

Supplementary Materials: Monoanionic Tin Oligomers Featuring Sn–Sn or Sn–Pb Bonds: Synthesis and Characterization of a Tris(Triheteroarylstannyl)Stannate and -Plumbate

Kornelia Zeckert

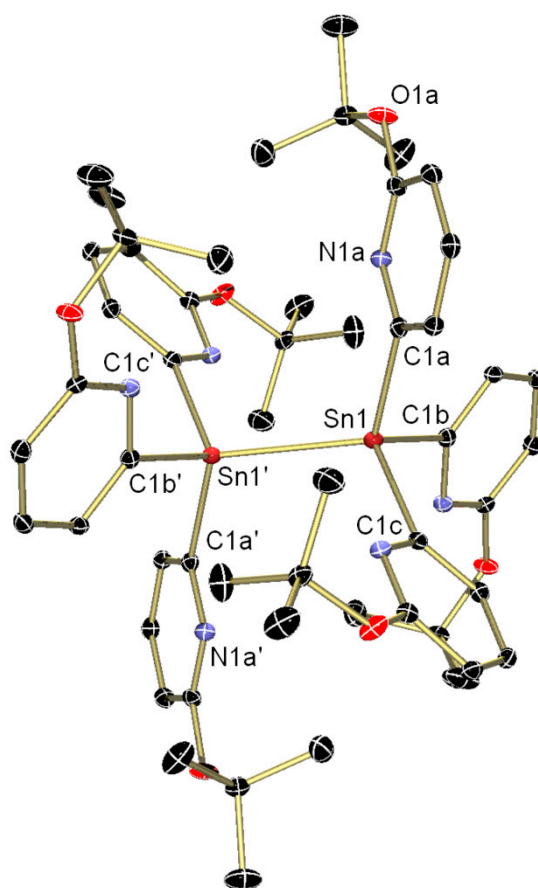
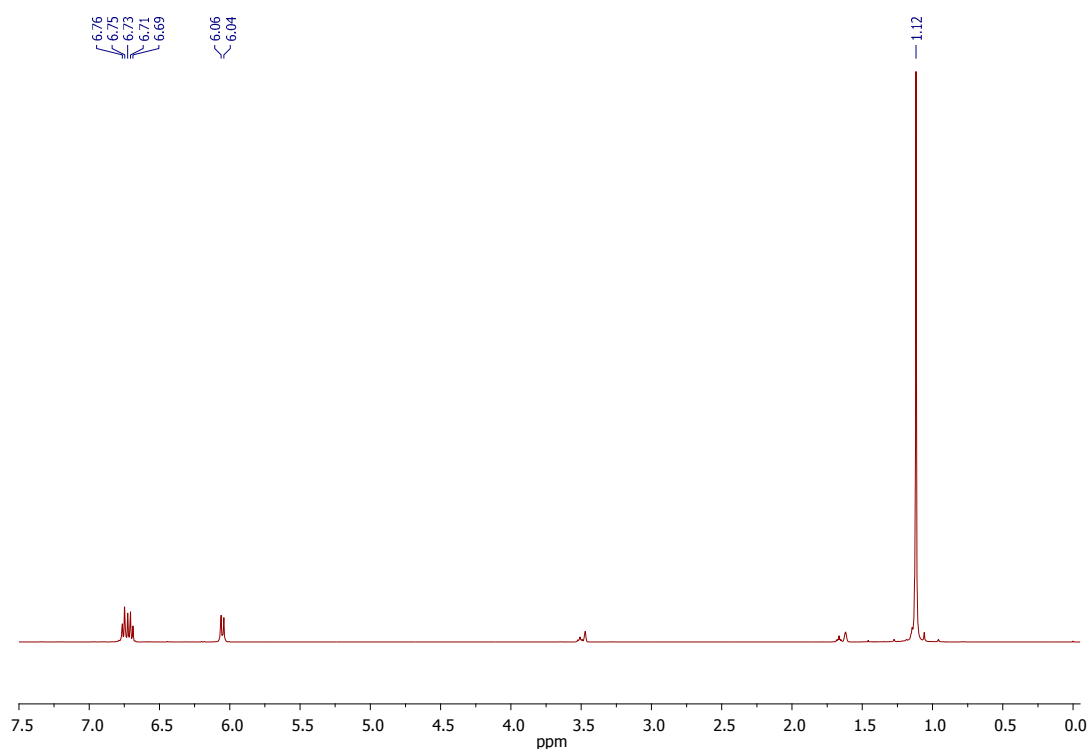


Figure S1. Molecular structure of $[\text{Sn}(\text{2-py}^{6\text{OtBu}})_3]_2$ (**4**) with 30% probability ellipsoids. Hydrogen atoms are omitted for clarity. Selected bond lengths (Å) and angles (°): Sn1–Sn1' 2.7631(6), Sn–C1a 2.154(2), C1a–Sn–C1b 106.65(7), C1a–Sn–Sn1' 112.16(6); equivalent atoms are generated by b: $-y+1, x-y-1, z$; c: $-x+y+2, -x+1, z$; ' : $-x+2, -y, -z+1$.

Table S1. Crystallographic data for compound **4**.

4 · 2 C₆H₆	
Formula	C ₆₆ H ₈₄ N ₆ O ₆ Sn
M _r (g·mol ⁻¹)	1294.77
Cryst system	trigonal
Space group	$P\bar{3}$
<i>a</i> (Å)	14.4547(3)
<i>b</i> (Å)	14.4547(3)
<i>c</i> (Å)	8.7666(3)
α (°)	90.0
β (°)	90.0
γ (°)	120.0
<i>V</i> (Å ³)	1586.28(7)
<i>Z</i>	1
F(000)	670
<i>T</i> (K)	−130(2)
Q _{calcd} (g·cm ³)	1.355
<i>M</i> (mm ⁻¹)	0.841
Reflns collected	3618
Reflns unique	2160
<i>R</i> _{int}	0.0257
Final <i>R</i> ₁ (<i>I</i> > 2σ(<i>I</i>))	0.0321
Final <i>wR</i> ₂ (<i>F</i> ²) (all data)	0.0621

**Figure S2.** ¹H NMR spectrum of [LiSn{Sn(2-py⁶O^tBu)₃}₃] (**2**) in *d*₈-THF.

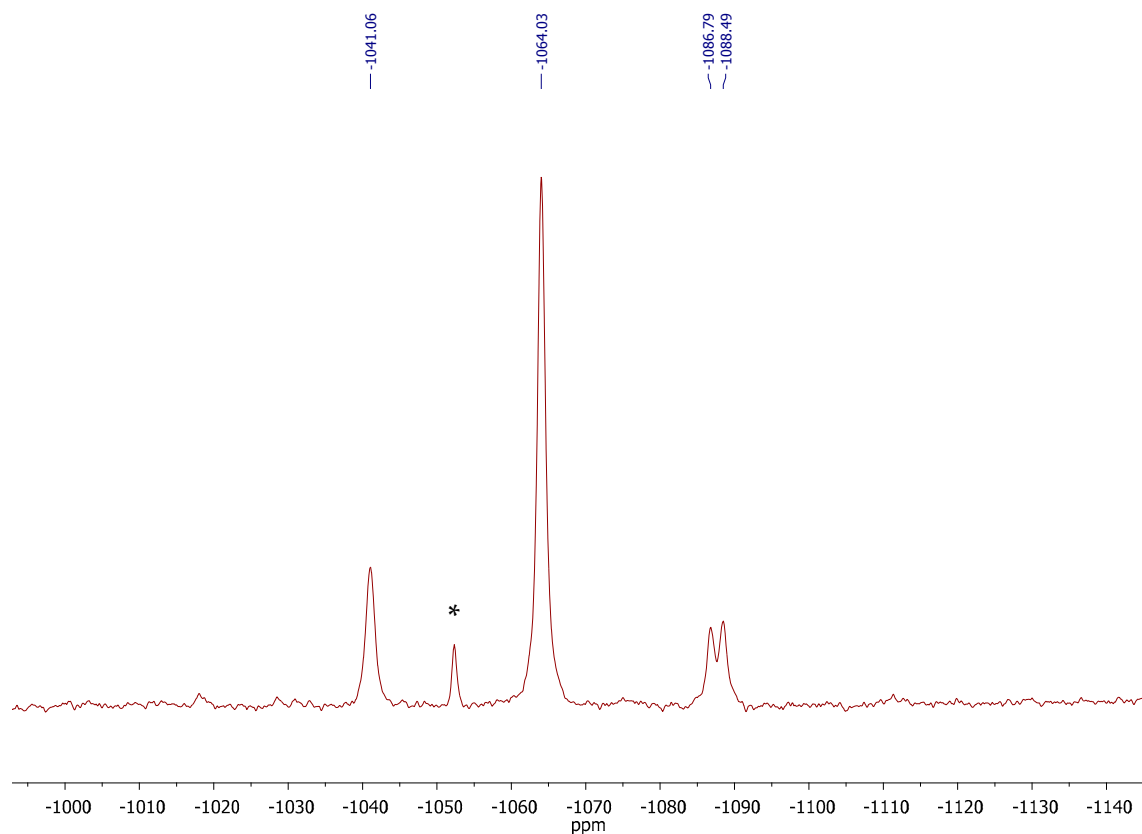


Figure S3. $^{119}\text{Sn}\{^1\text{H}\}$ NMR spectrum of $[\text{LiSn}\{\text{Sn}(\text{2-py}^{\text{6OtBu}})_3\}_3]$ (**2**) in d_8 -THF with the ^{119}Sn NMR resonance at -1064 ppm; * impurity.

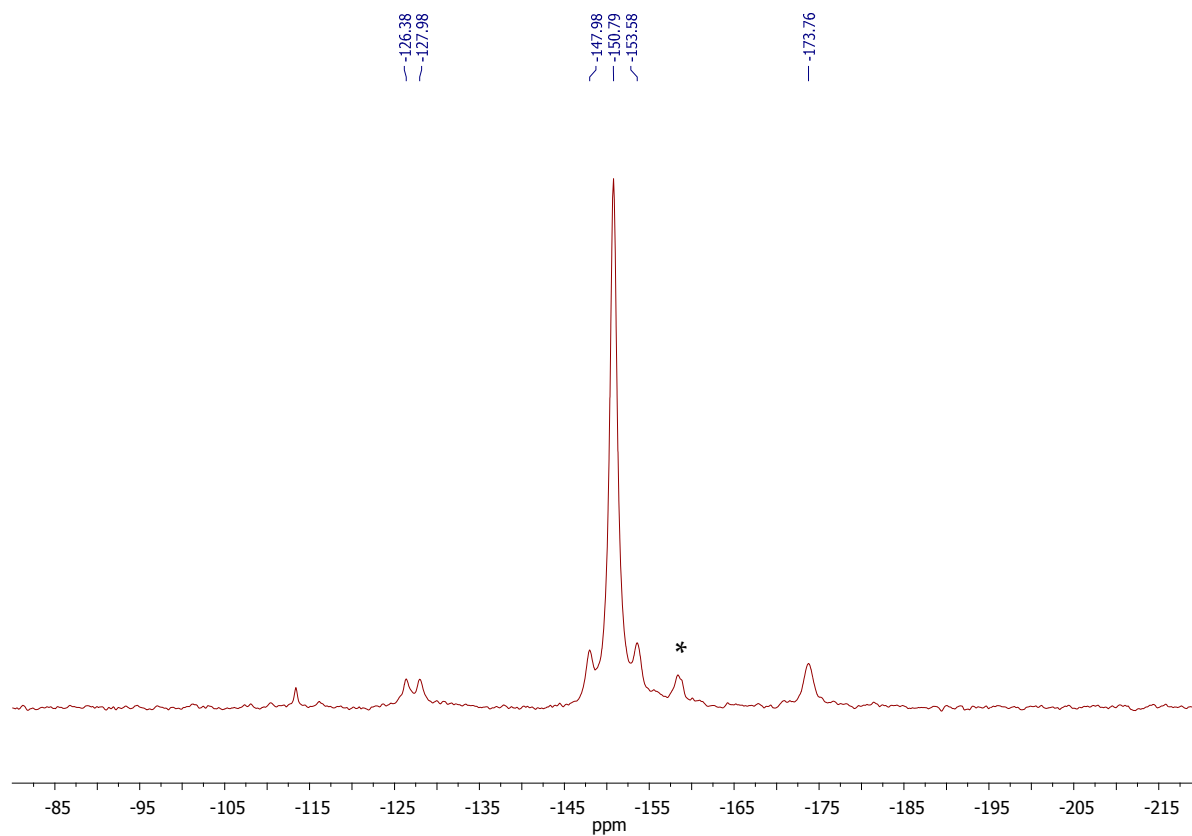


Figure S4. $^{119}\text{Sn}\{^1\text{H}\}$ NMR spectrum of $[\text{LiSn}\{\text{Sn}(\text{2-py}^{\text{6OtBu}})_3\}_3]$ (**2**) in d_8 -THF with the ^{119}Sn NMR resonance at -151 ppm; * impurity.

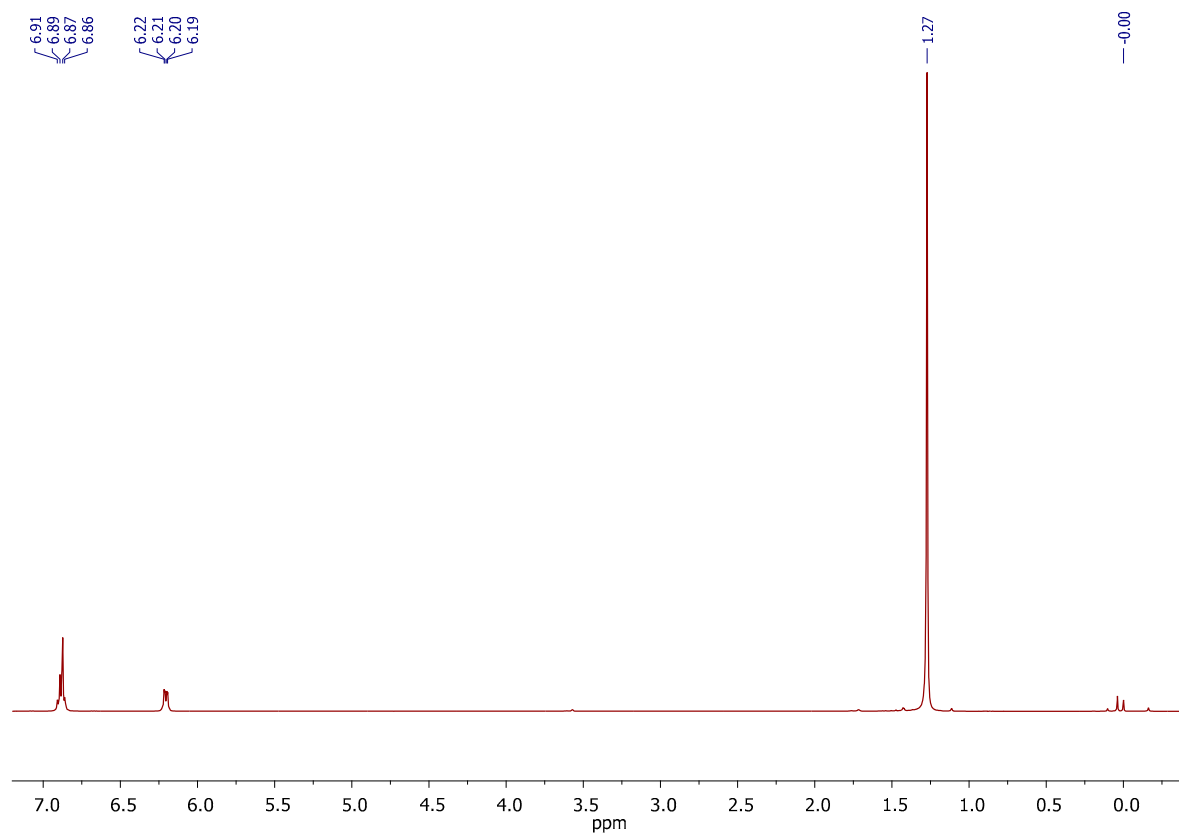


Figure S5. ^1H NMR spectrum of $[\text{LiPb}\{\text{Sn}(\text{2-py}^{6\text{OtBu}})_3\}_3]$ (3) in d_8 -THF.

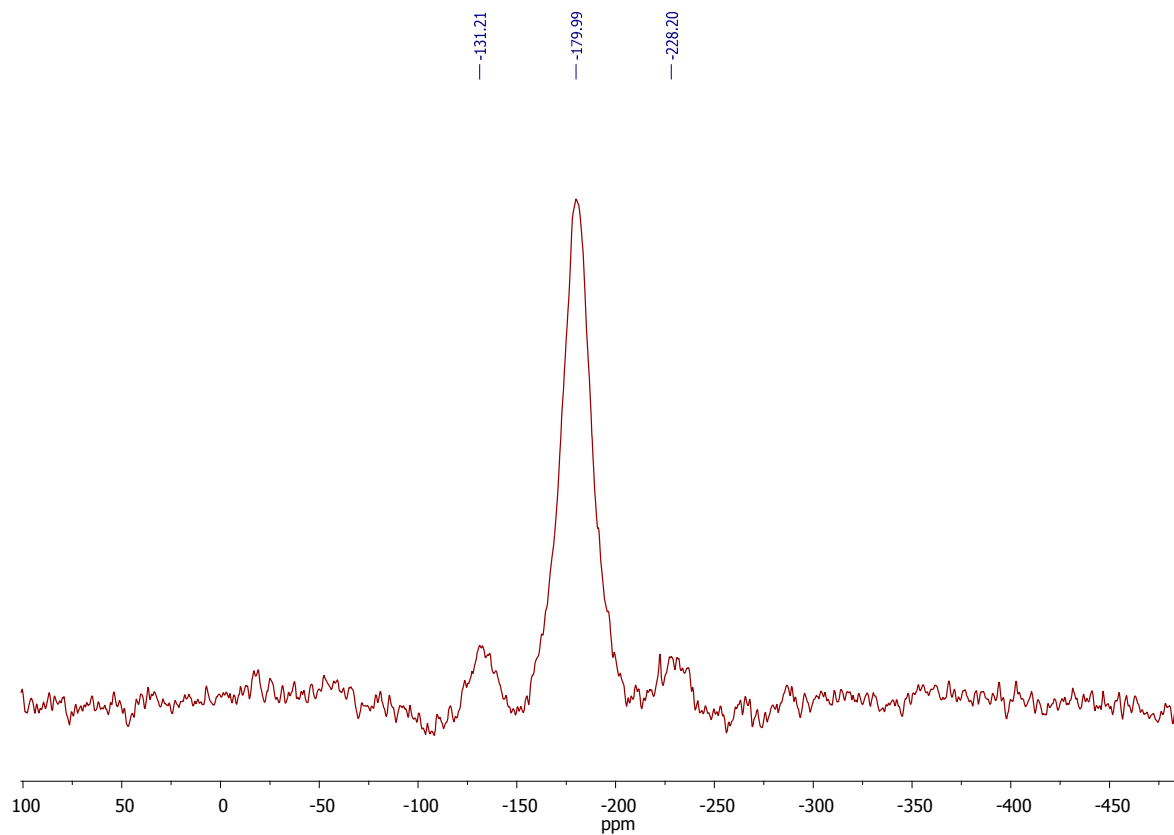


Figure S6. $^{119}\text{Sn}\{^1\text{H}\}$ NMR spectrum of $[\text{LiPb}\{\text{Sn}(\text{2-py}^{6\text{OtBu}})_3\}_3]$ (3) in d_8 -THF.

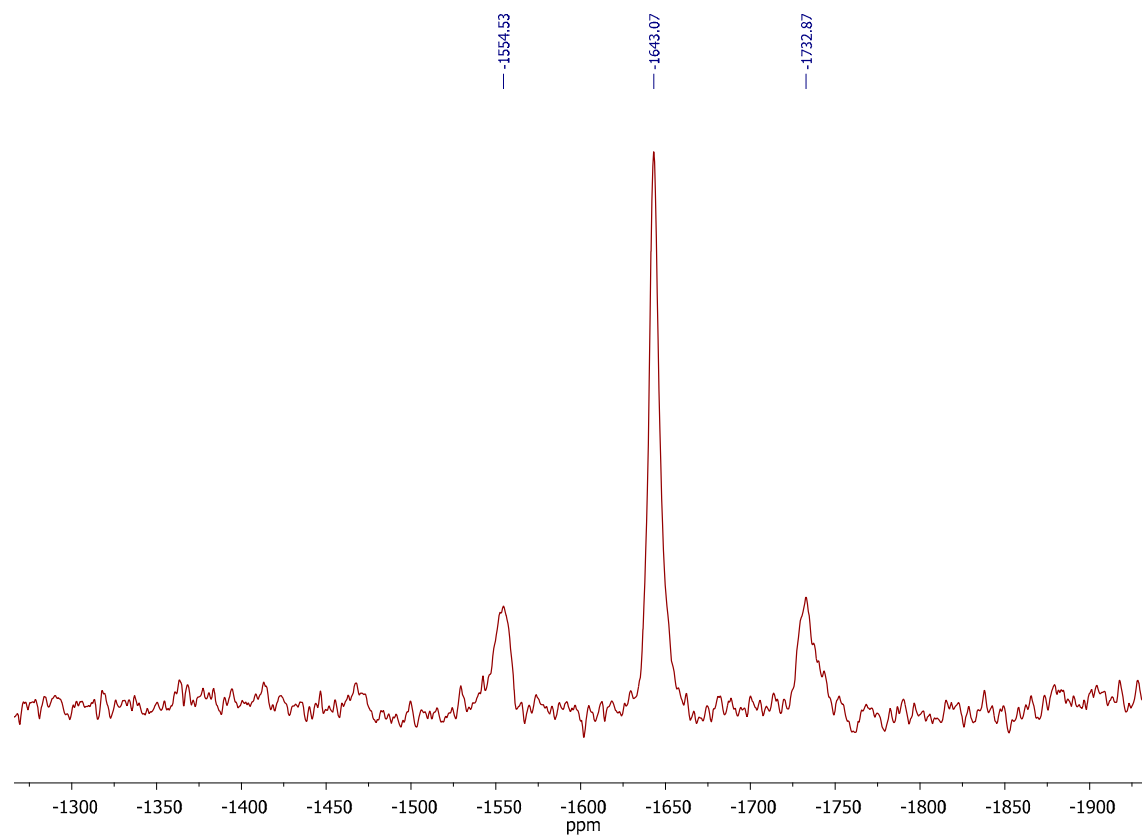


Figure S7. $^{207}\text{Pb}\{^1\text{H}\}$ NMR spectrum of $[\text{LiPb}\{\text{Sn}(\text{2-py}^{6\text{OtBu}})_3\}_3]$ (**3**) in d_8 -THF.