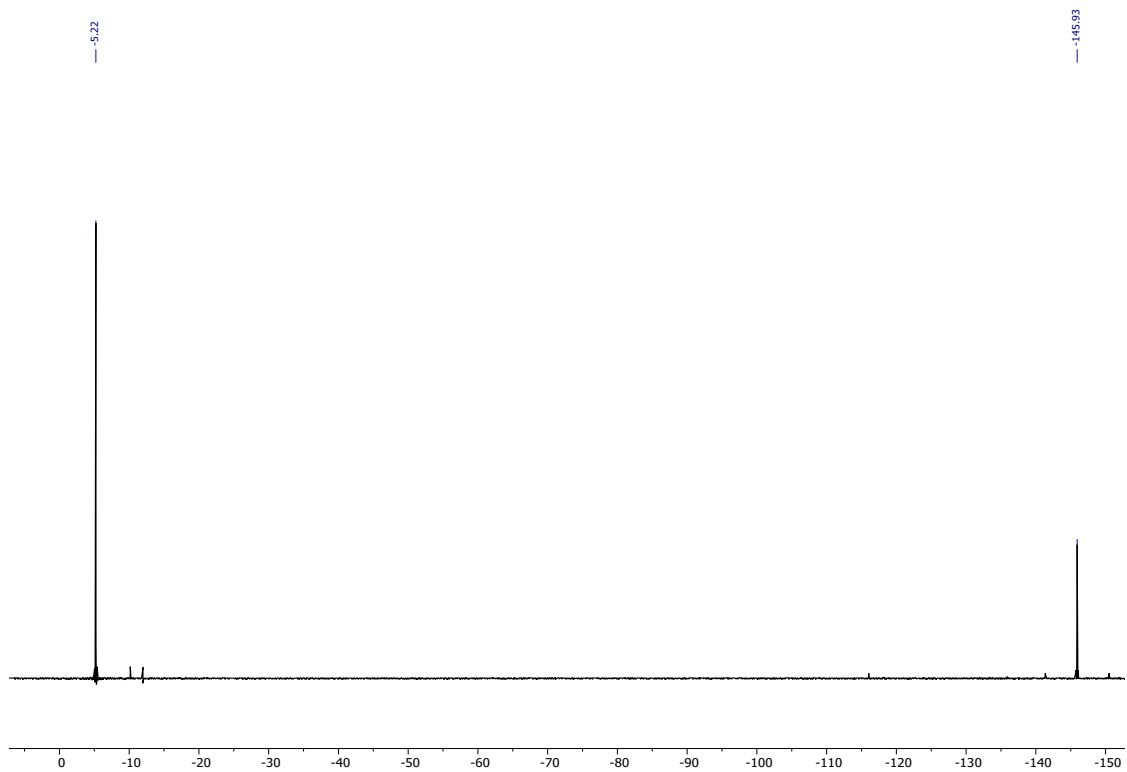
Figure S12. $^{29}Si\{^1H\}$ DEPT NMR spectrum (99.36 MHz, benzene-d_6, 300 K) of [Yb{Si(SiMe$_3$)$_3$}$_2$.(thf)$_3$] (**Yb-Si**).
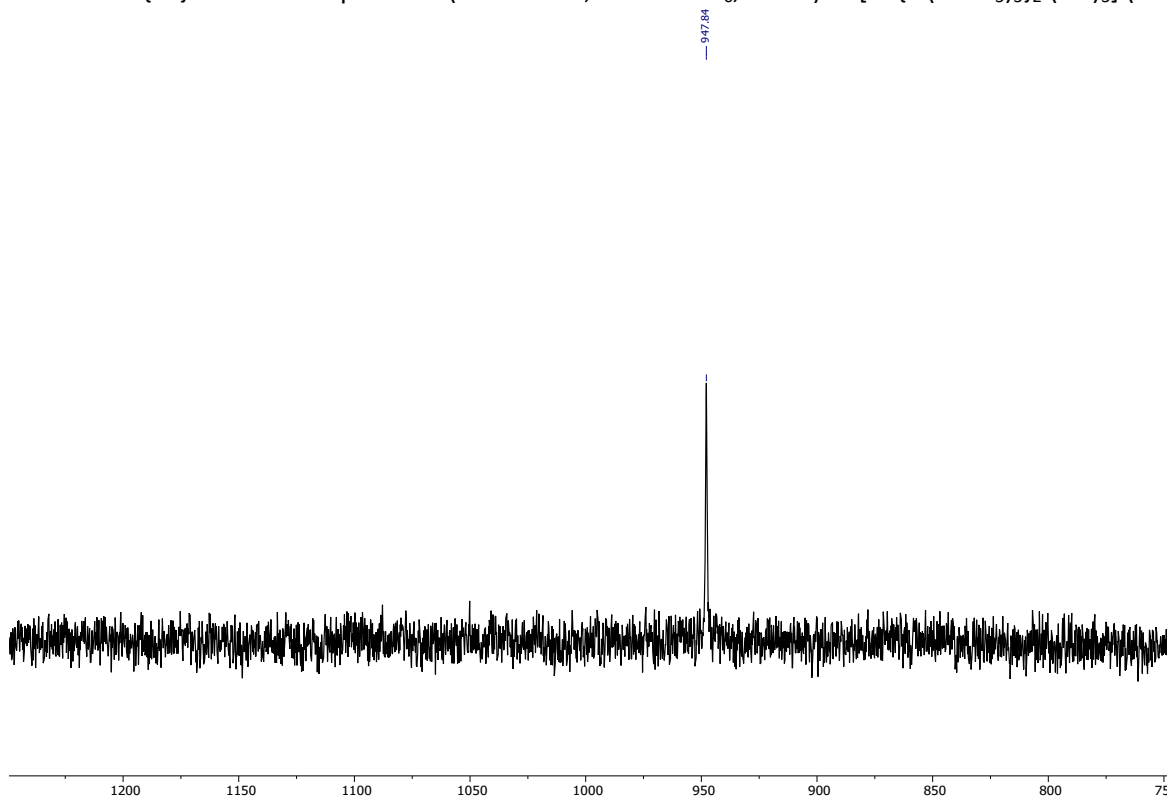
Figure S13. ^{171}Yb NMR spectrum (87.57 MHz, benzene-d_6, 300 K) of [Yb{Si(SiMe$_3$)$_3$}$_2$.(thf)$_3$] (**Yb-Si**).

X-ray diffraction crystallography details

Compound	Complex label	Experiment Number	CCDC Number
[Yb{Ge(SiMe$_3$)$_3$}$_2$}$_2$.(thf)$_3$]	Yb-Ge	PC05078	2060120
[Yb{Sn(SiMe$_3$)$_3$}$_2$}$_2$.(thf)$_4$]	Yb-Sn	PC04115	2060121

[Yb{Ge(SiMe$_3$)$_3$}$_2$}$_2$.(thf)$_3$] (**Yb-Ge**)

(C$_{30}$H$_{78}$Ge$_2$O$_3$Si$_6$Yb); M = 973.68. A suitable crystal for X-ray diffraction single crystal experiment (yellow prism, dimensions = 0.400 x 0.310 x 0.290 mm) was selected and mounted on the goniometer head of a D8 VENTURE Bruker AXS diffractometer equipped with a (CMOS) PHOTON 100 detector, using Mo-$K\alpha$ radiation (λ = 0.71073 Å, multilayer monochromator) at T = 150 K. The crystal structure has been described in orthorhombic symmetry and $P\,n\,a\,2_1$ (I.T. #33) space group. Cell parameters have been refined as follows: a = 18.943(3), b = 15.0354(17), c = 17.129(2) Å, V = 4878.6(11) Å^3. Number of formula unit Z is equal to 4 and calculated density d and absorption coefficient μ values are 1.326 g.cm^{-3} and 3.297 mm^{-1} respectively. The structure was solved by dual-space algorithm using the *SHELXT* program,[1] and then refined with full-matrix least-squares methods based on F^2 (*SHELXL*).[2] All non-hydrogen atoms were refined with anisotropic atomic displacement parameters. H atoms were finally included in their calculated positions and treated as riding on their parent atom with constrained thermal parameters. A final refinement on F^2 with 11236 unique intensities and 510 parameters converged at ωR_F^2 = 0.0516 (R_F = 0.0265) for 10170 observed reflections with $I > 2\sigma(I)$.

[Yb{Sn(SiMe$_3$)$_3$}$_2$}$_2$.(thf)$_4$] (**Yb-Sn**)

(C$_{34}$H$_{86}$O$_4$Si$_6$Sn$_2$Yb); M = 1137.98. D8 VENTURE Bruker AXS diffractometer equipped with a (CMOS) PHOTON 100 detector, Mo-$K\alpha$ radiation (λ = 0.71073 Å, multilayer monochromator), T = 150 K; orthorhombic $P\,b\,c\,a$ (I.T.#61), a = 13.2657(8), b = 19.8289(11), c = 40.652(2) Å, V = 10693.3(10) Å^3. Z = 8, d = 1.414 g.cm^{-3}, μ = 2.825 mm^{-1}. The structure was solved by dual-space algorithm using the *SHELXT* program,[1] and then refined with full-matrix least-squares methods based on F^2 (*SHELXL*).[2] All non-hydrogen atoms were refined with anisotropic atomic displacement parameters. H atoms were finally included in their calculated positions and treated as riding on their parent atom with constrained thermal parameters. A final refinement on F^2 with 12072 unique intensities and 489 parameters converged at ωR_F^2 = 0.0739 (R_F = 0.0378) for 9553 observed reflections with $I > 2\sigma(I)$.

References

1   G. M. Sheldrick, *Acta Cryst.*, 2015, **A71**, 3-8.

2   G. M. Sheldrick, *Acta Cryst.*, 2015, **C71**, 3-8.

Author Contributions

Peter. M. Chapple did all synthetic experimental work, analysis of the data and assisted in writing of the draft. Marie Cordier performed the X-ray analysis. Jean-Yves Saillard, Julien Cartron and Samia Kahlal carried out all computational work and took part in the writing of the draft. Jean-François Carpentier participated to the design of experiments and analysis of experimental data. Hassan Oulyadi and Ghanem Hamdoun designed, performed and interpreted the high-resolution NMR analysis. Yann Sarazin was the lead investigator; he participated to the design of experiments, analysis of experimental data and writing of the draft.