Electronic Supplementary Information

Reactivity of heavy carbene analogues towards oxidants: redox active ligand-enabled isolation of a paramagnetic stannylene

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1. General considerations. H_2L[1], $Pb(hmds)_2$,[2] **1b**,[3] and $MesN_3$,[4] were prepared according to the literature. Silver triflate was purchased from Sigma Aldrich. Trimethylamine-N-oxide dihydrate was purchased from Alfa Aesar and was dehydrated according to the literature.[5] All operations were performed using Schlenk techniques under dinitrogen or in a dinitrogen-filled glovebox. All glassware was either flame-dried or dried overnight in a 160 °C oven prior to use except for NMR tubes which were dried overnight in a 60 °C oven. THF, Et_2O, toluene, and C_6D_6 were distilled from Na/benzophenone under N_2. Pentane and hexanes were distilled from sodium under dinitrogen. All solvents were then stored over 3 Å molecular sieves prior to use. ^1H, ^{13}C, ^{119}Sn, and ^{207}Pb NMR spectra were recorded on a Varian 400 MHz, Agilent DD2 500 MHz, or Agilent DD2 600 MHz spectrometer. For ^1H and ^{13}C NMR spectra, chemical shifts are reported in ppm relative the residual protio-solvent peaks. ^{119}Sn and ^{207}Pb chemical shifts are reported in ppm relative to $SnMe_4$ and $PbMe_4$, respectively. Electron paramagnetic resonance (EPR) spectra were obtained at 298 K in toluene solution using a Bruker ECS-EMX X-band EPR spectrometer equipped with an ER4119HS cavity. The g values were determined using 2,2-diphenyl-1-picrylhydrazyl (dpph) as the reference (g = 2.0037). Simulation was carried out using PEST WinSIM software.[6] Elemental analyses were performed by ANALEST at the University of Toronto.

2. Synthesis of compounds 1a—4.

Synthesis of *N*,*N*'-bis(2,6-diisopropylphenyl)-benzimidazolin-2-plumbylene 1a:

A solution of H_2L (150 mg, 0.350 mmol, 1 eq) in toluene (1mL) was added to a solution of $Pb(hmds)_2$ (183 mg, 0.347 mmol) in toluene (1 mL). The mixture was diluted with toluene (1mL) before being heated in a Pyrex bomb to 105 °C for 15 h, which caused the mixture to turn purple. Volatiles were removed *in vacuo*, and the residue was recrystallized from toluene/hexanes (1:1 v/v) at -25 °C. Two crops of purple crystals were collected (117 mg, 0.185 mmol, 53%). ^1H NMR (500 MHz, C_6D_6) δ 7.36 (d, *J* = 7.7 Hz, 4H), 7.18 (t, *J* = 7.7 Hz, 2H), 6.44 (m, 2H), 6.21 (m, 2H), 2.97 (hept, *J* = 6.9 Hz, 4H), 1.15 (d, *J* = 7.0 Hz, 12H), 1.02 (d, *J* = 6.9 Hz, 12H). ^{13}C NMR (151 MHz, C_6D_6) δ 153.97, 147.19, 142.34, 127.03, 123.86, 118.87, 116.74, 27.50, 26.82, 24.39. ^{207}Pb NMR (105 MHz, C_6D_6, 25 °C) δ 3279.38. Anal. Calcd for $C_{30}H_{38}N_2Pb$: C, 56.85; H, 6.04; N, 4.42 Found: C, 57.68; H, 5.82; N, 4.43. Single crystals for X-ray were grown from a cold thf/pentane solution.

Synthesis of 2a:

1a (300 mg, 0.484 mmol) and $MesN_3$ (93.9 mg, 0.582 mmol) were dissolved in toluene (8 mL), transferred to a Pyrex bomb, and heated to 110 °C for 72 hours. Volatiles were removed *in vacuo*, and the burgundy residue was recrystallized from cold pentane/toluene of ratio *ca*. 4:1. The crystals were washed with cold pentane (3 x 1 mL), and dried under vacuum (139.8 mg, 0.1858 mmol, 38%). ^{1}H NMR (400 MHz, C_6D_6) δ 7.48 (dd, *J* = 7.7, 1.3 Hz, 1H), 7.43 (d, *J* = 8.0 Hz, 2H), 7.26 (t, *J* = 7.7 Hz, 1H), 7.23 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.03 (t, *J* = 7.8 Hz, 1H), 6.65 (s, 2H), 6.62 (m-overlapped, 2H), 6.34 (m, 1H), 6.27 (m, 1H), 3.46 (s, 1H), 3.40 – 3.19 (m, 3H), 2.08 (s, 3H), 1.85 (s, 6H), 1.46 (s, 3H), 1.28 (d, *J* = 7.0 Hz, 3H), 1.25 (d, *J* = 6.9 Hz, 5H), 1.17 (two overlapping doublets, 6H), 1.16 (s, overlapped, 3H), 1.13 (d, *J* = 6.9 Hz, 3H). ^{13}C NMR (126 MHz, C_6D_6) δ 153.48, 152.60, 150.21, 147.01, 146.44, 146.34, 144.42, 142.26, 139.86, 133.30, 131.81, 130.46, 126.03, 125.95, 125.29, 124.49, 123.87, 123.63, 117.47, 117.25, 115.95, 114.98, 60.26, 33.20, 28.73, 28.01, 27.67, 27.29, 27.26, 26.96, 26.75, 25.03, 24.43, 22.19, 20.56, 20.40. ^{207}Pb NMR (105 MHz, C_6D_6, 25 °C) δ 2656.68 Anal. Calcd for $C_{39}H_{49}N_3Pb$: C, 61.07; H, 6.44; N, 5.48 Found: C, 61.32; H, 6.42; N, 5.46. Single crystals for X-ray were grown from a cold pentane/hexamethyldisiloxane solution.

Synthesis of 2b:

1b (35.3 mg, 0.0647 mmol) and $MesN_3$ (20.2 mg, 0.125 mmol) were dissolved in toluene, transferred to a Pyrex bomb, and heated to 110 °C for 24 h. Volatiles were removed *in vacuo*, and the orange residue was recrystallized from pentane at -35 °C. The orange crystals of **2b** were dried under vacuum (15.0 mg, 0.0226 mmol, 34%). ^{1}H NMR (600 MHz, C_6D_6) δ 7.42 (m, 1H), 7.32 (m, 3H), 7.12 (m, 2H),), 6.81 (t, *J* = 7.1 Hz, 1H), 6.76 (t, *J* = 8.5 Hz, 1H), 6.54 (d, *J* = 7.7 Hz, 1H), 6.48 (d, *J* = 7.8 Hz, 1H) 3.63 (s, 1H), 3.44 (hept, *J* = 7.0 Hz, 1H), 3.33 (hept, *J* = 6.9 Hz, 1H), 3.21 (hept, *J* = 6.9 Hz, 1H), 2.05 (s, 3H), 1.88 (s, 6H), 1.40 (s, 3H), 1.26 (d, *J* = 7.4 Hz, 6H), 1.23 (d, *J* = 7.0 Hz, 6H), 1.20 (d, *J* = 6.9 Hz, 3H), 1.14 (s, 3H), 1.11 (d, *J* = 6.9 Hz, 3H). ^{13}C NMR (151 MHz, C_6D_6) δ 149.82, 146.38, 146.08, 145.78, 145.29, 144.96, 142.25, 141.95, 139.08, 133.71, 131.86, 130.61, 126.26, 126.21, 125.35, 124.76, 124.23, 123.73, 117.59, 117.22, 112.40, 111.38, 60.63, 33.32, 28.87, 28.58, 28.32, 27.82, 26.89, 26.68, 26.35, 24.89, 24.22, 22.09, 20.71, 20.54. ^{119}Sn NMR (224 MHz, C_6D_6) δ 69.13. Anal. Calcd for $C_{39}H_{49}N_3Sn$: C, 69.03; H, 7.28; N, 6.19 Found: C, 69.36; H, 7.24; N, 5.96. Single crystals for X-ray were grown from a cold pentane solution.

Synthesis of 3:

1a (87.5 mg, 0.141 mmol) was dissolved in toluene (4 mL) and added to a suspension of trimethylamine-N-oxide (10.6 mg, 0.141 mmol) in toluene (1 mL). After stirring at room temperature for 10 h the mixture changed colour from purple to blood-red. Volatile components were removed under reduced pressure. The residue was extracted into toluene (2 mL) and filtered through Celite; pentane (5 mL) was layered on top. Cooling to -25 °C overnight brought about the formation of orange microcrystals. The supernatant was decanted away and the crystals were washed with cold 30% v/v toluene/pentane (2 x 1 mL) and pentane (4 x 1 mL). Drying in vacuo yielded analytically pure **3** (69.7 mg, 0.0983 mmol, 70%). ^{1}H NMR (500 MHz, C_6D_6) δ 7.44 (d, *J* = 7.7 Hz, 4H), 7.28 (t, *J* = 7.6 Hz, 2H), 6.55 (m, 2H), 6.23 (m, 2H), 3.57 (hept, *J* = 6.9 Hz, 4H), 2.20 (s, 9H) 1.31 (d, *J* = 7.0 Hz, 12H), 1.20 (d, *J* = 6.8 Hz, 12H). ^{13}C NMR (126 MHz, C_6D_6) δ 153.86, 147.83, 146.22, 125.55, 123.89, 116.53, 116.33, 60.60, 27.56, 26.54, 25.44. ^{207}Pb NMR (126 MHz, C_6D_6, 25 °C) δ 2233.26 Anal. Calcd for $C_{33}H_{47}N_3OPb$: C, 55.91; H, 6.68; N, 5.93 Found: C, 56.33; H, 6.61; N, 5.81. Single crystals for X-ray were grown by slow evaporation of a cold pentane/Et_2O solution.

Synthesis of 4

Toluene (1.5 mL) was added to silver triflate (32.7 mg, 0.127 mmol), and the mixture was added dropwise to an orange solution of LSn (67.5 mg, 0.127 mmol) in toluene (1.5 mL). The reaction mixture turned brown and was stirred for 90 min. The reaction mixture was filtered through Celite and the filtrate was concentrated to *ca*. 1.5 mL. Hexanes (1.5 mL) was layered on top and the mixture was cooled to -35 °C overnight causing formation of brown X-ray quality crystals. The supernatant was decanted and the crystals were washed with cold pentane (3 x 1 mL). Drying *in vacuo* yielded analytically pure **4** (46.5 mg, 0.670 mmol, 53%). Anal. Calcd for $C_{31}H_{38}N_2O_3F_3SSn$: C, 53.61; H, 5.52; N, 4.03. Found: C, 53.44; H, 5.57; N, 4.06.

3. NMR Spectra

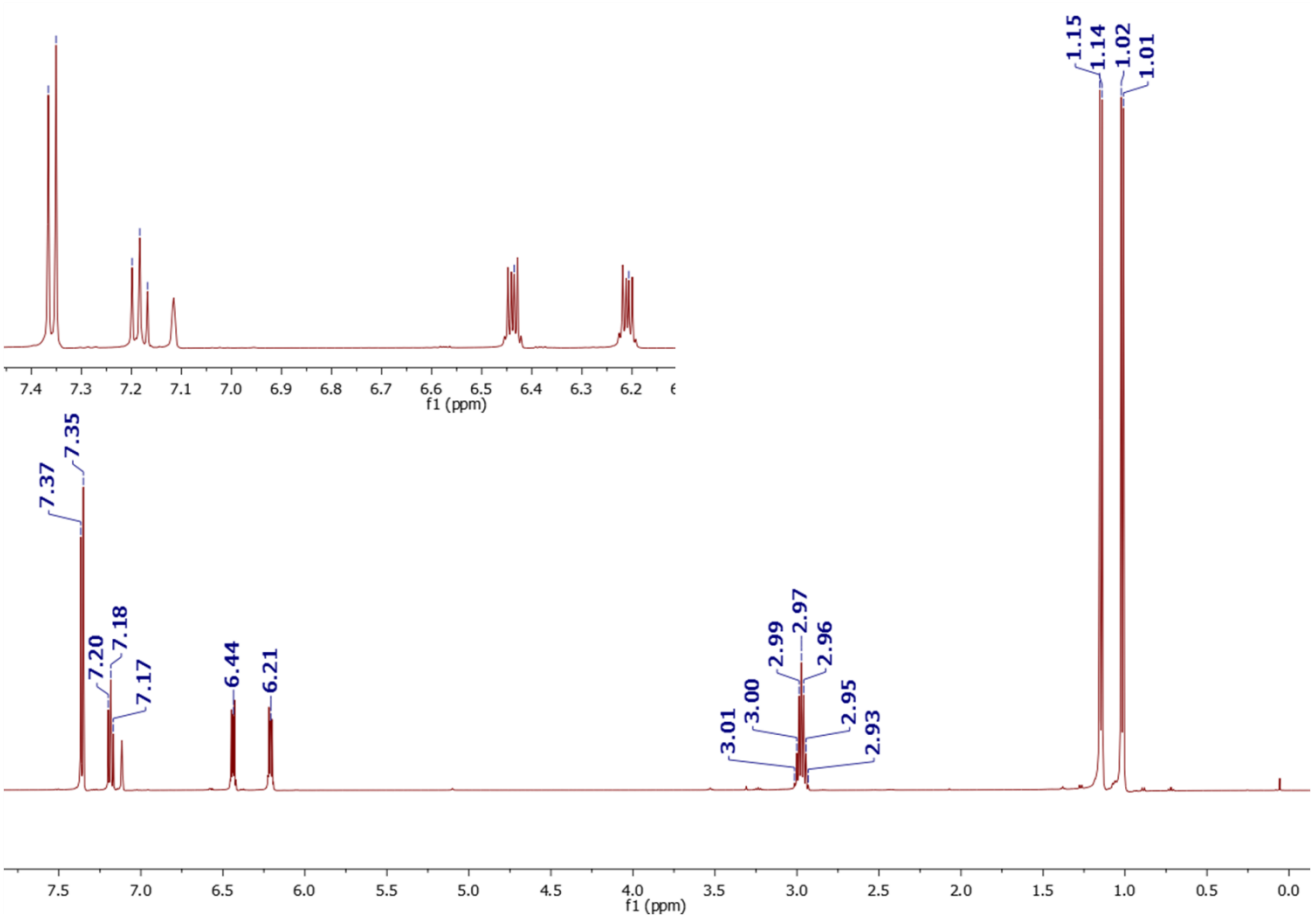

Figure S1. ^{1}H NMR Spectrum (500 MHz, 25 °C) of **1a** in C_6D_6. Inset: expanded aryl region.

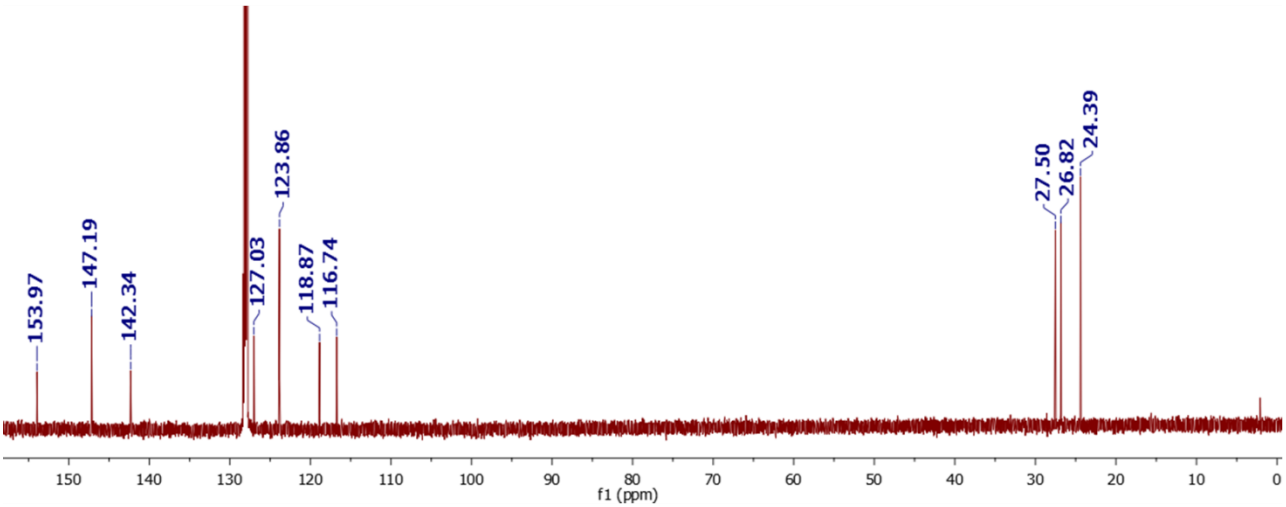

Figure S2. ^{13}C NMR Spectrum (151 MHz, 25 °C) of **1a** in C_6D_6.

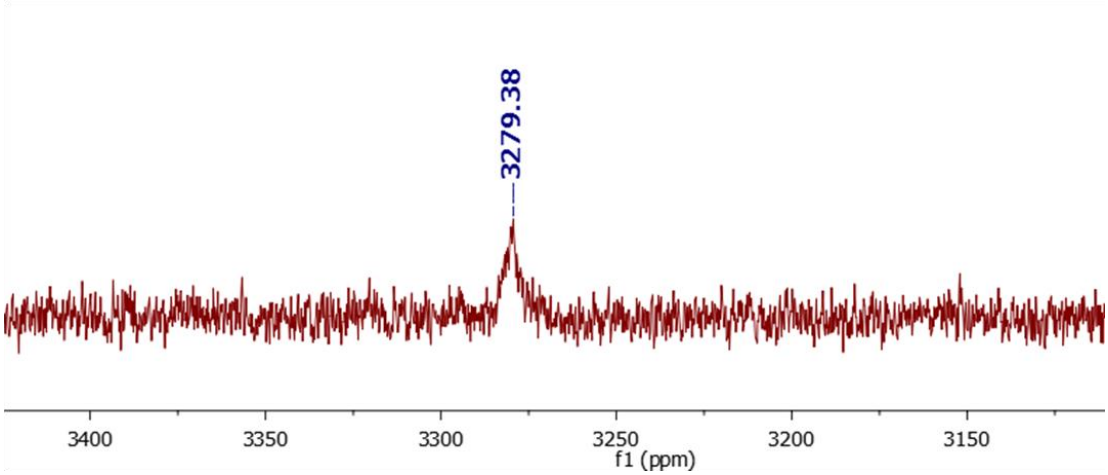

Figure S3. ^{207}Pb NMR Spectrum (105 MHz, 25 °C) of **1a** in C_6D_6.

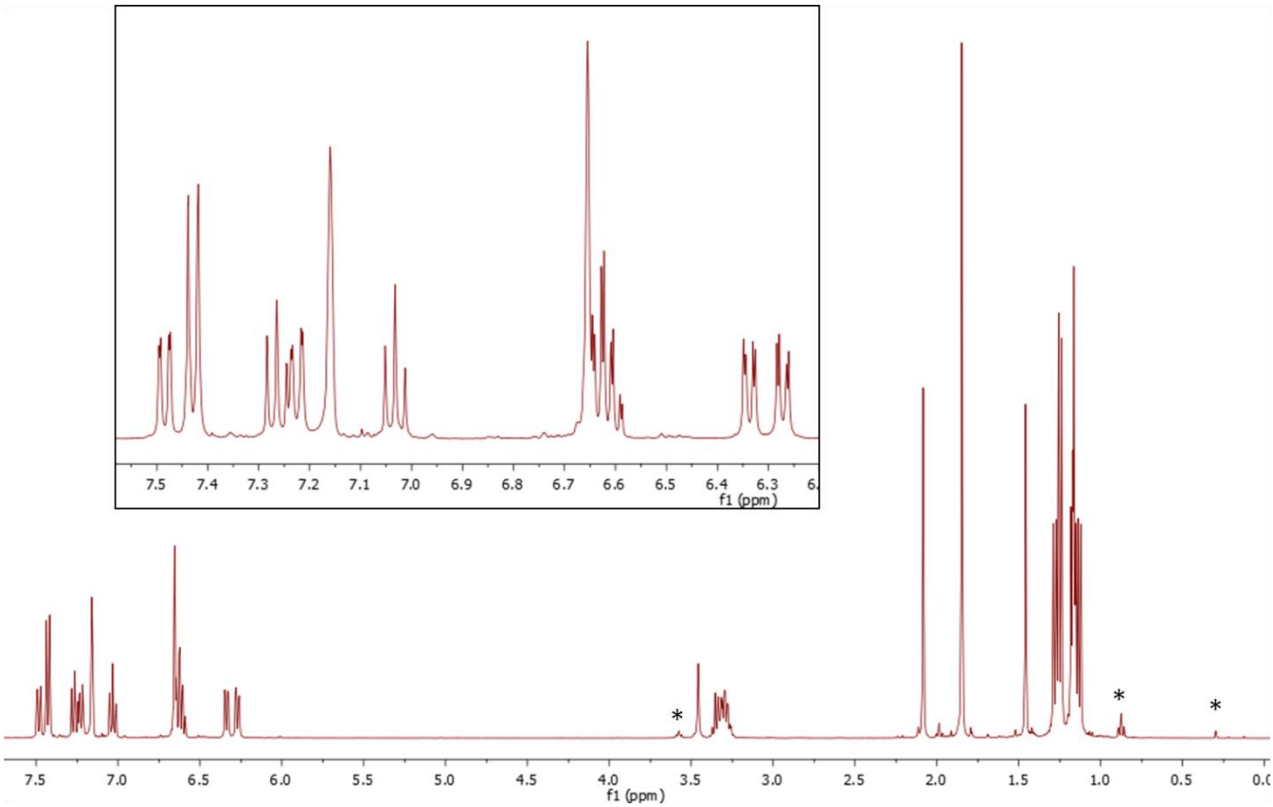

Figure S4. ^{1}H NMR Spectrum (400 MHz, 25 °C) of **2a** in C_6D_6. Note: spectrum contains resonances due to trace thf, pentane, and grease marked with an asterisk. Inset: expanded aryl region.

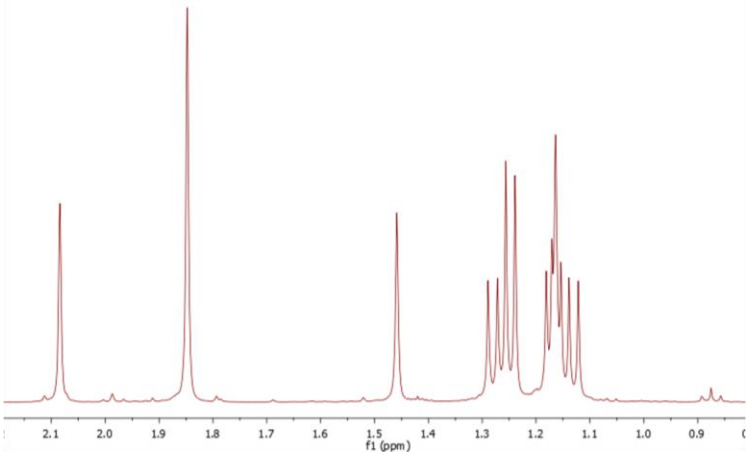

Figure S5. Expanded high-field region of ^{1}H NMR Spectrum (400 MHz, 25 °C) of **2a** in C_6D_6.

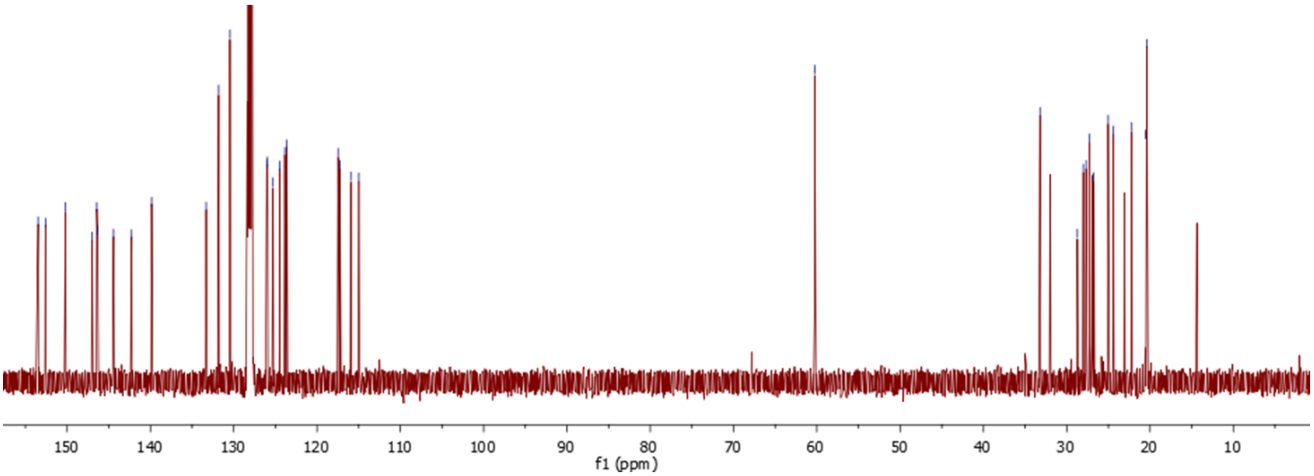

Figure S6. ^{13}C NMR Spectrum (126 MHz, 25 °C) of **2a** in C_6D_6.

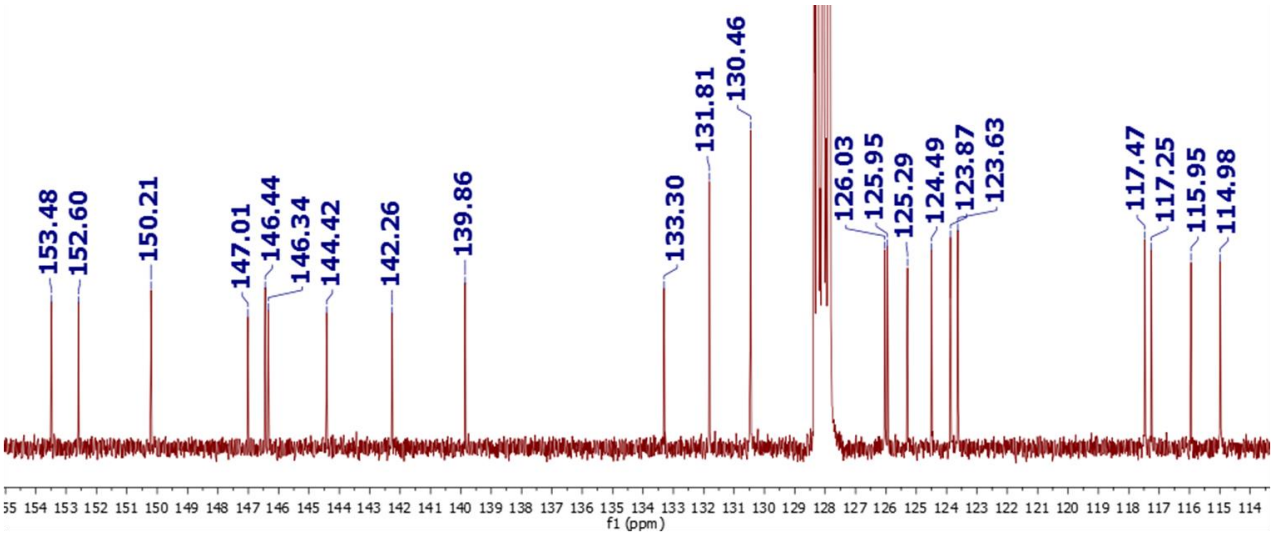

Figure S7. Expanded aryl region of ^{13}C NMR Spectrum (126 MHz, 25 °C) of **2a** in C_6D_6

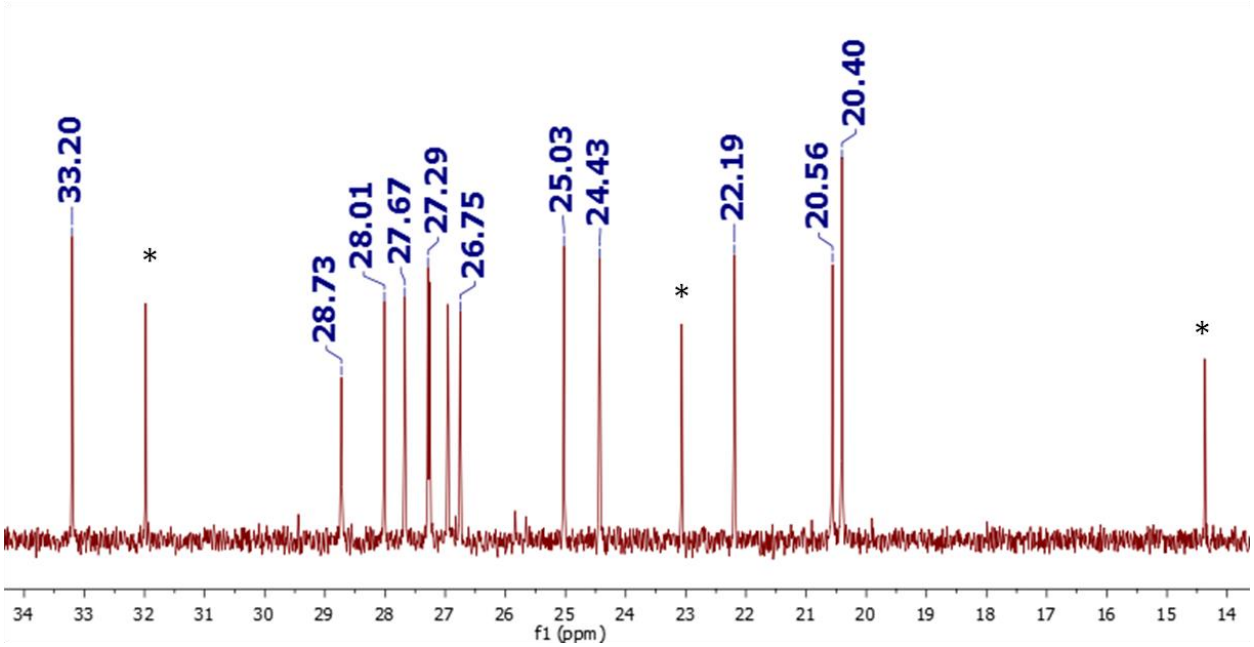

Figure S8. Expanded alkyl region of ^{13}C NMR Spectrum (126 MHz, 25 °C) of **2a** in C_6D_6. Note: residual *n*-hexane is marked with an asterisk.

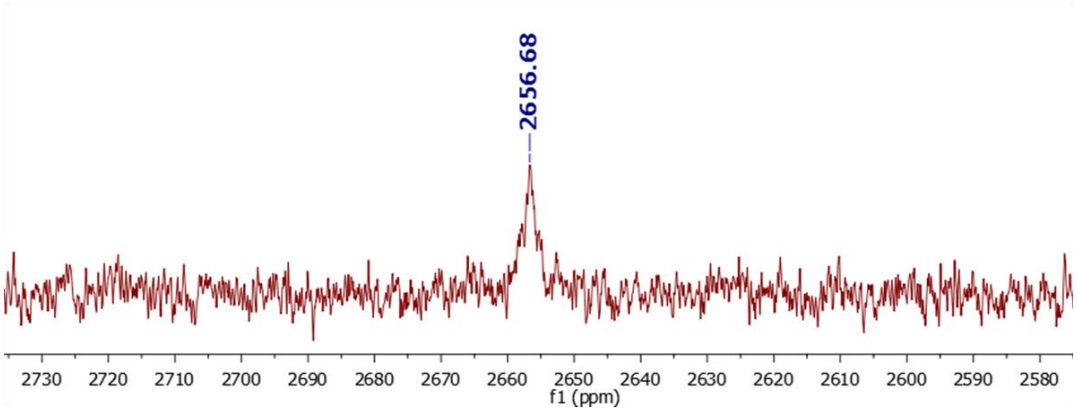

Figure S9. ^{207}Pb NMR Spectrum (105 MHz, 25 °C) of **2a** in C_6D_6.

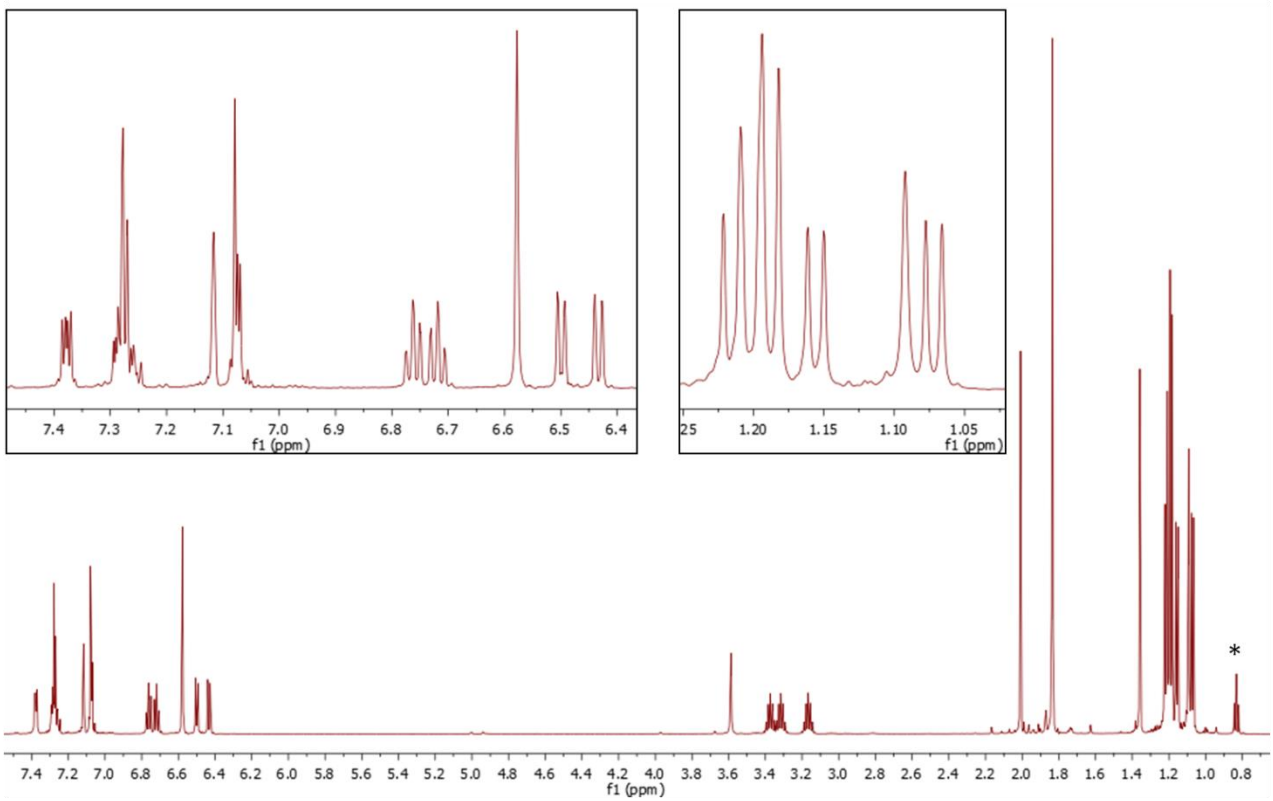

Figure S10. ^{1}H NMR Spectrum (600 MHz, 25 °C) of **2b** in C_6D_6.Note: residual pentane resonance marked with an asterisk. Left inset: expanded aryl region. Right inset: expanded alkyl region.

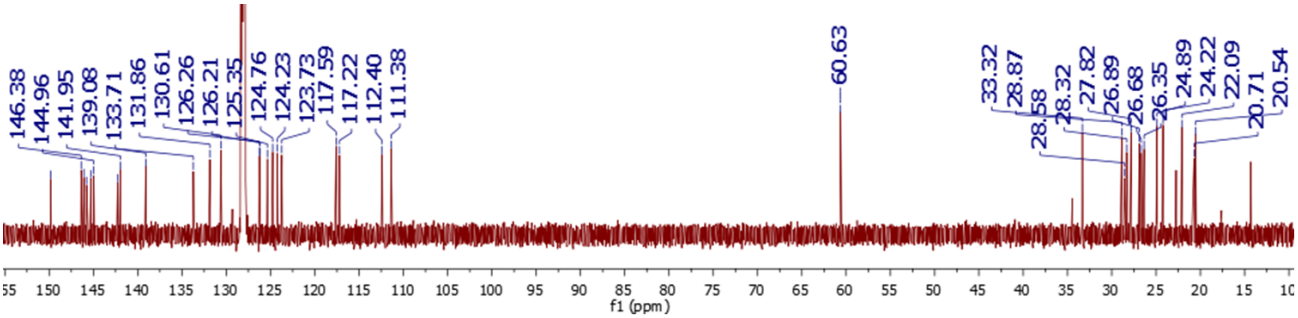

Figure S11. ^{13}C NMR Spectrum (151 MHz, 25 °C) of **2b** in C_6D_6.

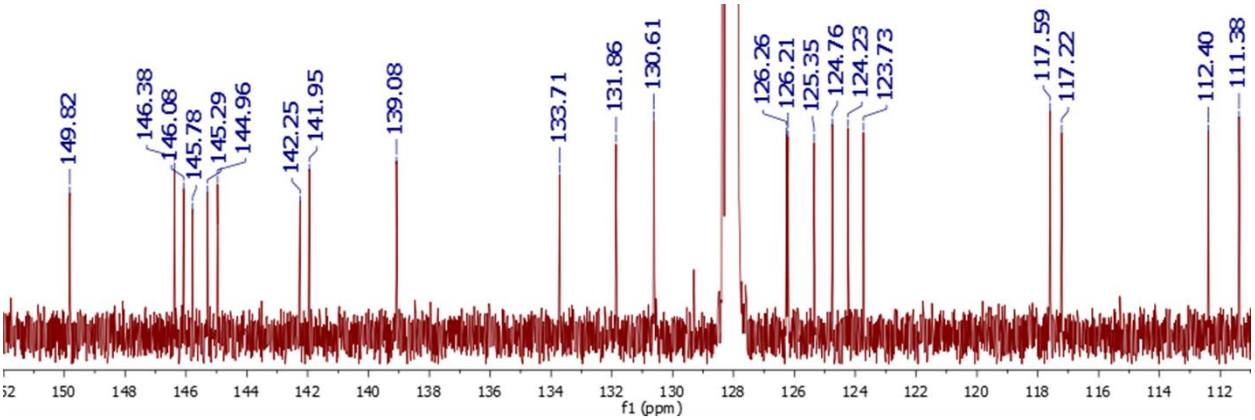

Figure S12. Expanded aryl region of ^{13}C NMR Spectrum (151 MHz, 25 °C) of **2b** in C_6D_6.

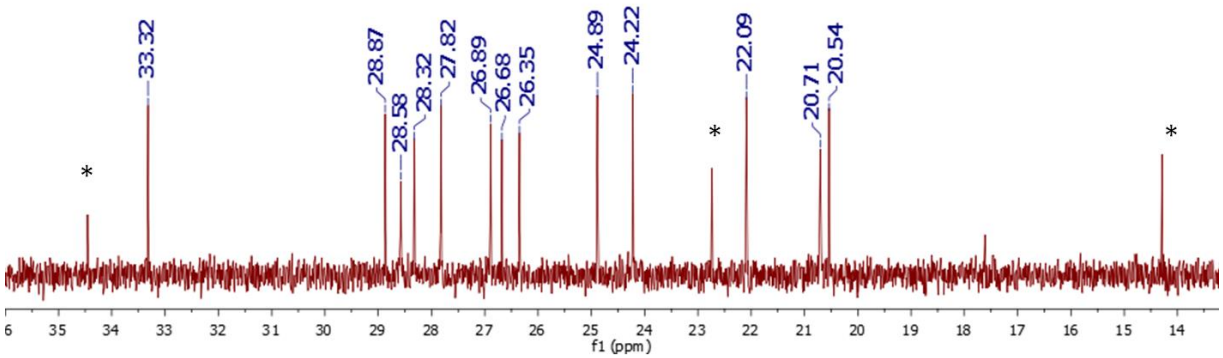

Figure S13. Expanded alkyl region of ^{13}C NMR Spectrum (151MHz, 25 °C) of **2b** in C_6D_6. Note: residual pentane is marked with an asterisk.

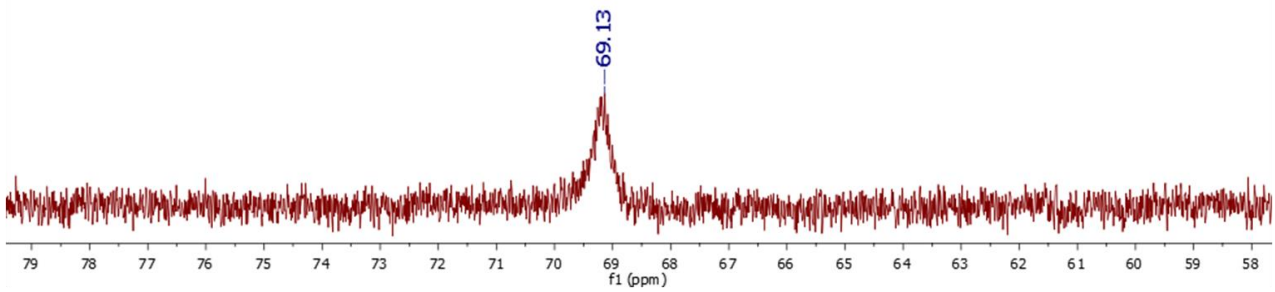

Figure S14. ^{119}Sn NMR Spectrum (224 MHz, 25 °C) of **2b** in C_6D_6.

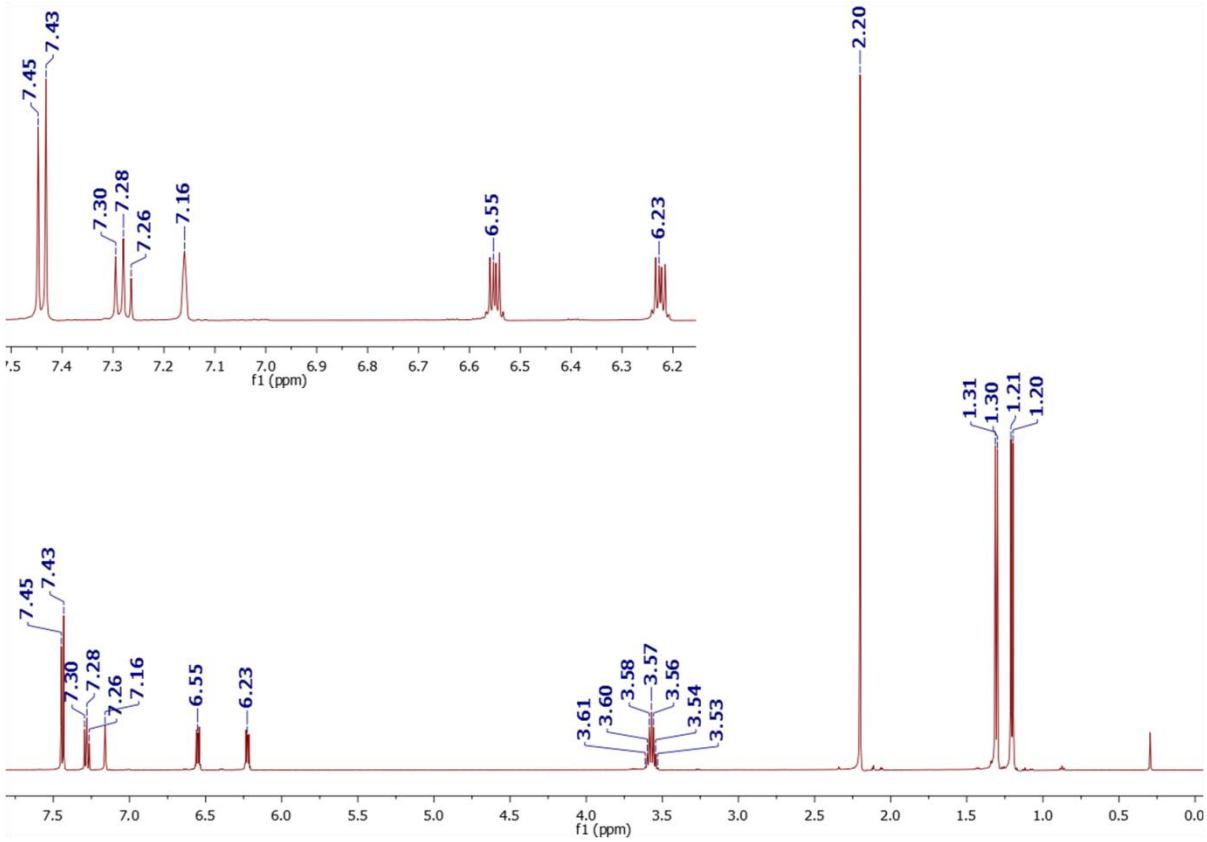

Figure S15. ^{1}H NMR Spectrum (500 MHz, 25 °C) of **3** in C_6D_6. Inset: expanded aryl region.

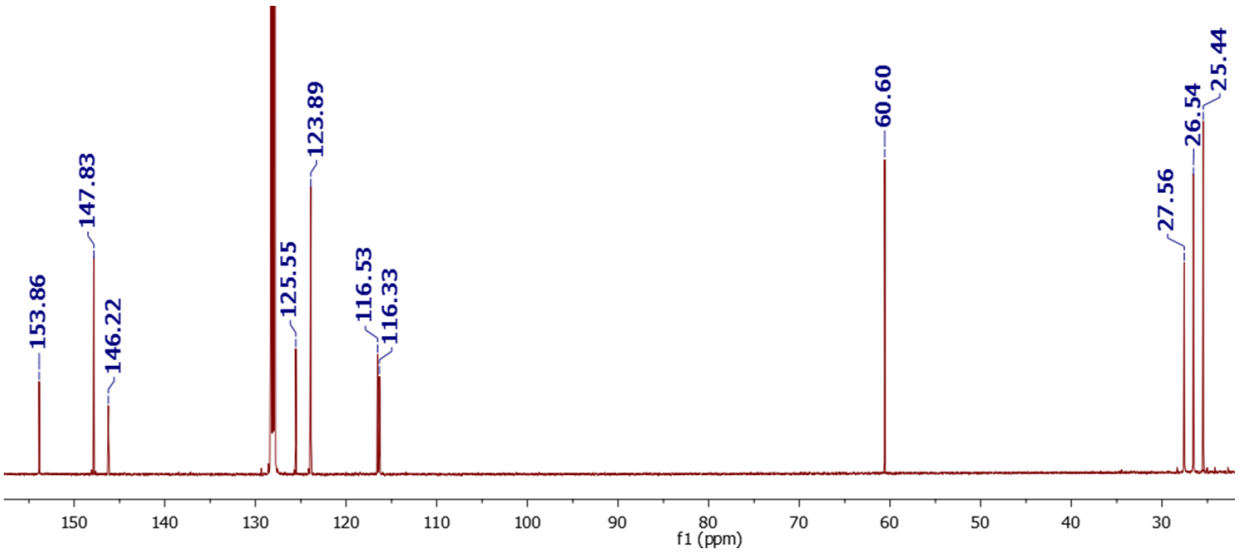

Figure S16. ^{13}C NMR Spectrum (126 MHz, 25 °C) of **3** in C_6D_6.

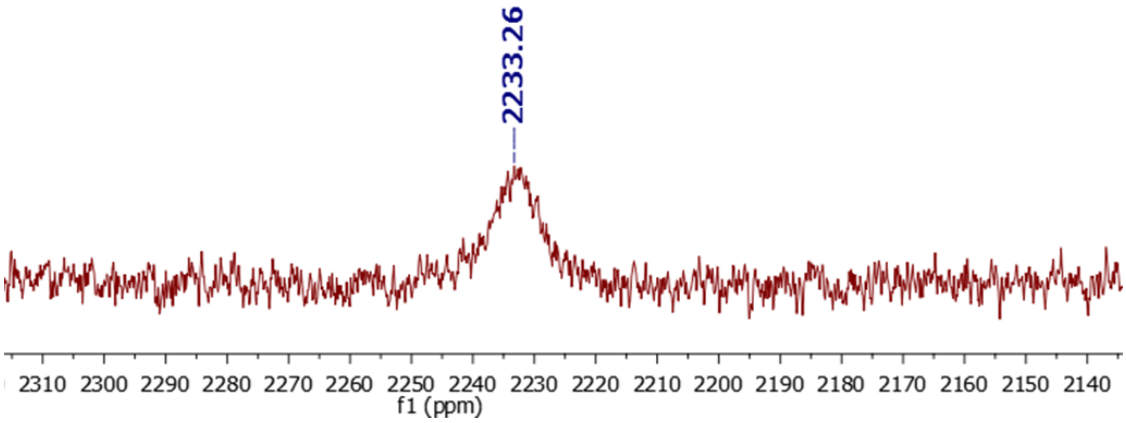

Figure S17. ^{207}Pb NMR Spectrum (126 MHz, 25 °C) of **3** in C_6D_6.

4. X-ray Crystallography

The X-ray diffraction data were collected on a Bruker Kappa Apex II diffractometer with graphite-monochromated Mo Kα radiation (λ = 0.71073 Å) at 150 K controlled by an Oxford Cryostream 700 series low-temperature system and processed with the Bruker Apex 2 software package.[7] The structures were solved by direct methods and refined using SHELXL-2014/7 and SHELXL-2016/6.[8, 9] N-H atoms in **2a** and **2b** were located directly from the difference Fourier map, while all other H atoms were calculated with the riding model. Non-hydrogen atoms were refined anisotropically, except for atoms involved in the disordered isopropyl moieties in **1a**, **3**, and **4**, the disordered $ONMe_3$ ligand in **3**, and the disordered CF_3 group in **4**. The diffuse residual electron density from disordered solvent molecules in the lattice of **3** was removed with the SQUEEZE function of PLATON,[10] and were not included in the formula. Selected crystallographic data are listed in Table 1S.

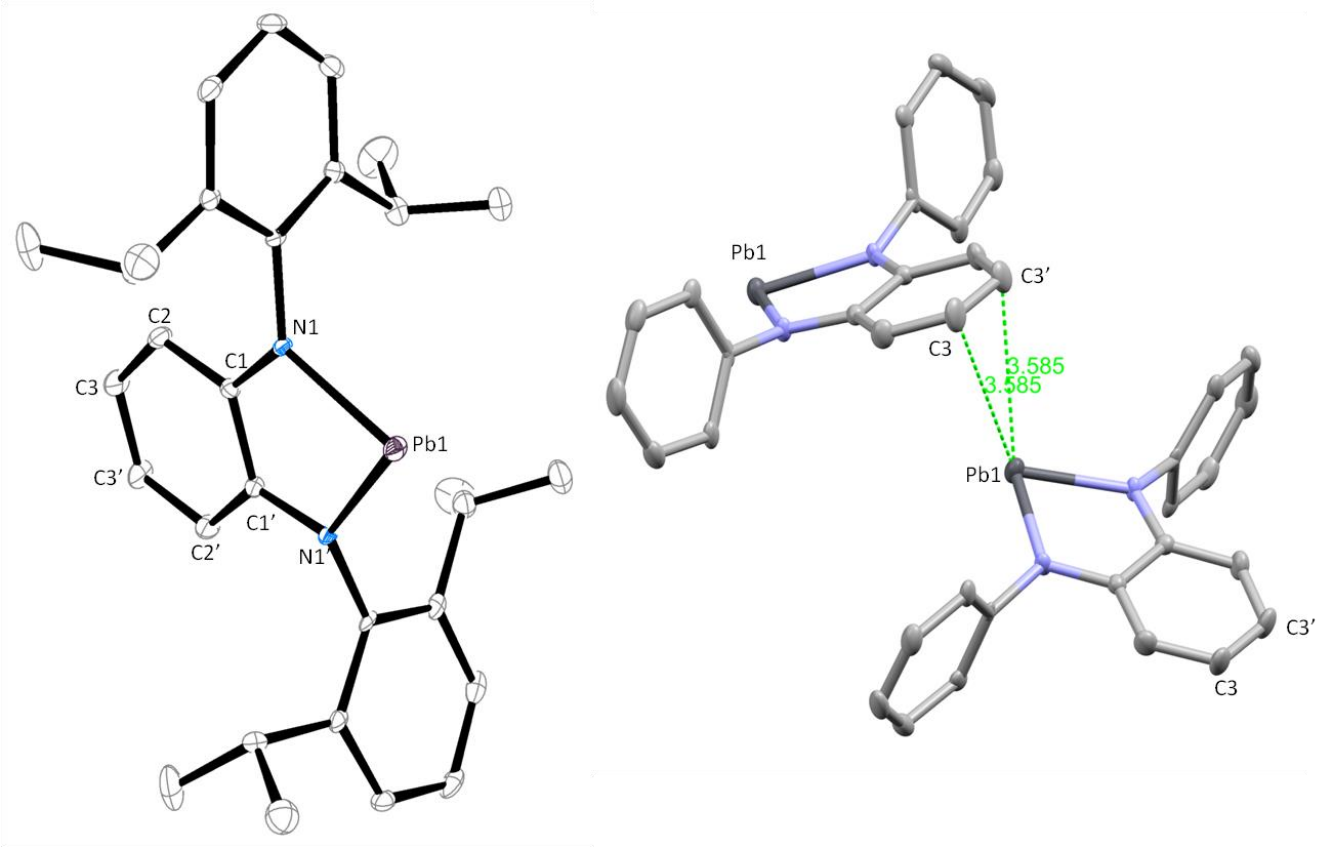

Figure S18. Molecular structure of **1a** with 30% probability ellipsoids (left), and crystal packing of **1a** with 50% probability ellipsoids (right). Hydrogen atoms omitted for clarity. Only one orientation of disordered isopropyl groups shown at left; isopropyl groups are omitted for clarity at right. Selected bond lengths (Å) and angles (°): Pb1-N1 2.134(3), C1-N1 1.330(4), C1-C1' 1.422(7), C1-C2 1.353(5), C2-C3 1.337(5), C3-C3' 1.362(8); intermolecular distance Pb1---C3(C3') 3.58; N1-Pb1-N1' 77.6(2).

Table 1S Selected crystallographic data

	1a	**2a**	**2b**	**3**	**4**
Formula	$C_{30}H_{38}N_2Pb$	$C_{39}H_{49}N_3Pb$	$C_{39}H_{49}N_3Sn$	$C_{33}H_{47}N_3OPb$	$C_{31}H_{38}F_3N_2O_3SSn$
F.W.	633.81	767.00	678.50	708.92	694.38
T (K)	150(2)	150(2)	150(2)	150(2)	150(2)
Space group	*Pnma*	$P2_1/n$	*Cc*	$P2_1/c$	$C2/c$
a (Å)	10.9016(7)	11.2497(8)	10.2651(16)	14.8076(12)	30.2756(12)
b (Å)	21.6336(17)	22.1876(18)	22.732(3)	26.177(2)	11.6808(5)
c (Å)	11.6083(8)	13.7655(10)	15.116(2)	20.3861(17)	17.9498(7)
α (°)	90	90	90	90	90
β (°)	90	93.600(3)	100.724(6)	92.810(4)	94.9769(18)
γ (°)	90	90	90	90	90
V (Å^3)	2737.7(3)	3429.1(4)	3465.8(9)	7892.7(11)	6323.9(4)
Z	4	4	4	8	8
D_c (g·cm^{-3})	1.538	1.486	1.300	1.193	1.459
μ (mm^{-1})	6.181	4.950	0.767	4.298	0.925
no. reflns collcd	24612	30953	16085	63320	28694
no. indept reflns	3219	7823	7845	15512	7288
GOF on F^2	1.019	1.016	0.977	0.997	1.039
R [I > 2σ (I)]	R_1 = 0.0275	R_1 = 0.0263	R_1 = 0.0426	R_1 = 0.0663	R_1 = 0.0320
	wR_2 = 0.0571	wR_2 = 0.0498	wR_2 = 0.0672	wR_2 = 0.1341	wR_2 = 0.0634
R (all data)	R_1 = 0.0429	R_1 = 0.0430	R_1 = 0.0601	R_1 = 0.1590	R_1 = 0.0497
	wR_2 = 0.0614	wR_2 = 0.0535	wR_2 = 0.0719	wR_2 = 0.1673	wR_2 = 0.0697

5. Computation

All computations were performed using Gaussian 09, Revision B.01[11] with B3LYP[12] method. The 6-31G* basis set was used for carbon, hydrogen, nitrogen, oxygen, fluorine, and sulfur, while the SDD basis set was used for tin and lead with effective core potential. All structures were optimized in the gas phase. Frequency analysis was then performed to confirm that the structure is a ground state. NBO analyses showed that the occupancies of the Pb 6s orbital (in compound **3**) and the Sn 5s orbital (in compound **4**) are 1.85 and 1.80 electrons, respectively. This result is consistent with the +2 oxidation state assignment for Pb and Sn. The HOMO−3 of compound **3** has the lead-based lone pair character (Figure S19), while the SOMO−3 and SOMO−4 of compound **4** have the tin-based lone pair character (Figure S20). The SOMO and spin density distribution of compound **4** are shown in Figures S21 and S22, respectively.

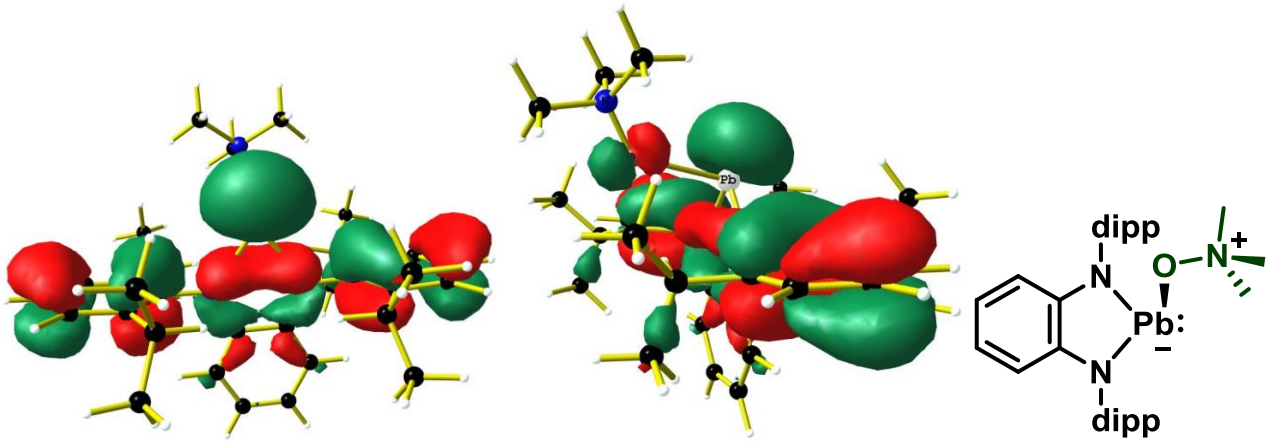

Figure S19 Plots of HOMO−3 of compound **3** at two orientations showing the presence of a lone pair on Pb.

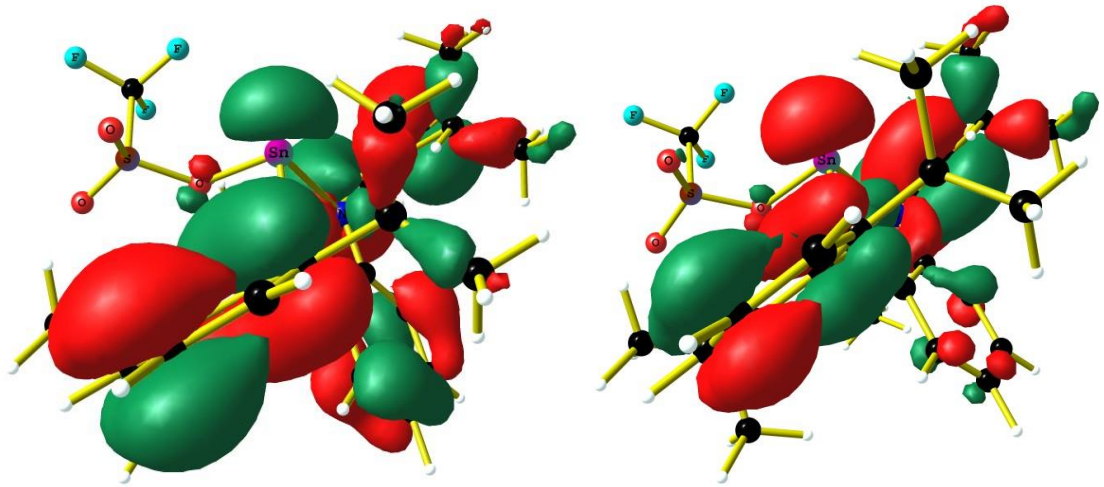

Figure S20 Plots of SOMO−3 (left) and SOMO−4 (right), showing the lone pair on Sn.

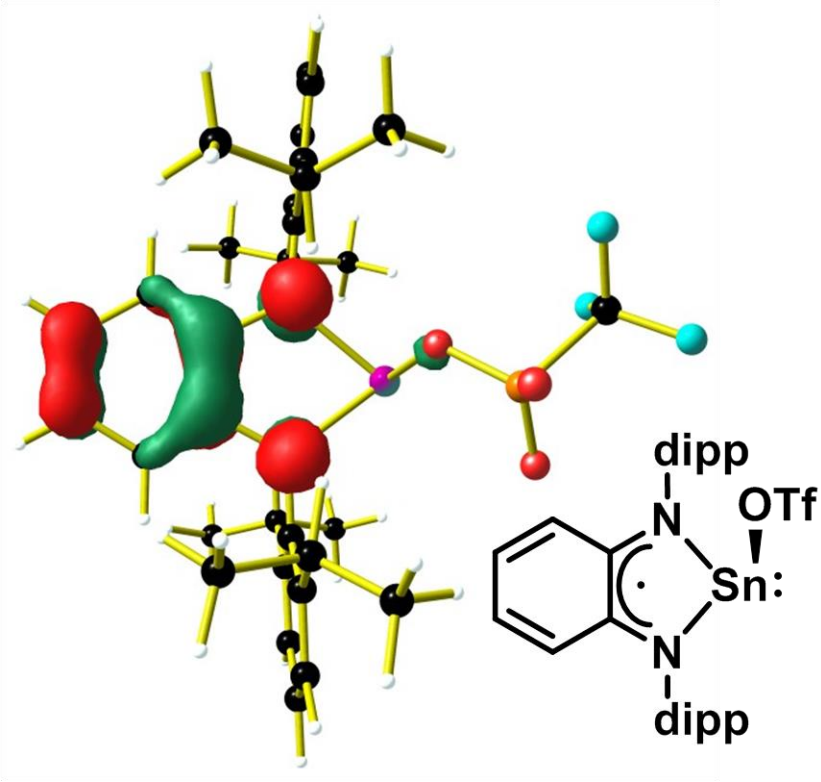

Figure S21 Singly occupied molecular orbital (SOMO) of **4** showing delocalization across the *o*-phenylene framework and the two N atoms.

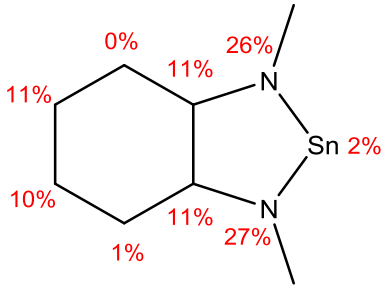

Figure S22 Spin density distribution based on DFT results for compound **4**.

Optimized geometry of 3:

Pb	-3.700576000	22.480686000	14.100241000
O	-1.146511000	22.069131000	14.748588000
N	-4.486449000	23.064881000	16.090096000
N	-4.512577000	20.602350000	14.949119000
N	-0.019848000	22.428293000	14.032268000
C	-5.105024000	22.035522000	16.801206000
C	-5.120355000	20.736363000	16.198289000
C	-5.766692000	19.684466000	16.872581000
H	-5.790243000	18.703122000	16.409311000
C	-6.381427000	19.883947000	18.110347000

H	-6.875841000	19.051097000	18.603807000
C	-6.363965000	21.148157000	18.699015000
H	-6.843425000	21.317160000	19.659821000
C	-5.732800000	22.210131000	18.048134000
H	-5.729228000	23.196238000	18.501815000
C	1.173127000	21.973373000	14.820607000
H	1.114559000	22.459659000	15.793636000
H	2.101884000	22.234771000	14.303756000
H	1.081351000	20.895306000	14.944971000
C	0.030698000	23.917929000	13.854991000
H	-0.009581000	24.361547000	14.848267000
H	-0.850195000	24.212564000	13.285011000
H	0.944451000	24.212390000	13.329830000
C	-0.027960000	21.757507000	12.689581000
H	-0.094258000	20.685074000	12.865398000
H	0.876898000	22.007889000	12.127392000
H	-0.917070000	22.098399000	12.159570000
C	-4.493397000	24.390003000	16.618392000
C	-3.447660000	26.165076000	17.903660000
H	-2.632900000	26.525043000	18.526237000
C	-4.501505000	27.024251000	17.604363000
H	-4.504132000	28.041758000	17.987495000
C	-5.552489000	26.568816000	16.814971000
H	-6.376780000	27.239521000	16.584402000
C	-5.574726000	25.259678000	16.317993000
C	-6.765271000	24.807262000	15.476872000
H	-6.601670000	23.759128000	15.212974000
C	-6.870635000	25.607140000	14.163523000
H	-5.948374000	25.530698000	13.574671000
H	-7.053374000	26.671959000	14.352567000
H	-7.697921000	25.232477000	13.548046000
C	-8.085624000	24.873964000	16.269006000
H	-8.027709000	24.262490000	17.175098000
H	-8.916550000	24.498129000	15.659265000
H	-8.329613000	25.901410000	16.566132000
C	-3.416079000	24.849568000	17.423102000
C	-2.246423000	23.940908000	17.795845000
H	-2.230026000	23.111509000	17.083705000
C	-0.884744000	24.653727000	17.695336000
H	-0.070856000	23.923453000	17.789120000
H	-0.773488000	25.178606000	16.738871000
H	-0.741928000	25.394555000	18.491167000
C	-4.509807000	19.333481000	14.296900000
C	-5.554856000	19.004738000	13.394311000
C	-5.515791000	17.773231000	12.728225000
H	-6.310757000	17.520108000	12.030698000
C	-4.486384000	16.864091000	12.949437000
H	-4.476451000	15.909223000	12.429571000
C	-3.471962000	17.184506000	13.847611000
H	-2.675210000	16.466610000	14.024897000
C	-3.456225000	18.408573000	14.528292000
C	-2.326299000	18.704245000	15.512090000
H	-2.352911000	19.773881000	15.734111000
C	-0.937785000	18.399936000	14.920185000
H	-0.803883000	18.889133000	13.948765000
H	-0.773223000	17.325554000	14.774135000
H	-0.153974000	18.758056000	15.599483000
C	-2.513762000	17.939097000	16.838407000
H	-3.461697000	18.202008000	17.315650000
H	-1.704150000	18.181079000	17.538728000
H	-2.501998000	16.854084000	16.672811000
C	-6.726949000	19.947929000	13.137519000
H	-6.584222000	20.827154000	13.771396000
C	-6.762558000	20.427430000	11.673139000
H	-5.826160000	20.924896000	11.392127000
H	-7.583541000	21.138492000	11.518535000

H	-6.911631000	19.591438000	10.979076000
C	-8.071888000	19.313349000	13.541502000
H	-8.063224000	19.021277000	14.596513000
H	-8.297208000	18.421461000	12.943880000
H	-8.891345000	20.027708000	13.394337000
C	-2.421759000	23.342574000	19.207463000
H	-1.583673000	22.676297000	19.449164000
H	-2.452521000	24.134295000	19.967285000
H	-3.345756000	22.762808000	19.280385000

Optimized geometry of 4:

Sn	3.141688000	5.405703000	1.163096000
O	3.431384000	3.219619000	1.387403000
O	4.384374000	1.439488000	2.857413000
O	3.879112000	3.765071000	3.755380000
N	3.116143000	5.020383000	-1.042269000
N	5.209499000	5.860330000	0.443491000
C	4.229981000	5.392823000	-1.703009000
C	5.363419000	5.852024000	-0.897661000
C	6.546076000	6.278421000	-1.570529000
H	7.383167000	6.620215000	-0.973226000
C	6.624980000	6.250588000	-2.944148000
H	7.537471000	6.572841000	-3.437275000
C	5.523669000	5.808934000	-3.725473000
H	5.602088000	5.804079000	-4.808743000
C	4.358225000	5.394470000	-3.123558000
H	3.512784000	5.066096000	-3.717013000
C	1.959190000	4.541856000	-1.748751000
C	1.872363000	3.173116000	-2.103327000
C	0.714868000	2.739128000	-2.762096000
H	0.630974000	1.694231000	-3.046823000
C	-0.329513000	3.611573000	-3.053198000
H	-1.218538000	3.248437000	-3.561857000
C	-0.230267000	4.950620000	-2.689071000
H	-1.046735000	5.629797000	-2.919255000
C	0.906782000	5.443404000	-2.037119000
C	0.975973000	6.927495000	-1.683314000
H	1.926811000	7.108452000	-1.170978000
C	-0.151827000	7.340618000	-0.717711000
H	-0.052052000	8.396942000	-0.441131000
H	-1.139967000	7.208211000	-1.172985000
H	-0.129292000	6.744766000	0.201898000
C	0.974549000	7.811642000	-2.946278000
H	1.070960000	8.869438000	-2.673997000
H	1.806564000	7.553745000	-3.610280000
H	0.043659000	7.696516000	-3.513557000
C	2.984401000	2.169333000	-1.805083000
C	2.465938000	0.945714000	-1.026247000
H	3.304852000	0.295015000	-0.754589000
H	1.964920000	1.243562000	-0.102200000
H	1.764384000	0.349078000	-1.621852000
C	3.698915000	1.722304000	-3.097335000
H	4.134639000	2.571373000	-3.634346000
H	4.509038000	1.023114000	-2.858967000
H	3.006939000	1.211651000	-3.778327000
C	6.235333000	6.408287000	1.292039000
C	7.201130000	5.543861000	1.859270000
C	8.180978000	6.107518000	2.686173000
H	8.935632000	5.462699000	3.126379000
C	8.203354000	7.471302000	2.961822000
H	8.971814000	7.884201000	3.609893000
C	7.233675000	8.302946000	2.410820000
H	7.251129000	9.365997000	2.635695000
C	6.235488000	7.796727000	1.569190000
C	5.196146000	8.755335000	0.990684000

C	4.381080000	9.449661000	2.099727000
H	3.893634000	8.719096000	2.755132000
H	5.016275000	10.084873000	2.727430000
H	3.603743000	10.087101000	1.661647000
C	5.838201000	9.791816000	0.047455000
H	5.070446000	10.445356000	-0.383662000
H	6.555079000	10.426565000	0.581181000
H	6.369601000	9.302857000	-0.775866000
C	7.217617000	4.042281000	1.583338000
H	6.258305000	3.773434000	1.130141000
C	8.324262000	3.672870000	0.573422000
H	8.307604000	2.595692000	0.370078000
H	8.198353000	4.198914000	-0.378981000
H	9.315931000	3.924684000	0.969484000
C	7.364110000	3.211475000	2.872627000
H	7.219305000	2.149556000	2.649899000
H	8.359159000	3.326129000	3.319483000
H	6.616505000	3.497633000	3.617786000
S	3.590061000	2.660797000	2.825668000
C	1.841200000	2.146006000	3.207306000
F	1.016405000	3.194050000	3.050584000
F	1.446953000	1.165121000	2.388994000
F	1.764745000	1.719453000	4.468084000
H	4.492024000	8.170930000	0.389085000
H	3.721765000	2.660523000	-1.166006000

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