

Supporting information for

Lithium Salt of 2,5-Bis(trimethylsilyl)Stannolyl Anion: Synthesis, Structure, and Nonaromatic Character

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1. Packing structure of **2**

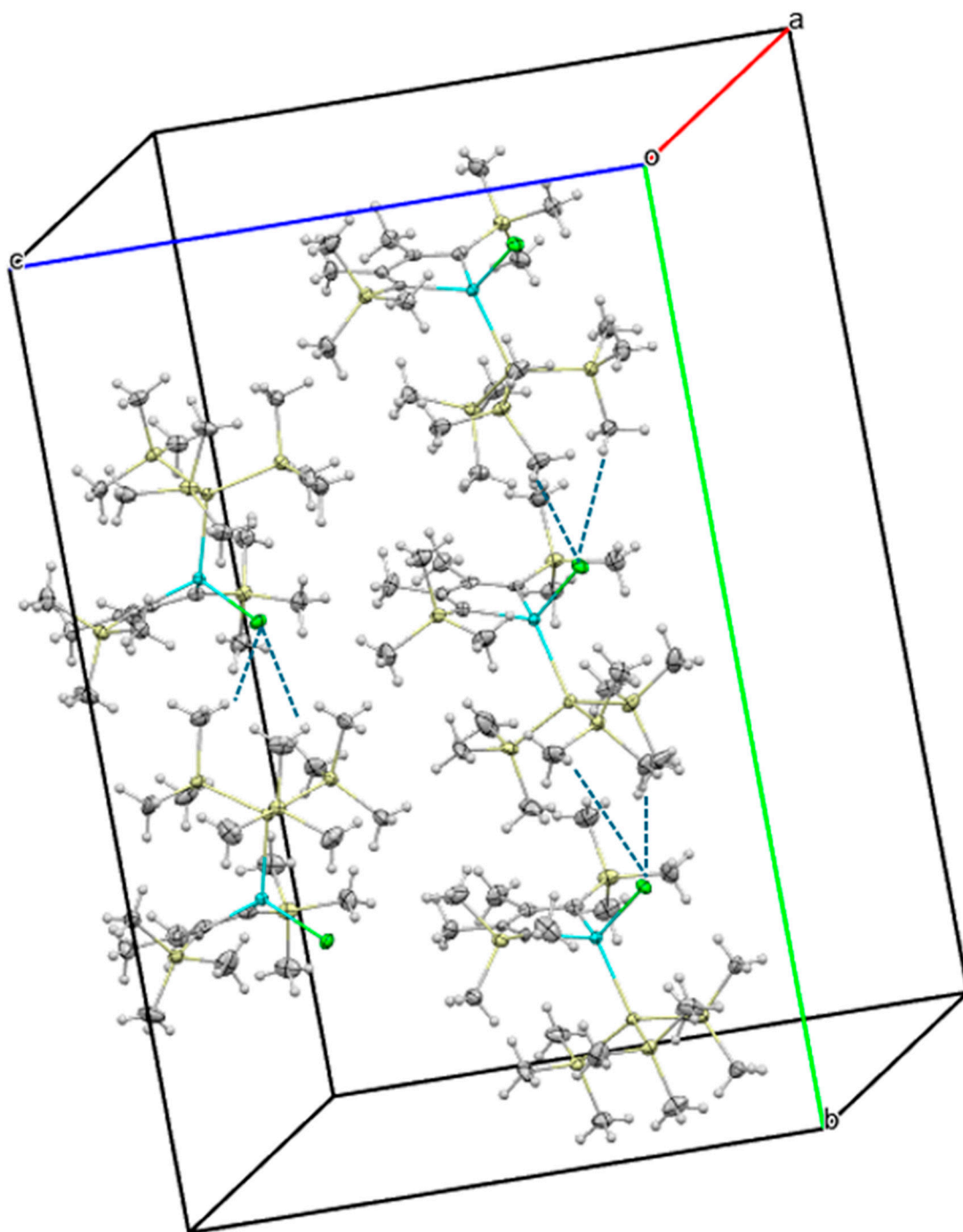


Figure S1. Packing structure of **2**. CH...Cl bonds are shown by blue broken lines.

2. X-ray crystallographic data for **2** and **3·(thf)₃**

Table S1. Crystallographic data for **2** and **3·(thf)₃**.

	2	3·(thf)₃
CCDC	2337714	2337715
formula	C ₂₁ H ₅₁ ClSi ₆ Sn	C ₃₃ H ₇₅ Li O ₃ Si ₆ Sn
Mw	626.29	814.10
crystal dimension	0.25 × 0.15 × 0.15	0.14 × 0.13 × 0.10
crystal system	monoclinic	monoclinic
space group	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> 2 ₁ / <i>n</i>
<i>a</i> [Å]	18.826(2)	13.3363(11)
<i>b</i> [Å]	28.856(3)	19.6417(18)
<i>c</i> [Å]	18.810(2)	17.7954(16)
α [deg]	90	90
β [deg]	97.7770(10)	91.4530(10)
γ [deg]	90	90
<i>V</i> [Å ³]	10124.5(19)	4660.0(7)
<i>Z</i>	12	4
ρ_{calcd} [g cm ⁻³]	1.233	1.16
<i>F</i> (000)	3936	1736
μ [cm ⁻¹]	10.57	7.29
transmission factors	0.947 – 0.9694	0.8623 – 1
range		
index range	-24 ≤ <i>h</i> ≤ 24	-17 ≤ <i>h</i> ≤ 13
	-35 ≤ <i>k</i> ≤ 37	-24 ≤ <i>k</i> ≤ 25
	-24 ≤ <i>l</i> ≤ 19	-23 ≤ <i>l</i> ≤ 23
no. reflections	82916	37674
unique (<i>R_{int}</i>)	23037 (0.0729)	10667 (0.0437)
<i>I</i> > 2σ(<i>I</i>)	18698	8924
no. parameters	1243	452
<i>R</i> ₁ (<i>I</i> > 2σ(<i>I</i>)) ^a	0.0619	0.0437
<i>wR</i> ₂ (all data) ^b	0.1272	0.0952
GOF ^c	1.121	1.103
max diff peak	1.073/–1.01	1.155/–0.849
/ hole [e Å ⁻³]		

^a $R1 = \sum ||F_o| - |F_c|| / \sum |F_o|$. ^b $wR2 = [\sum \{w(F_o^2 - F_c^2)^2\} / \sum w(F_o^2)^2]^{1/2}$, $w = 1 / [^2F_o^2 + (aP)^2 + bP]$ (*a* and *b* are constants suggested by the refinement program; $P = [\max(F_o^2, 0) + 2F_c^2] / 3$). ^c $GOF = [\sum w(F_o^2 - F_c^2)^2 / (N_{\text{obs}} - N_{\text{params}})]^{1/2}$.

3. NMR spectra of **1**, **2**, and **3**·(thf)

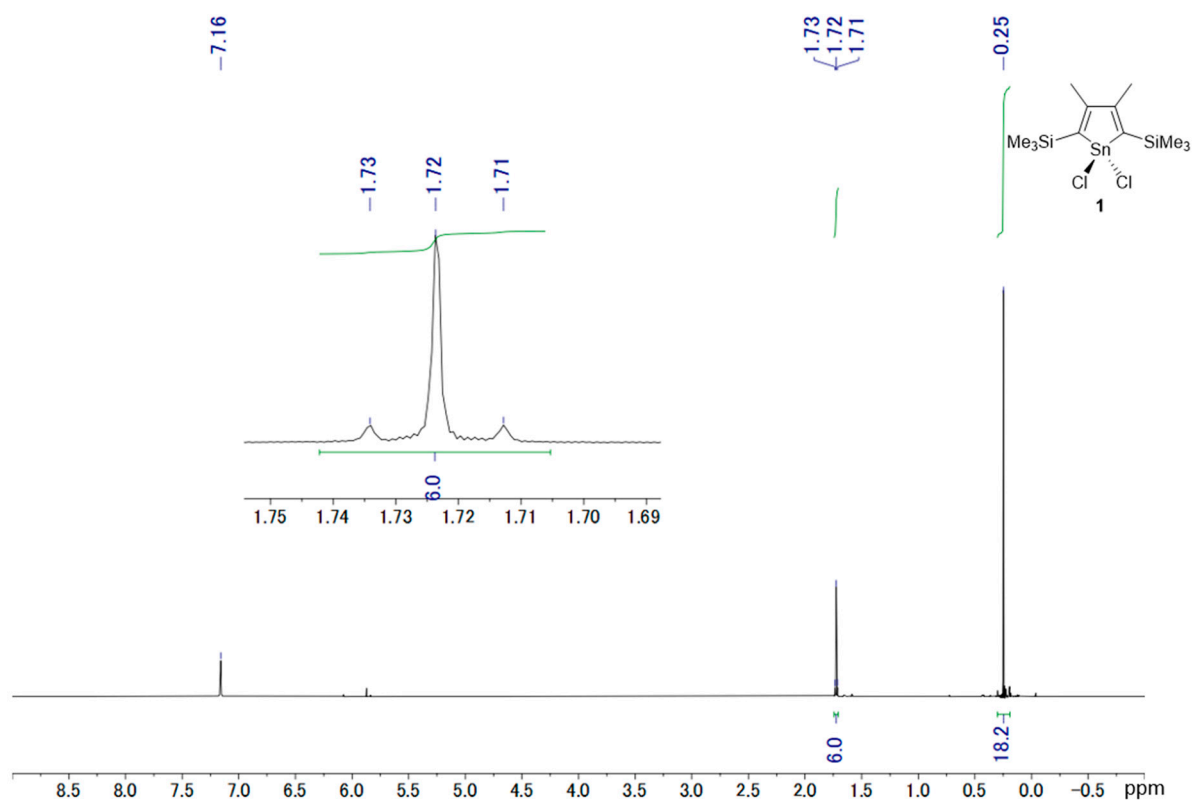


Figure S2. ¹H NMR spectrum of **1** (500 MHz, C₆D₆).

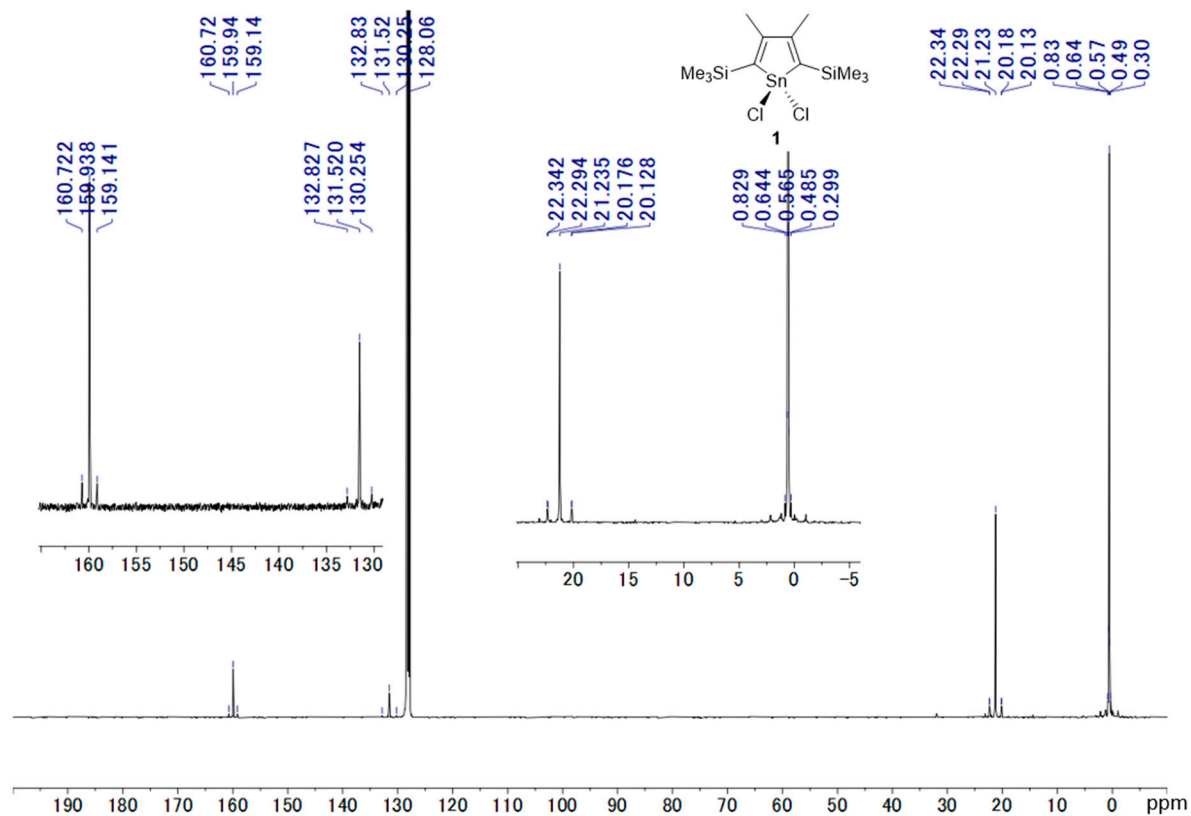


Figure S3. ¹³C{¹H} NMR spectrum of **1** (100 MHz, C₆D₆).

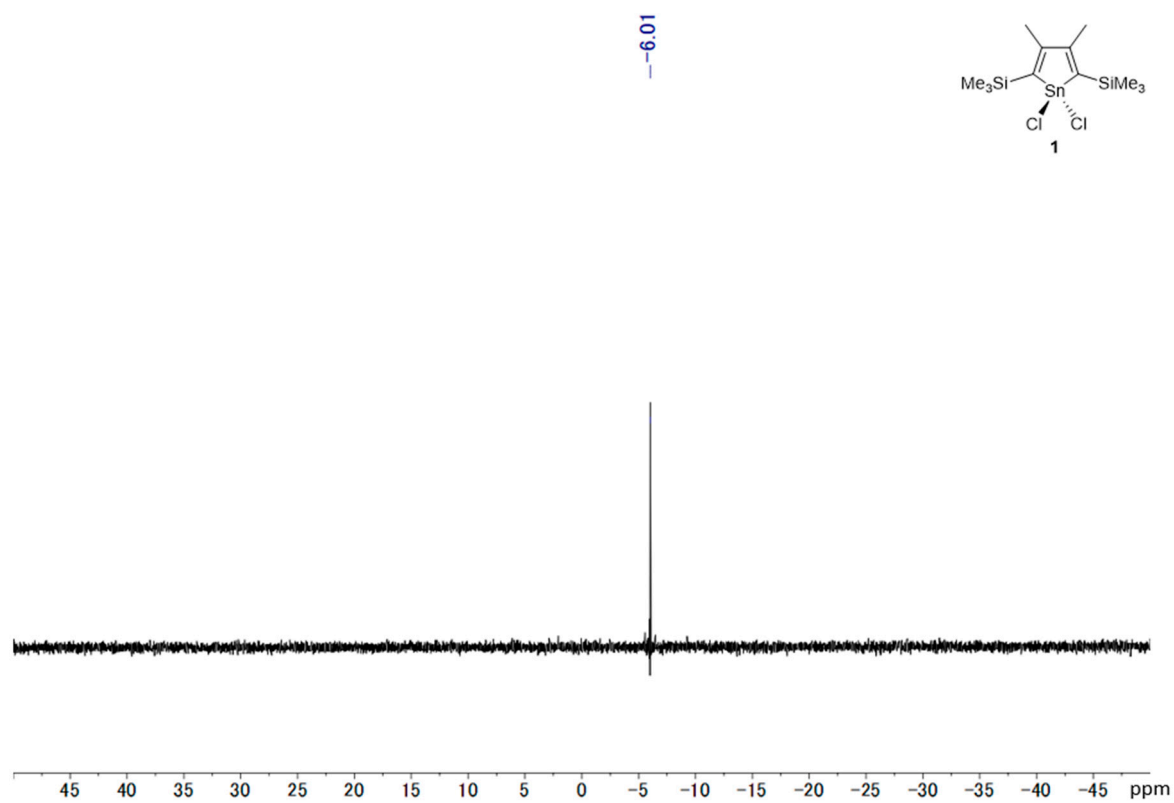


Figure S4. ²⁹Si{¹H} NMR spectrum of **1** (99 MHz, CDCl₃).

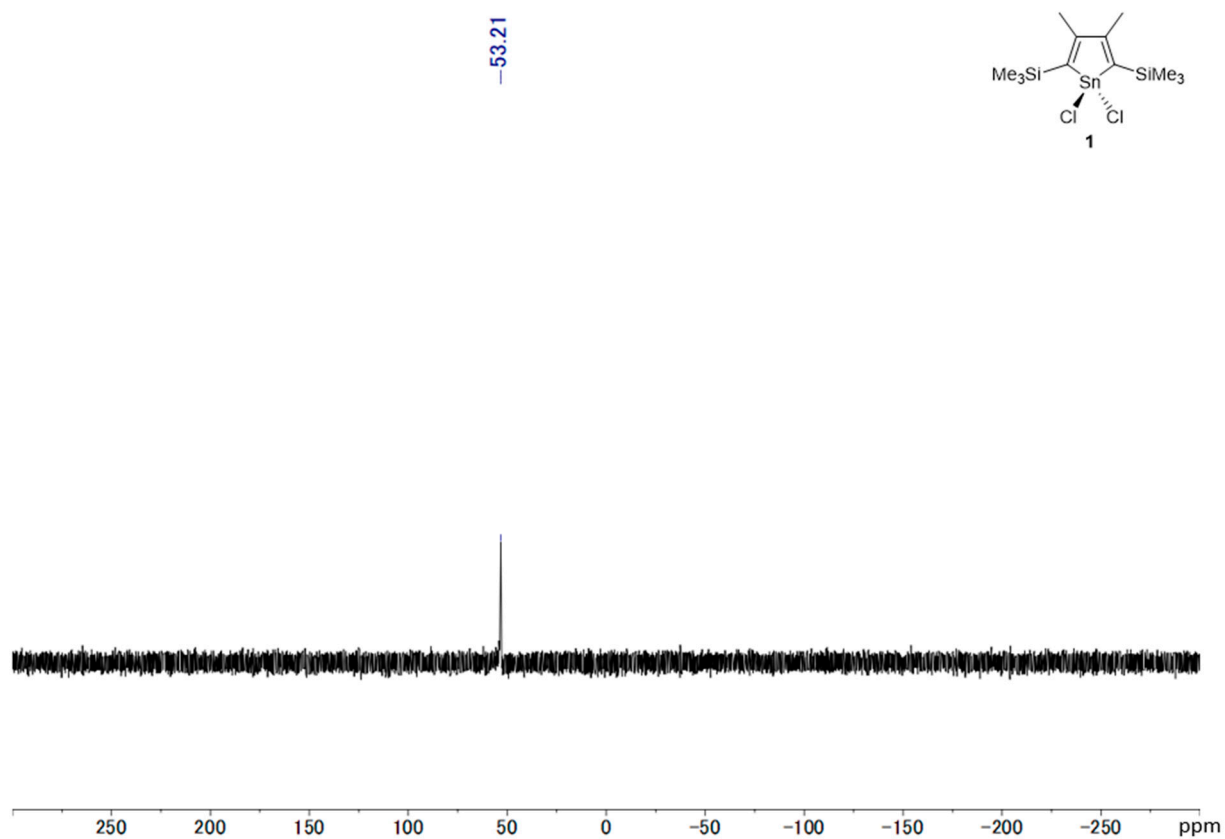


Figure S5. ¹¹⁹Sn{¹H} NMR spectrum of **1** (186 MHz, C₆D₆).

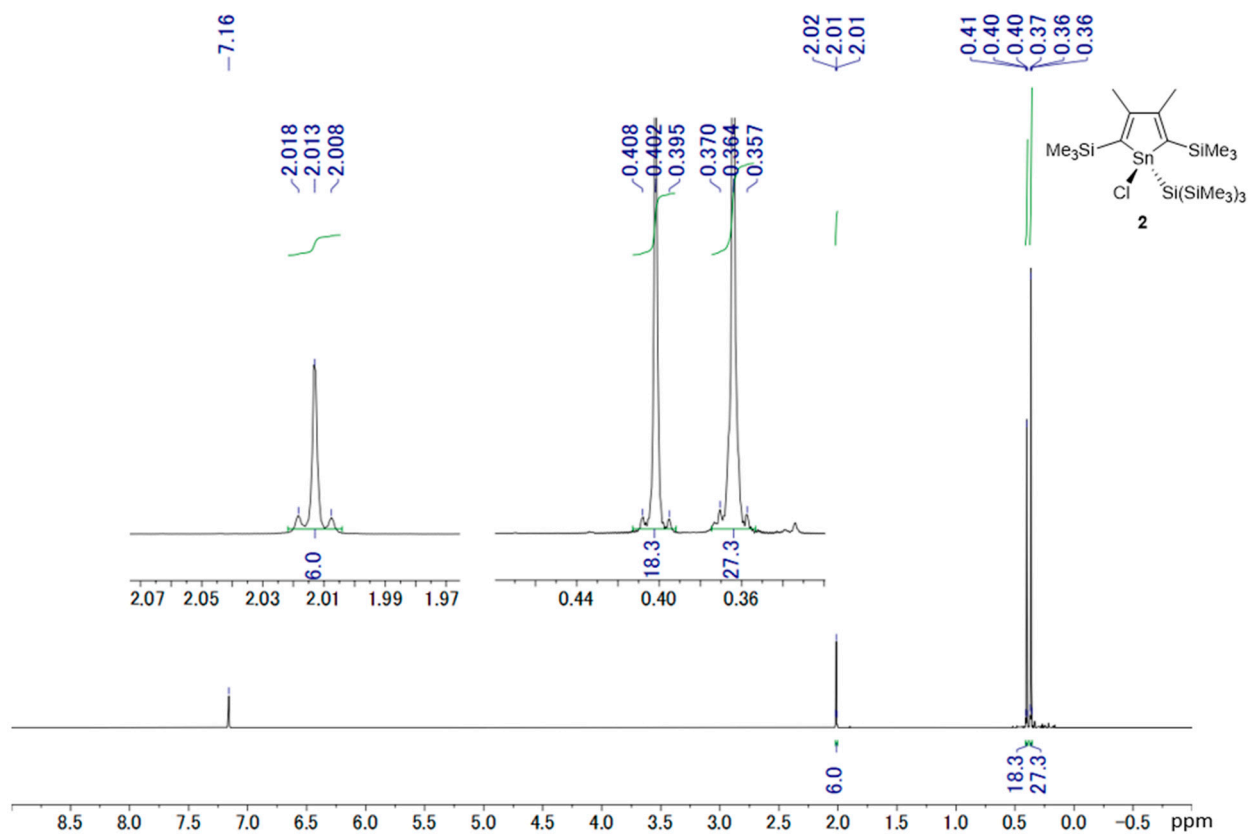


Figure S6. ¹H NMR spectrum of **2** (500 MHz, C₆D₆).

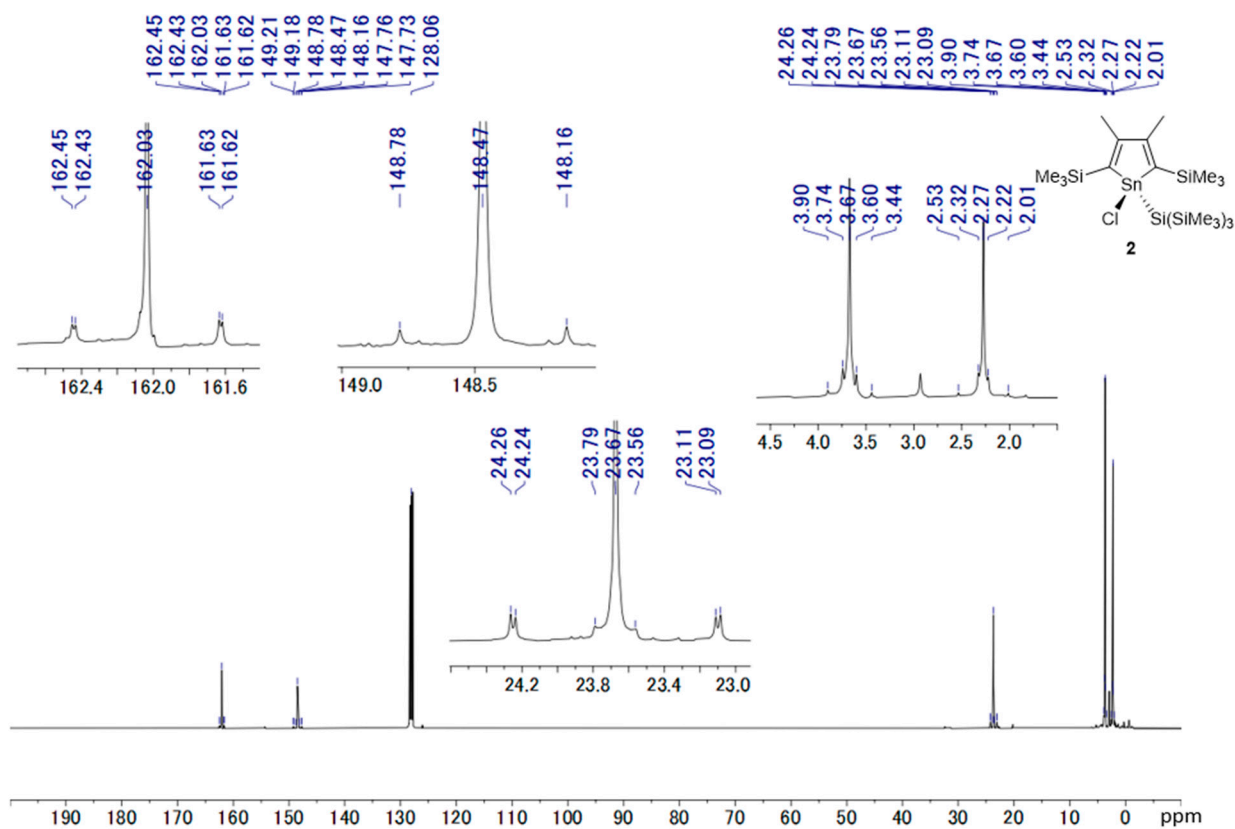


Figure S7. ¹³C{¹H} NMR spectrum of **2** (100 MHz, C₆D₆).

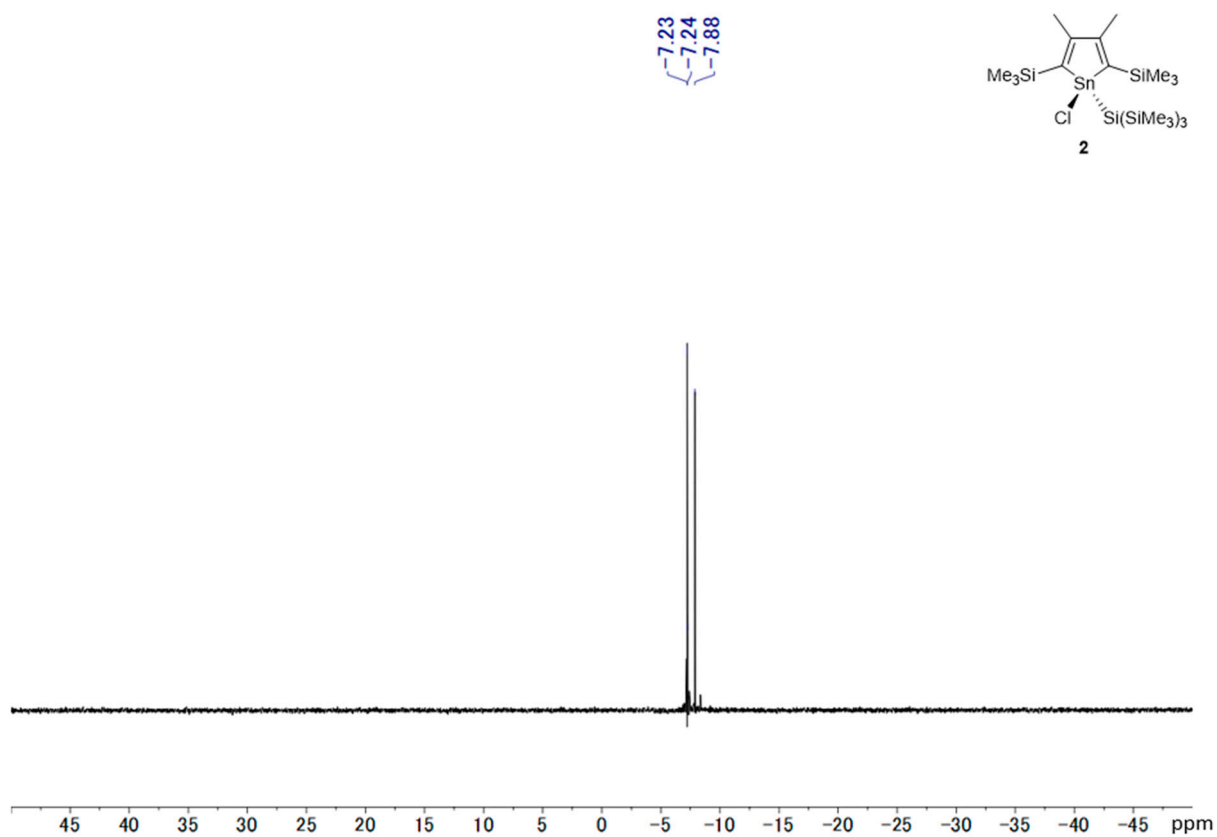


Figure S8. ²⁹Si{¹H} NMR spectrum of **2** (99 MHz, CDCl₃).

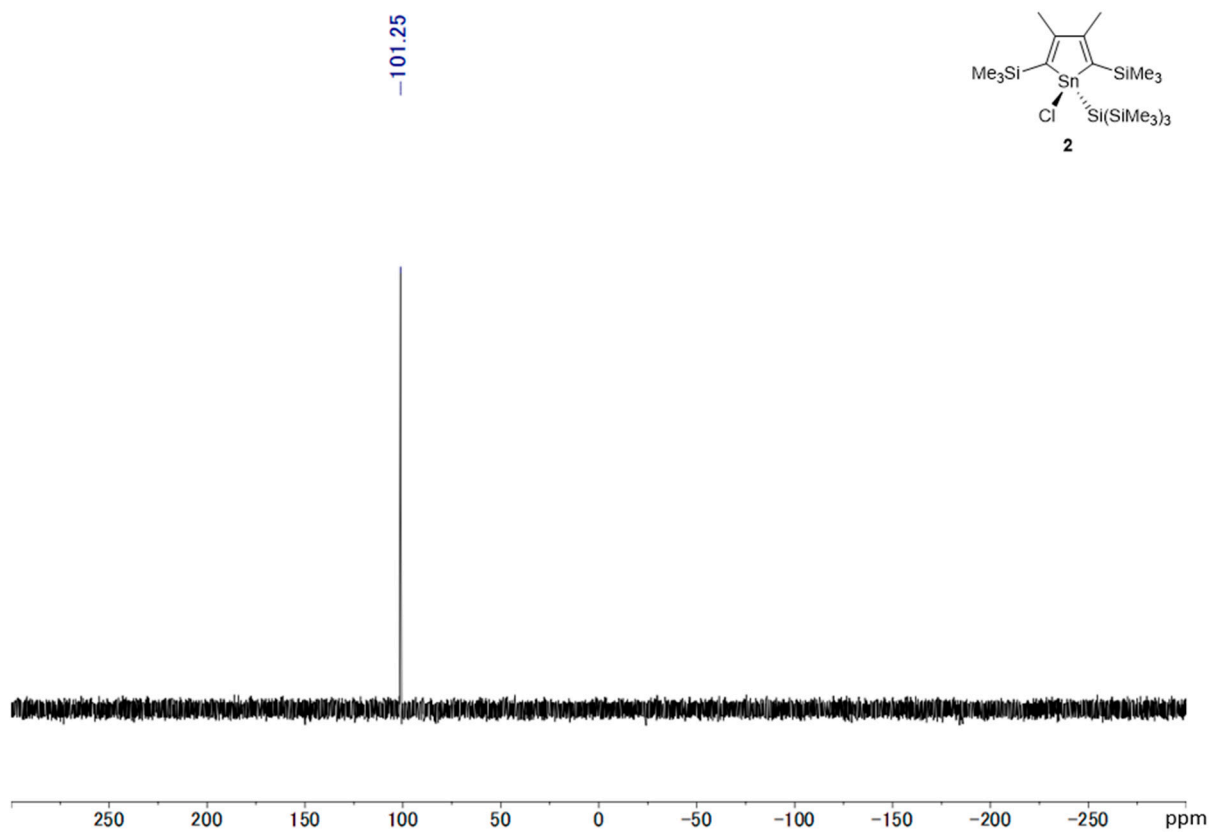


Figure S9. ¹¹⁹Sn{¹H} NMR spectrum of **2** (186 MHz, C₆D₆).

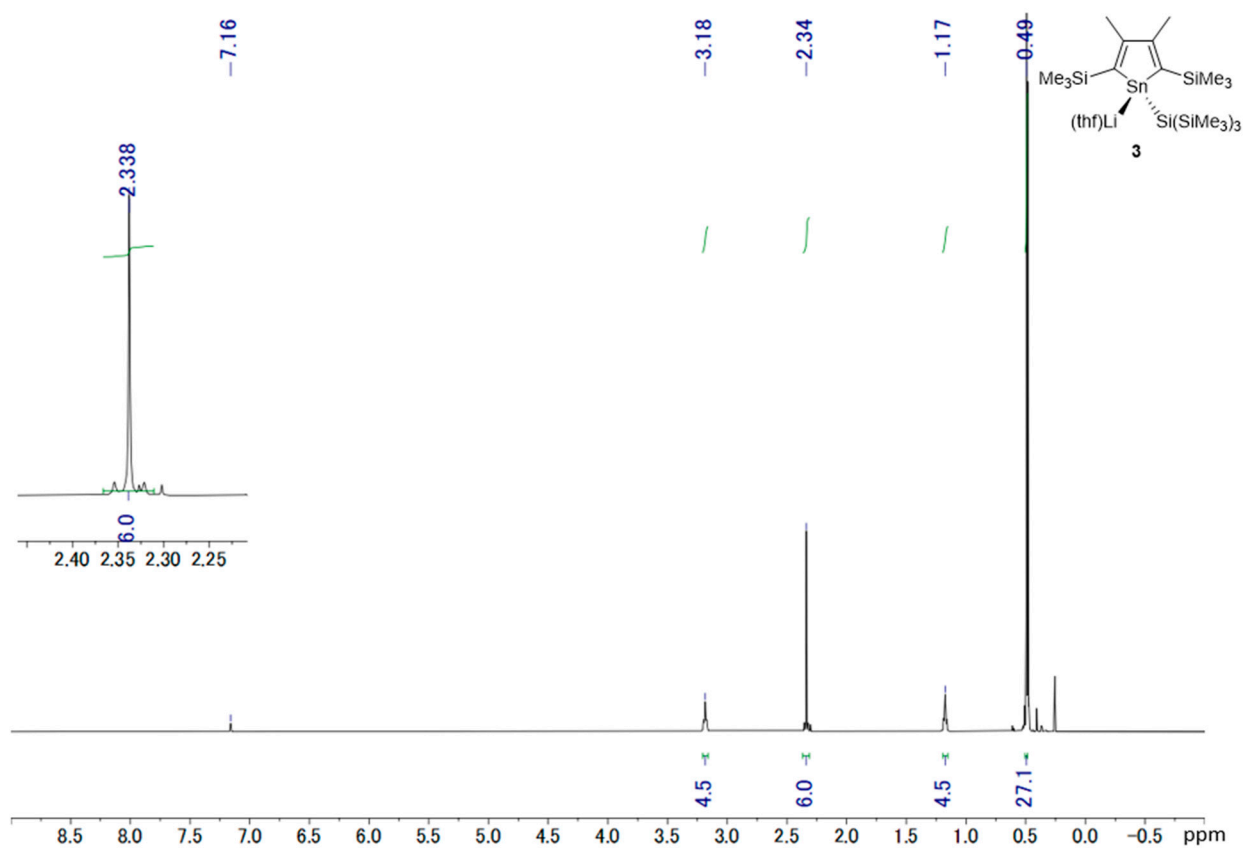


Figure S10. ¹H NMR spectrum of **3**·thf (500 MHz, C₆D₆).

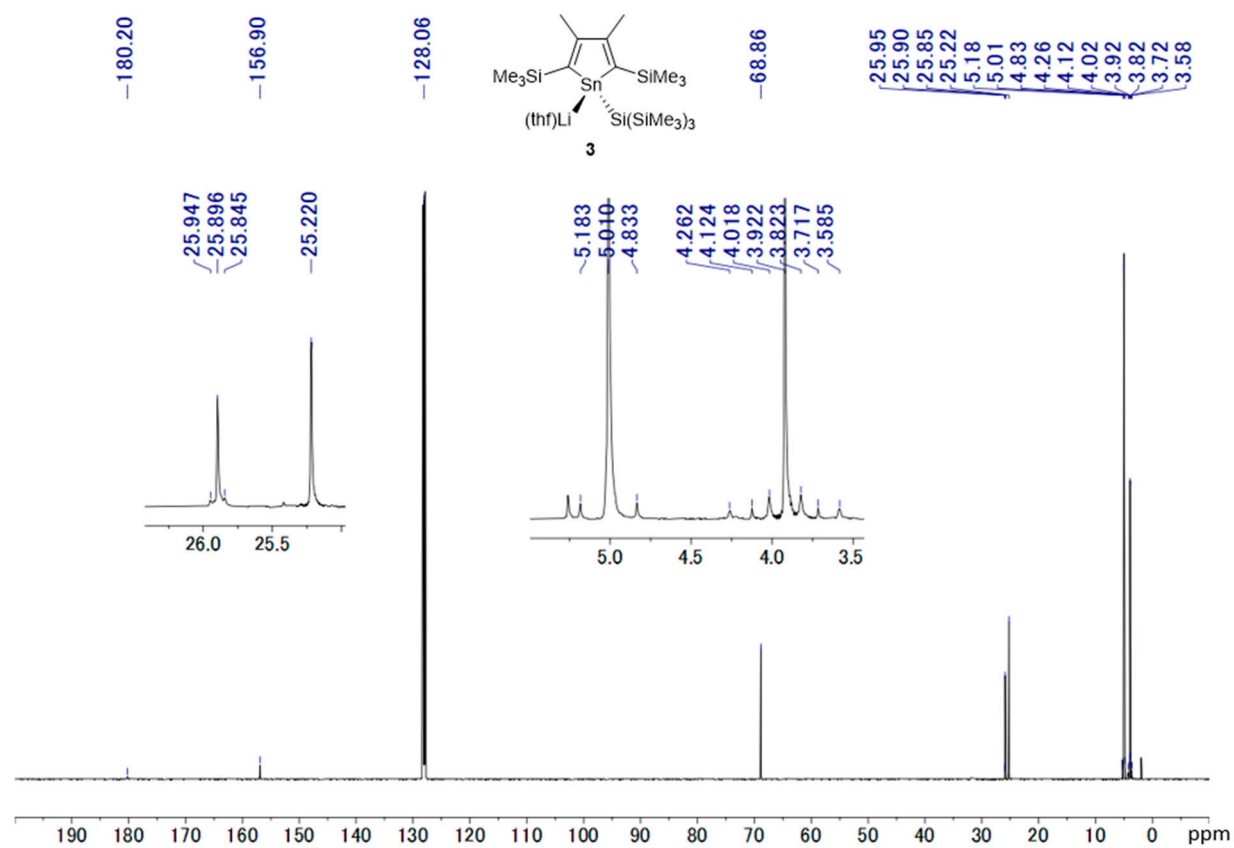


Figure S11. ¹³C{¹H} NMR spectrum of **3**·thf (125 MHz, C₆D₆).

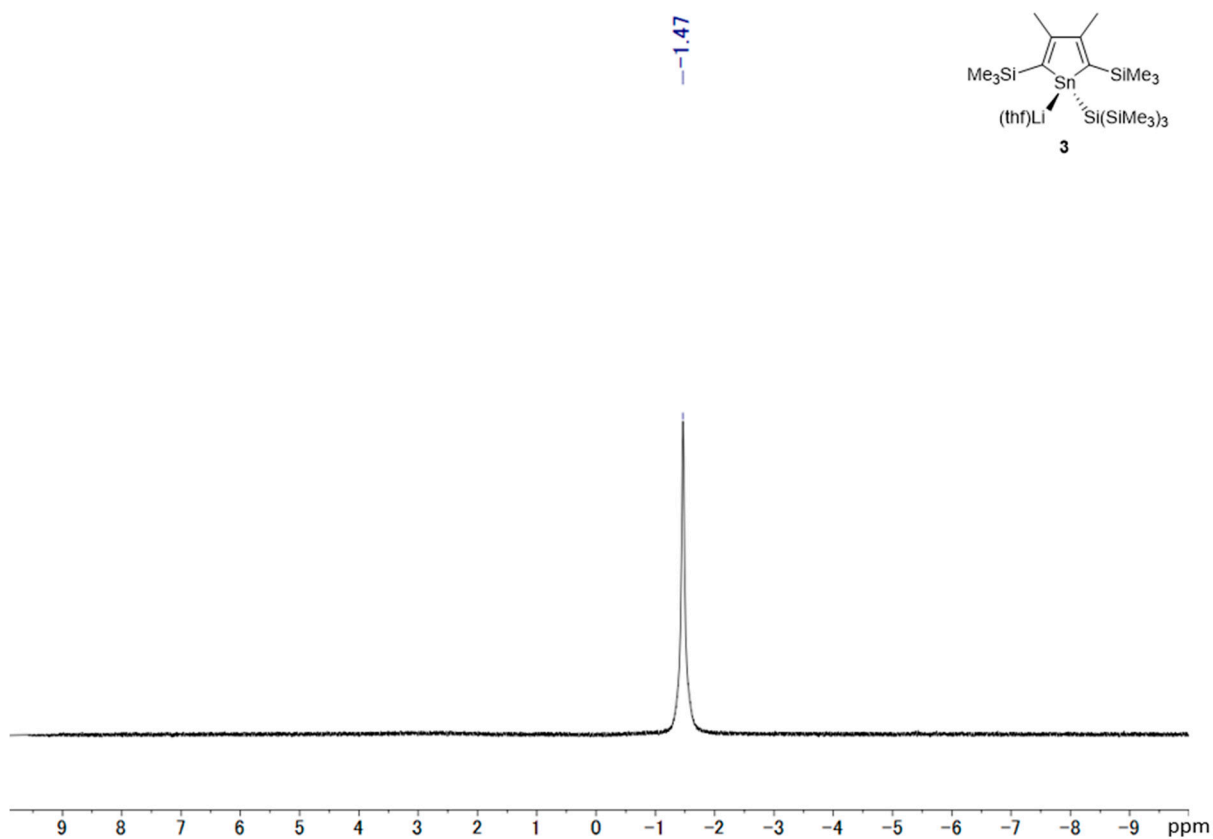


Figure S12. ${}^7\text{Li}\{{}^1\text{H}\}$ NMR spectrum of **3**·thf (194 MHz, C₆D₆).

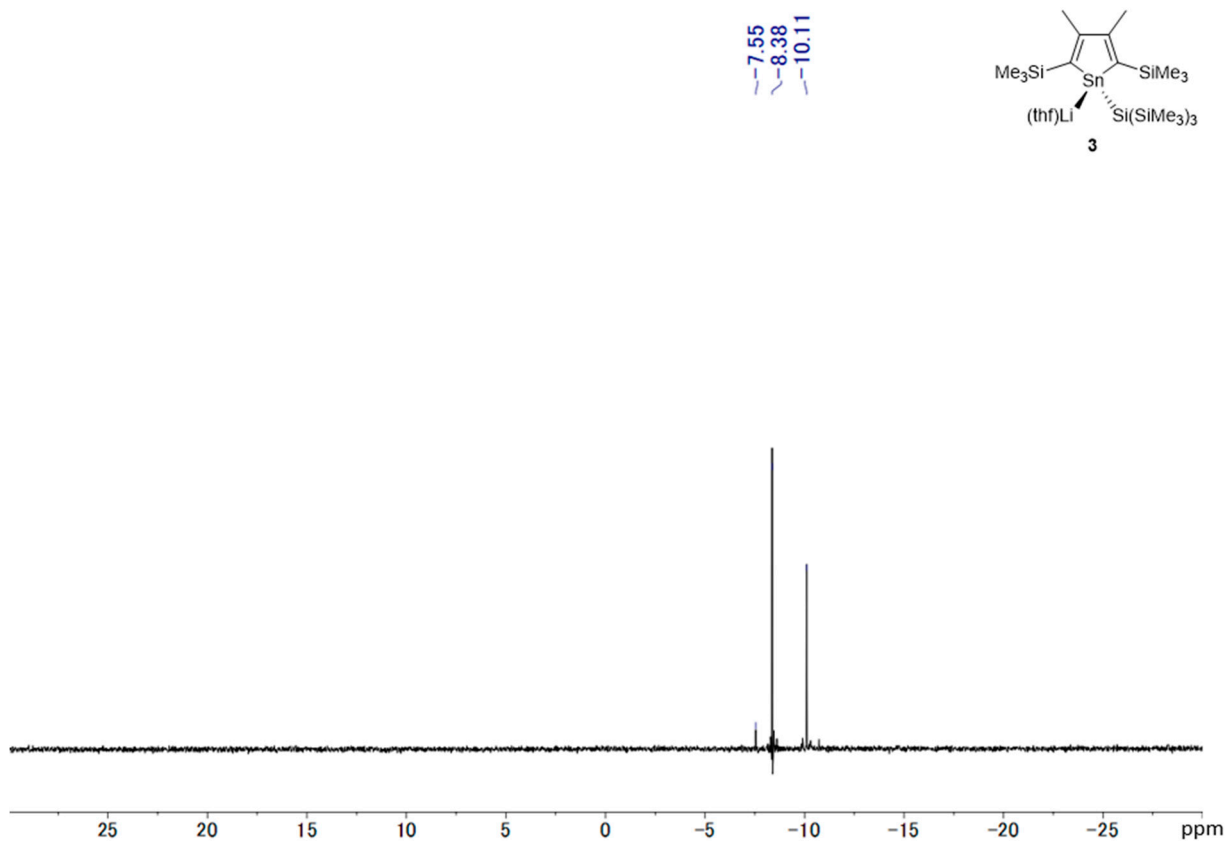


Figure S13. ${}^{29}\text{Si}\{{}^1\text{H}\}$ NMR spectrum of **3**·thf (99 MHz, C₆D₆).

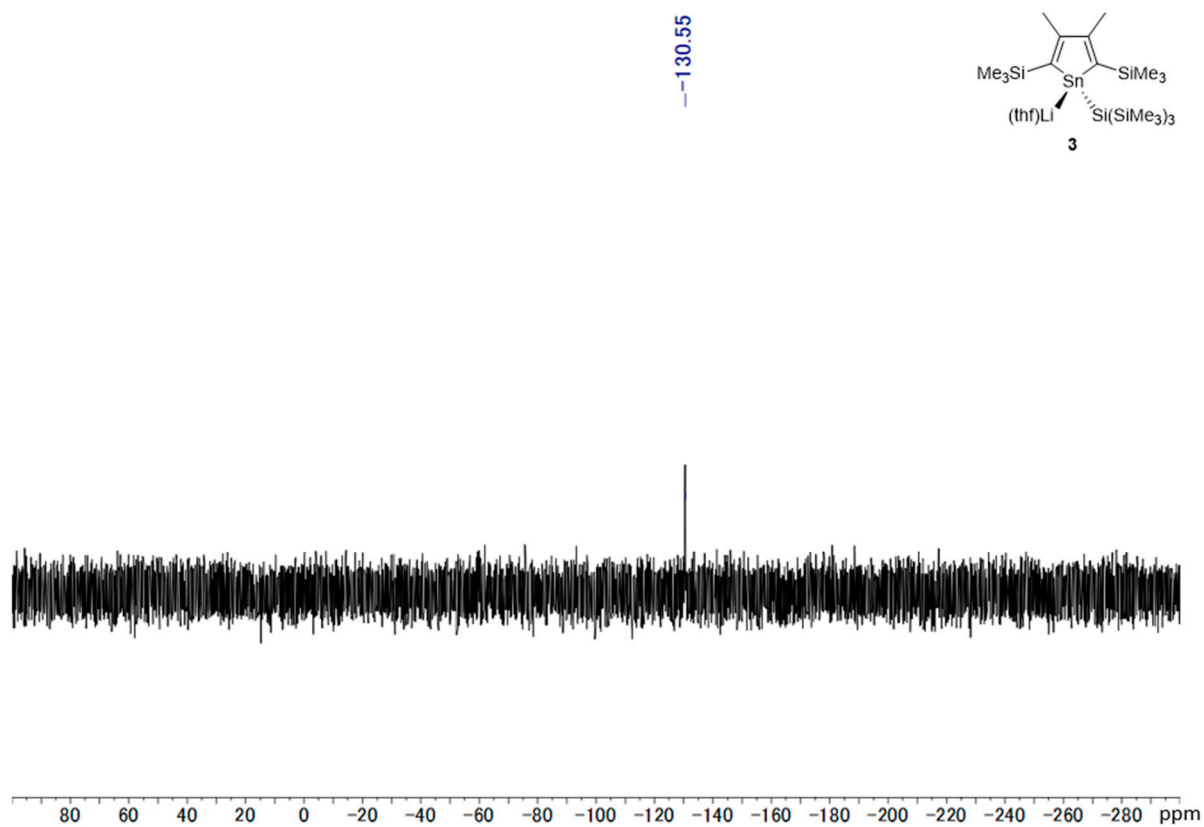


Figure S14. $^{119}\text{Sn}\{^1\text{H}\}$ NMR spectrum of **3**·thf (186 MHz, C_6D_6).