Electronic Supplementary Material (ESI) for Dalton Transactions.

Supplementary Information

for

Bis(di-*tert*-butylindenyl)tetrelocenes

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NMR Spectra

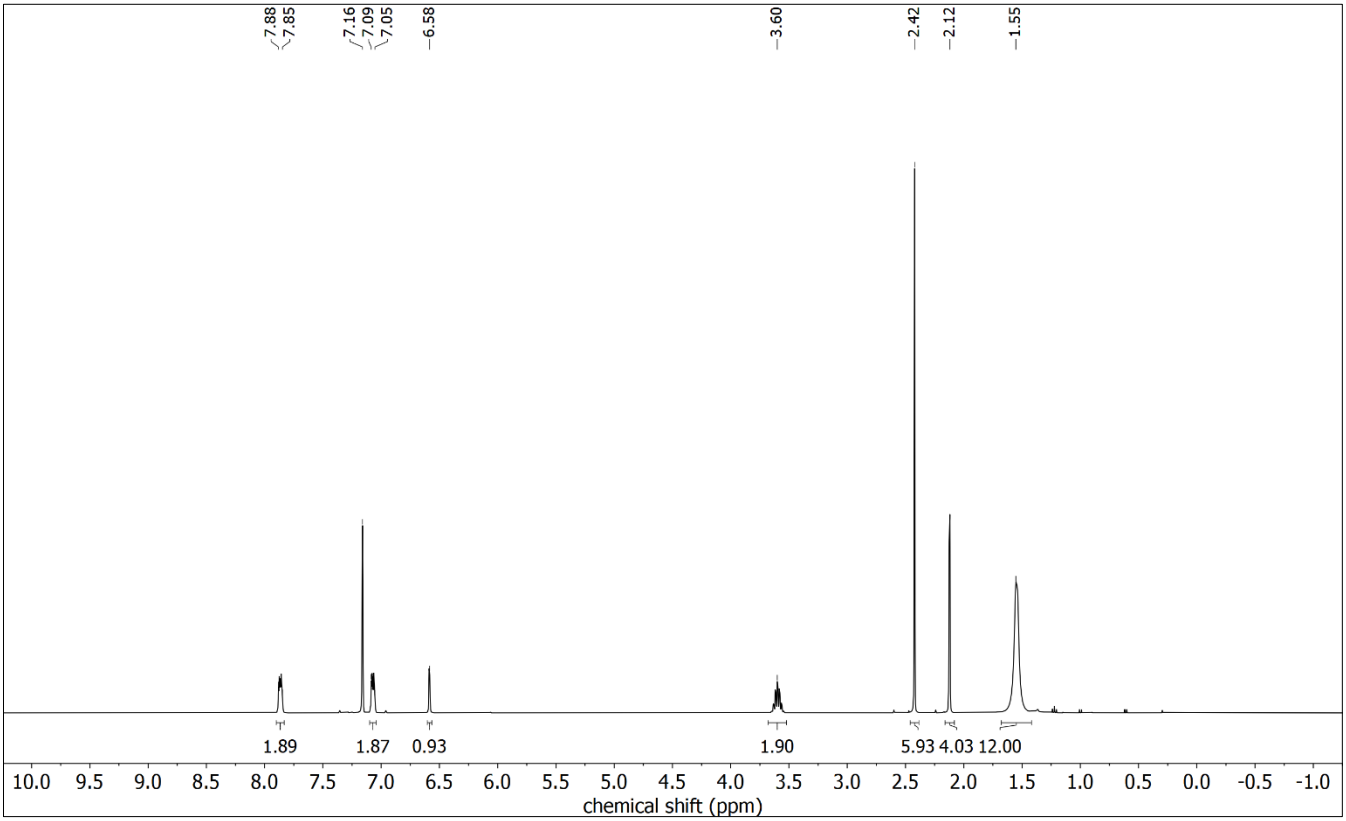

Figure S1. ^{1}H NMR spectrum (400 MHz, C_6D_6, 295 K) of lithium dimethoxyethane diisopropylindenide, **1a**·(dme).

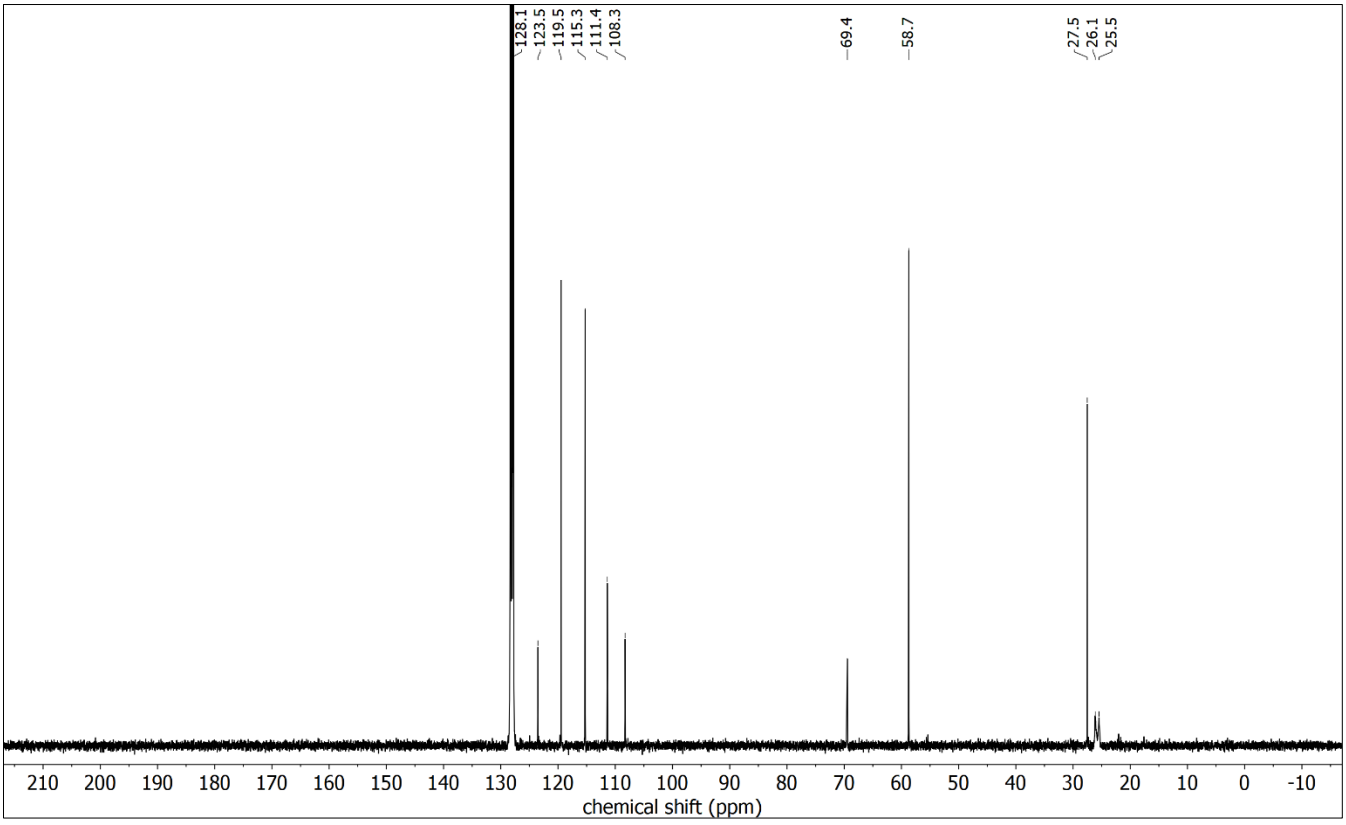

Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, C_6D_6, 295 K) of lithium dimethoxyethane diisopropylindenide, **1a**·(dme).

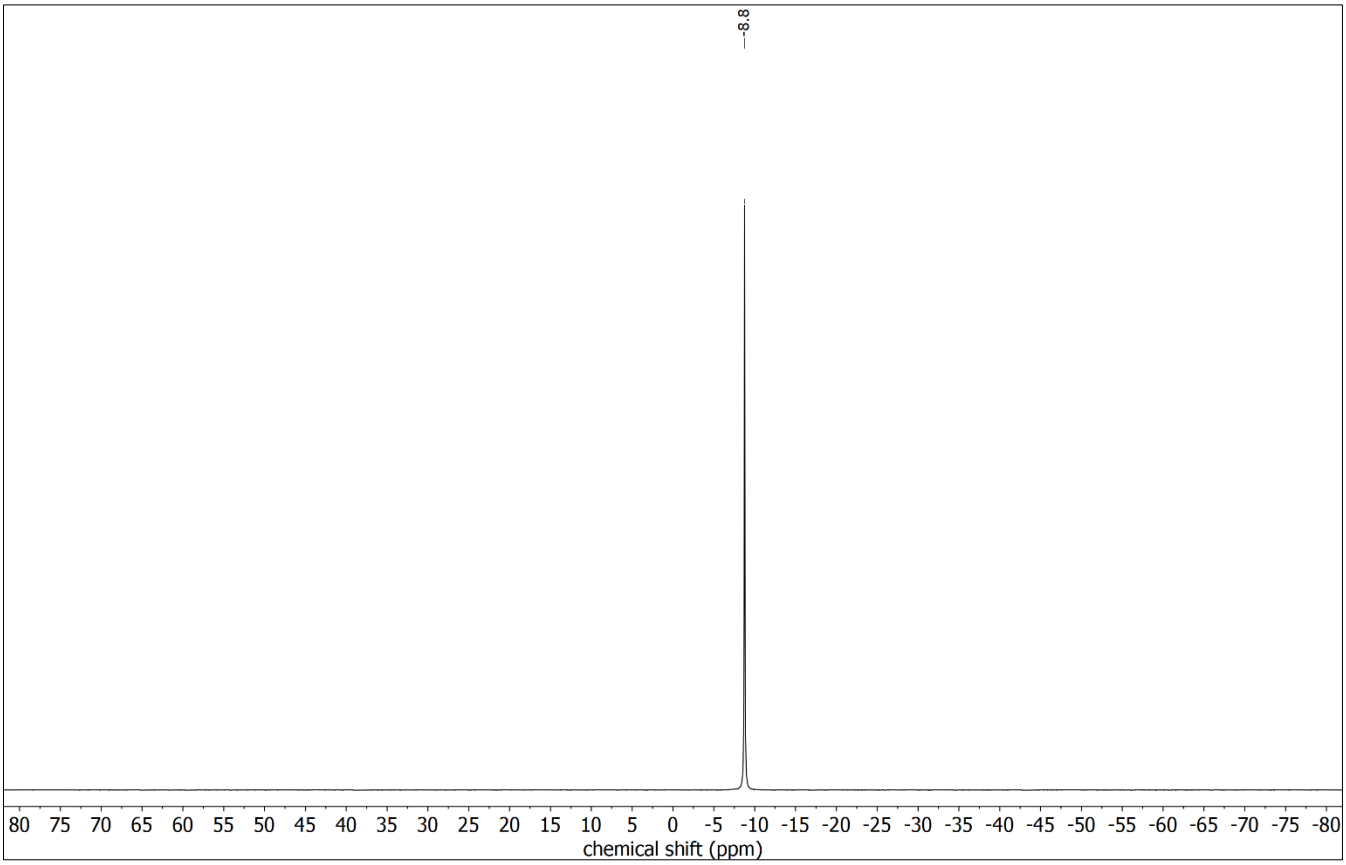

Figure S3. $^{7}Li\{^{1}H\}$ NMR spectrum (156 MHz, C_6D_6, 295 K) of lithium dimethoxyethane diisopropylindenide, **1a**·(dme).

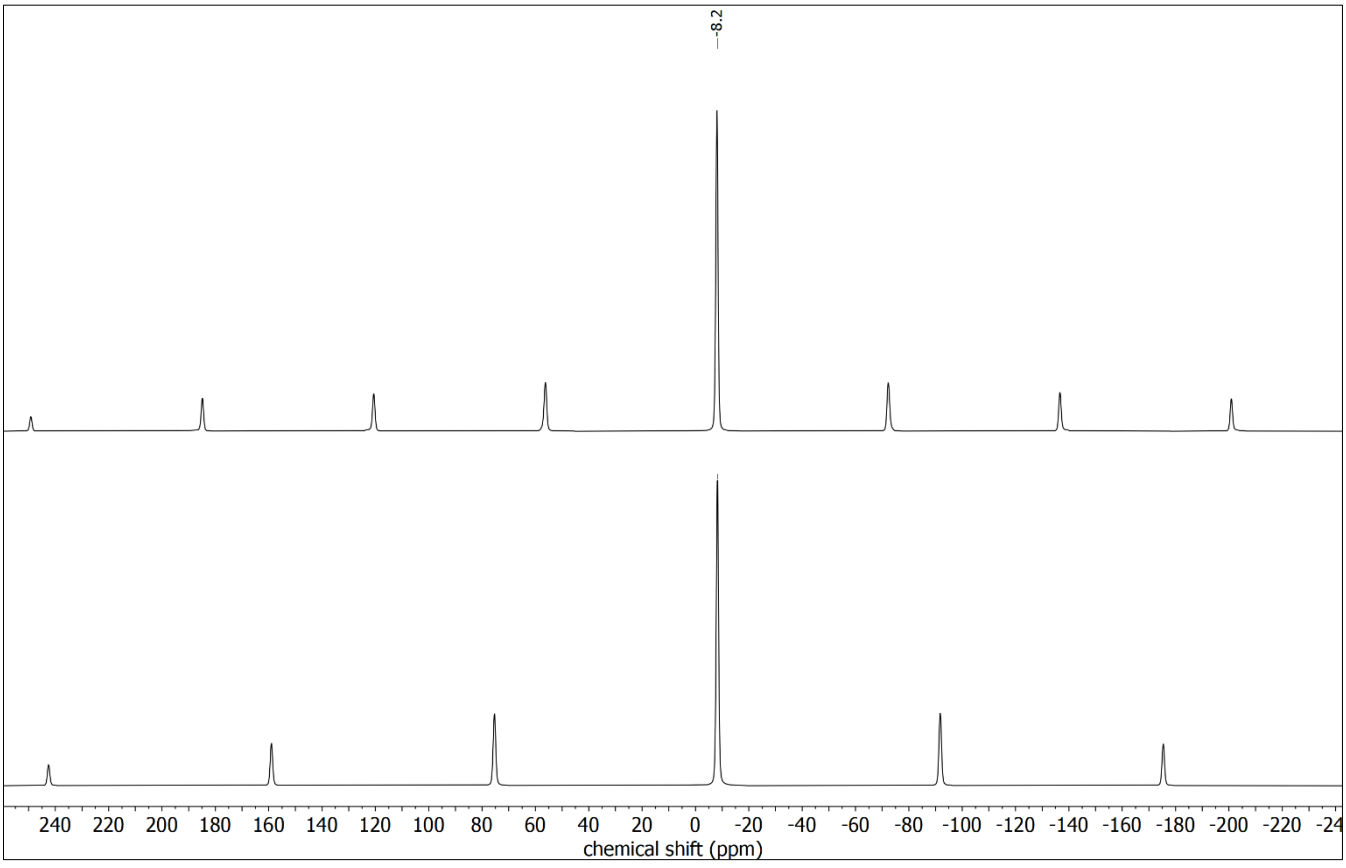

Figure S4. $^{7}Li\{^{1}H\}$ CP-MAS(upper trace: 10 kHz; lower trace: 13 kHz) NMR spectra (156 MHz, 297 K) of lithium dimethoxyethane diisopropylindenide, **1a**·(dme).

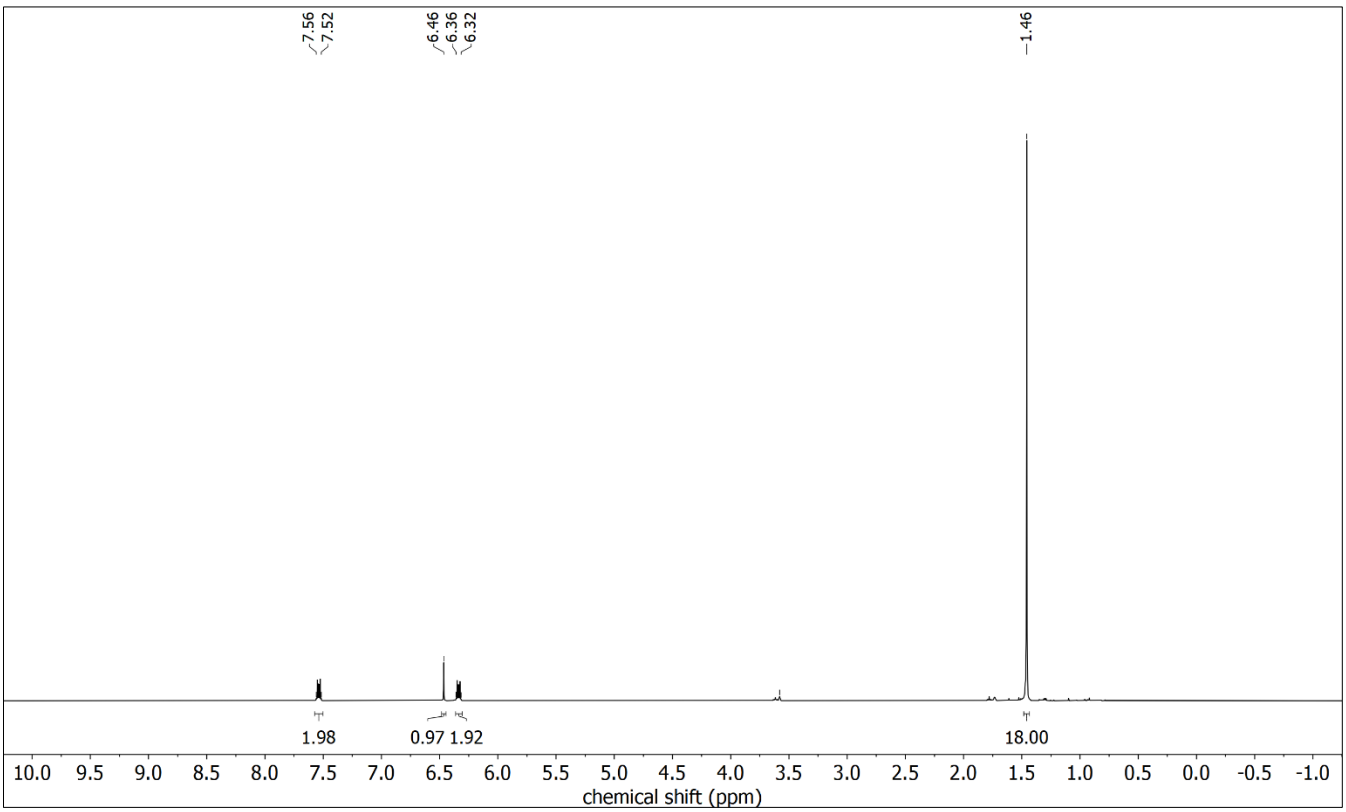

Figure S5. ^{1}H NMR spectrum (400 MHz, THF-D8, 295 K) of sodium di-*tert*-butylindenide, **1b**.

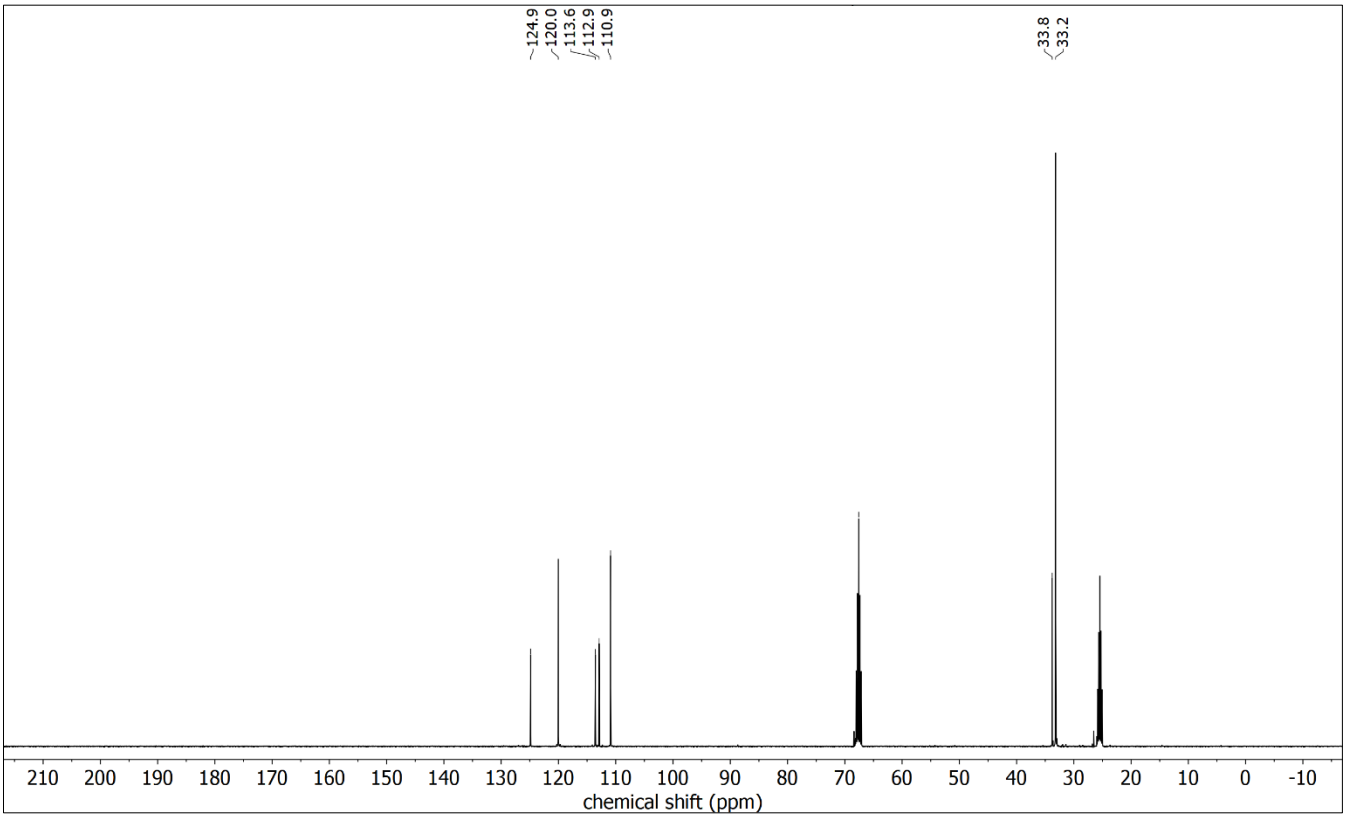

Figure S6. $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, THF-D8, 295 K) of sodium di-*tert*-butylindenide, **1b**.

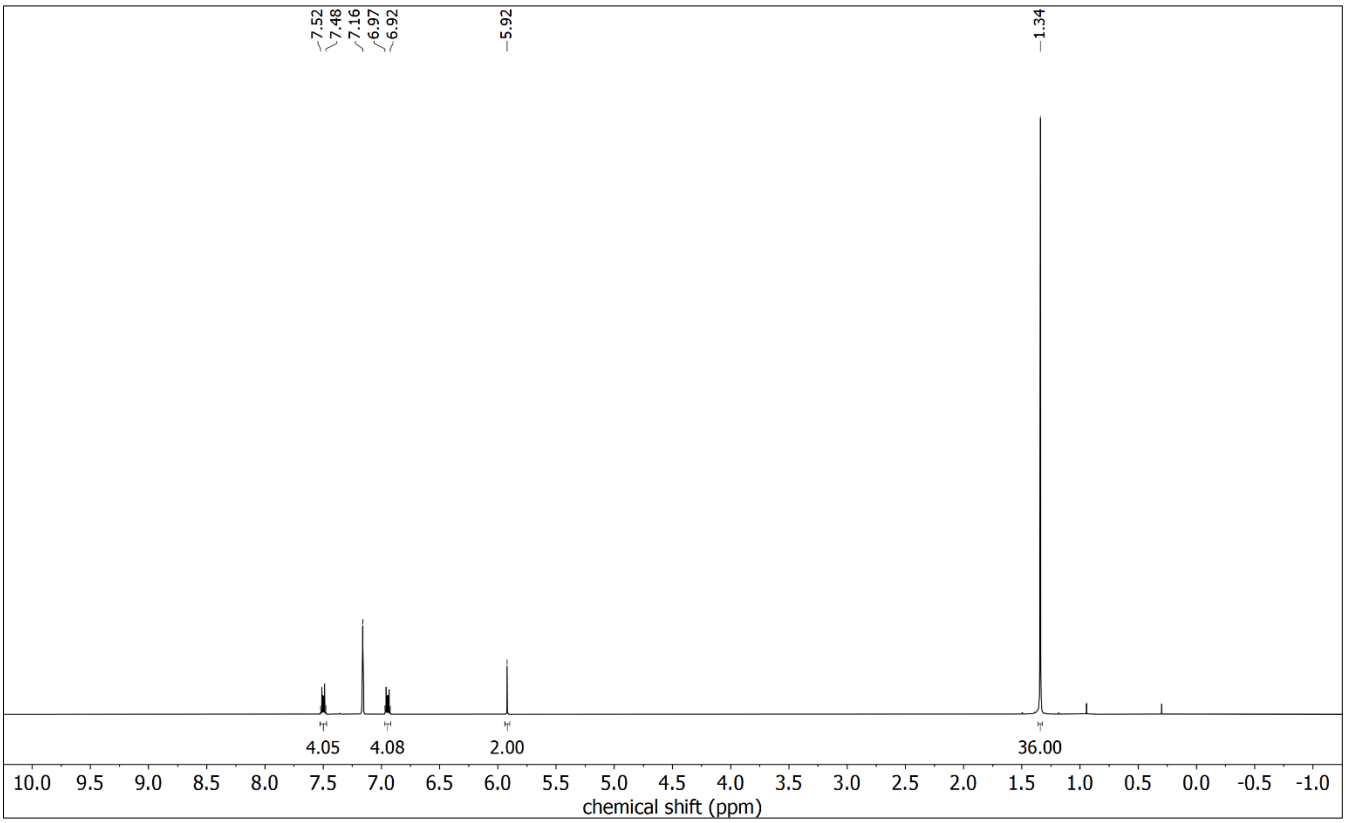

Figure S7. ^{1}H NMR spectrum (400 MHz, C_6D_6, 295 K) of bis(di-*tert*-butylindenyl)germanocene, **2a**.

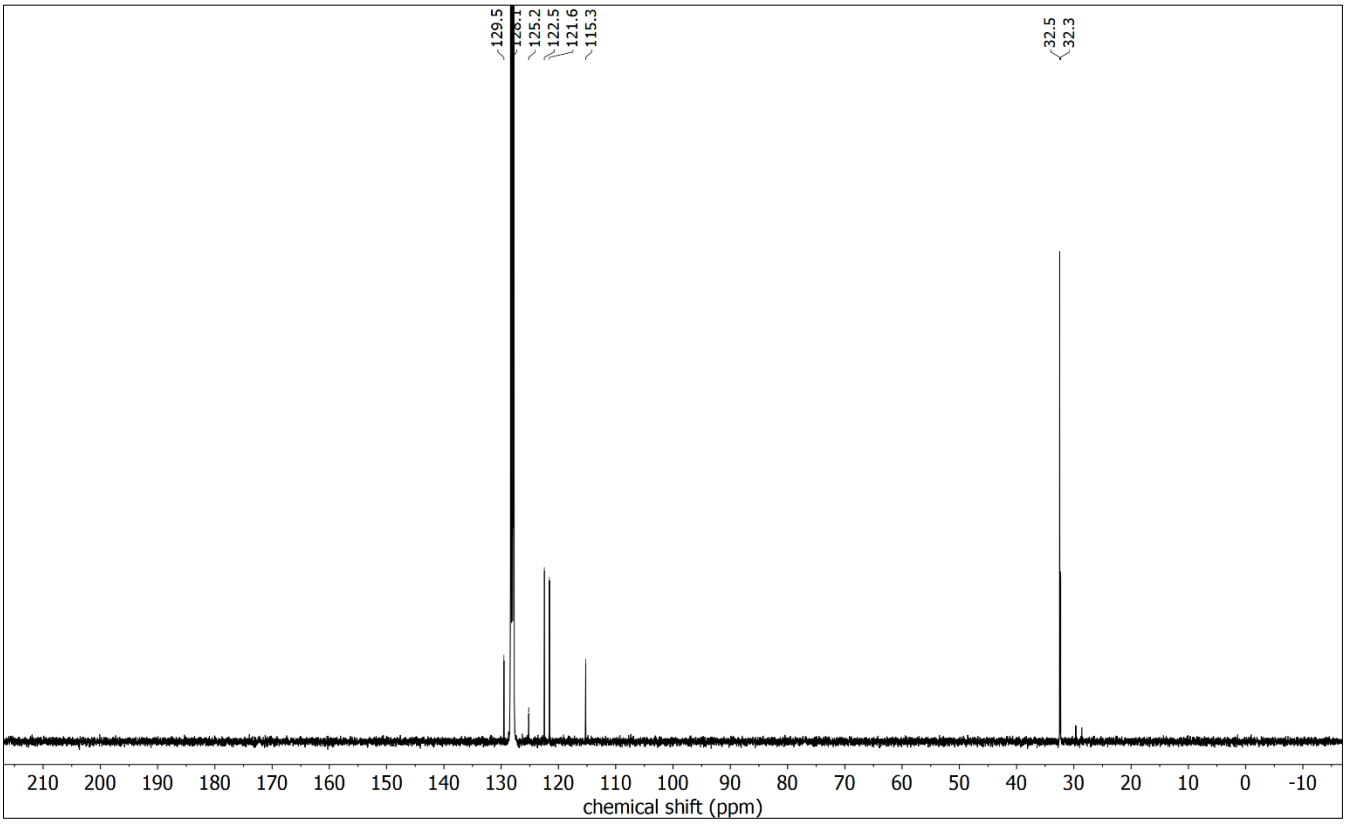

Figure S8. $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, C_6D_6, 295 K) of bis(di-*tert*-butylindenyl)germanocene, **2a**.

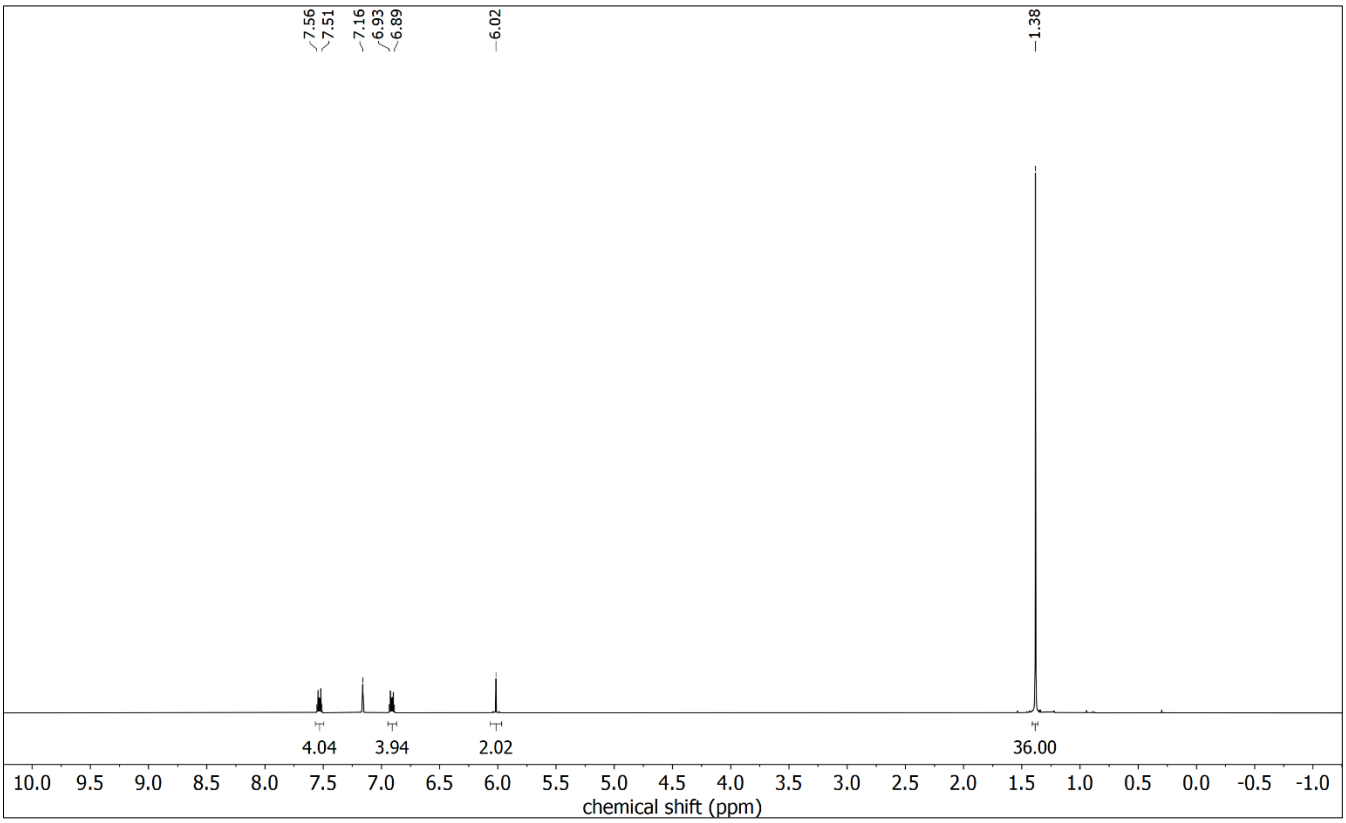

Figure S9. ^{1}H NMR spectrum (400 MHz, C_6D_6, 295 K) of bis(di-*tert*-butylindenyl)stannocene, **2b**.

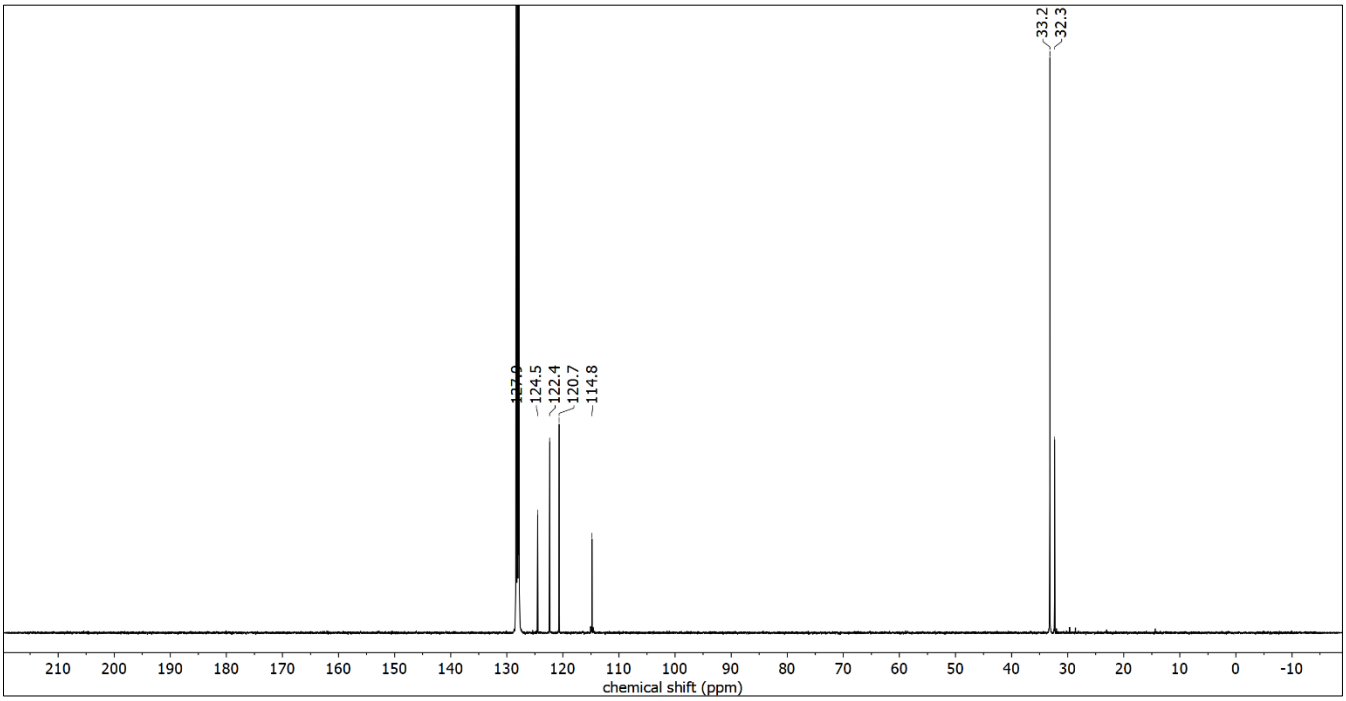

Figure S10. $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, C_6D_6, 296 K) of bis(di-*tert*-butylindenyl)stannocene, **2b**.

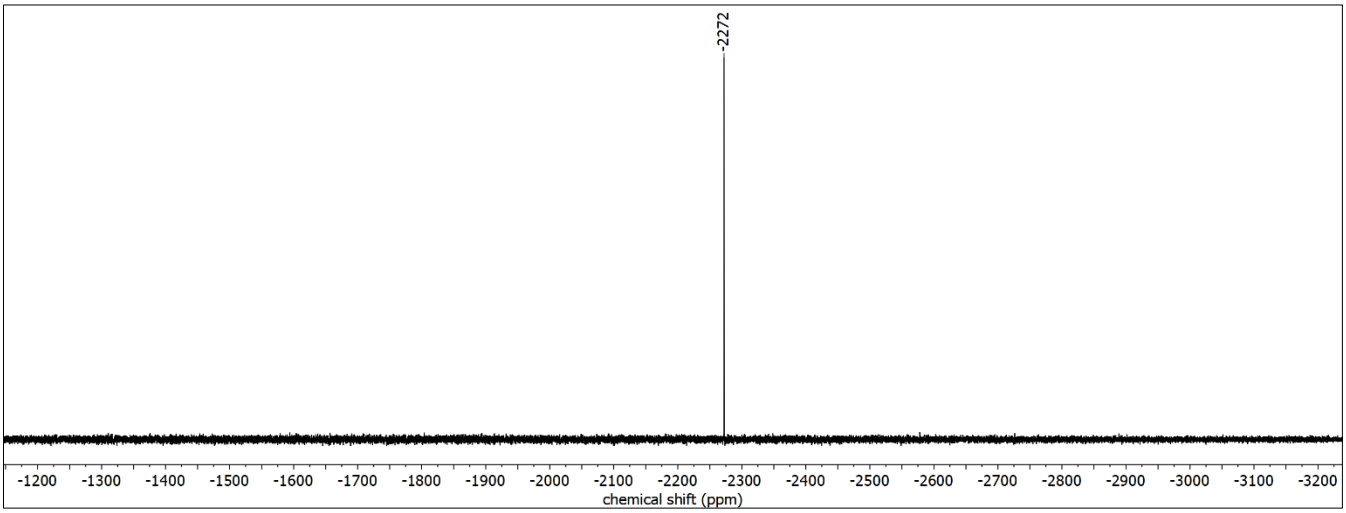

Figure S11. $^{119}Sn\{^{1}H\}$ NMR spectrum (149 MHz, C_6D_6, 295 K) of bis(di-*tert*-butylindenyl)stannocene, **2b**.

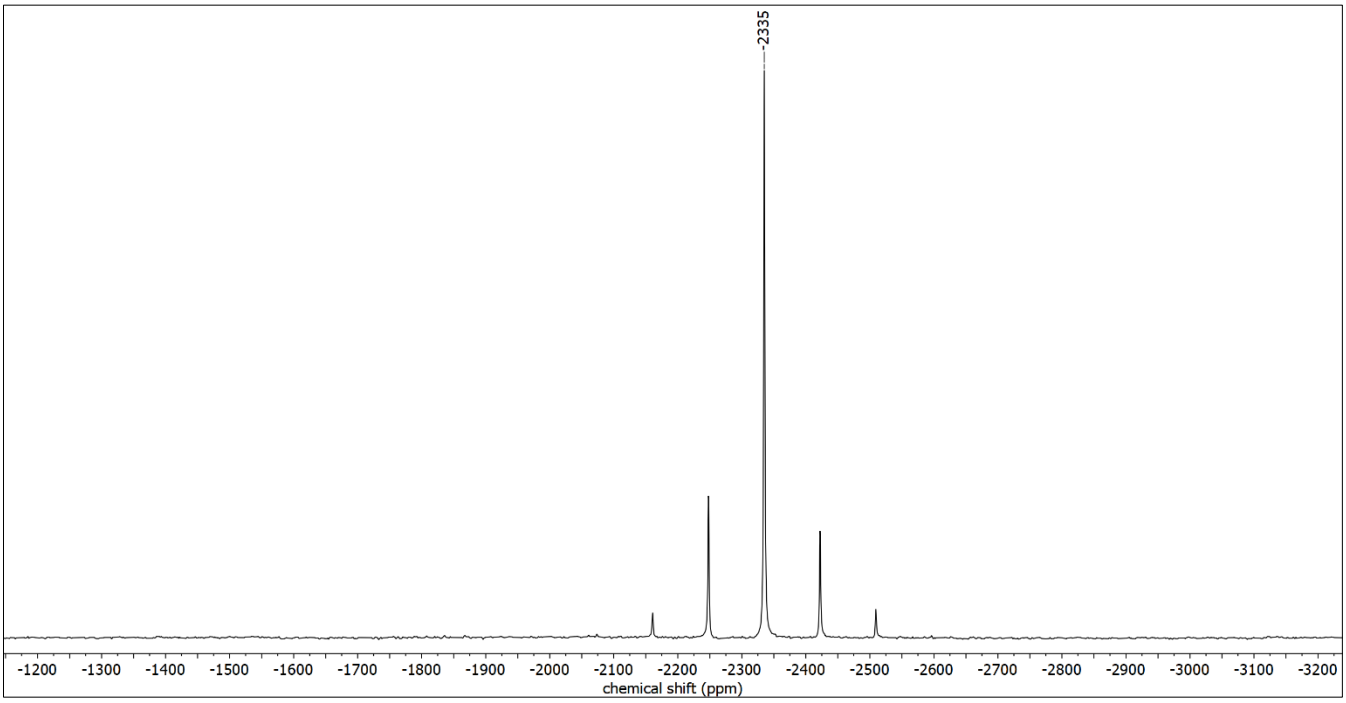

Figure S12. $^{119}Sn\{^{1}H\}$ CP-MAS(13 kHz) NMR spectra (149 MHz) of bis(di-*tert*-butylindenyl)stannocene, **2b**.

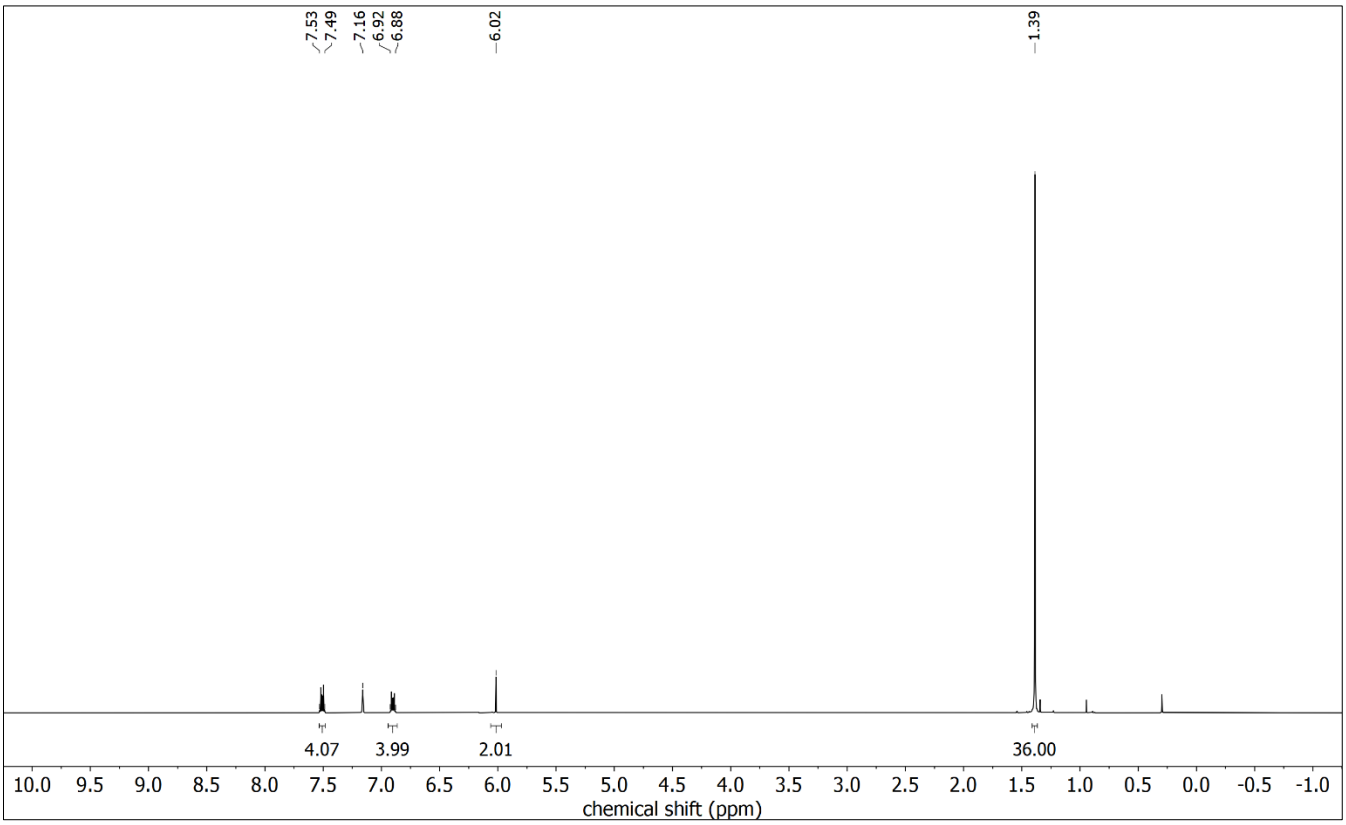

Figure S13. ^{1}H NMR spectrum (400 MHz, C_6D_6, 294 K) of bis(di-*tert*-butylindenyl)plumbocene, **2c**.

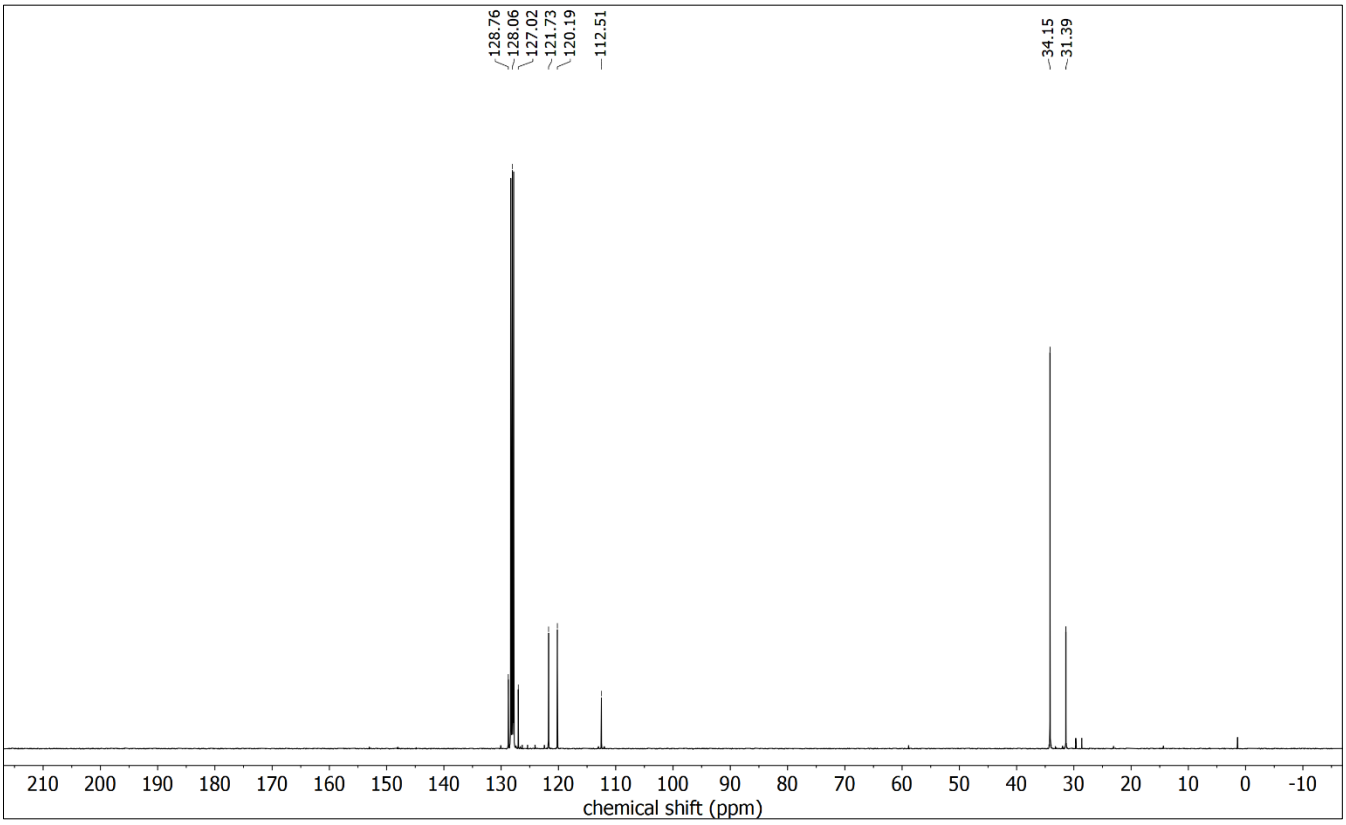

Figure S14. $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, C_6D_6, 294 K) of bis(di-*tert*-butylindenyl)plumbocene, **2c**.

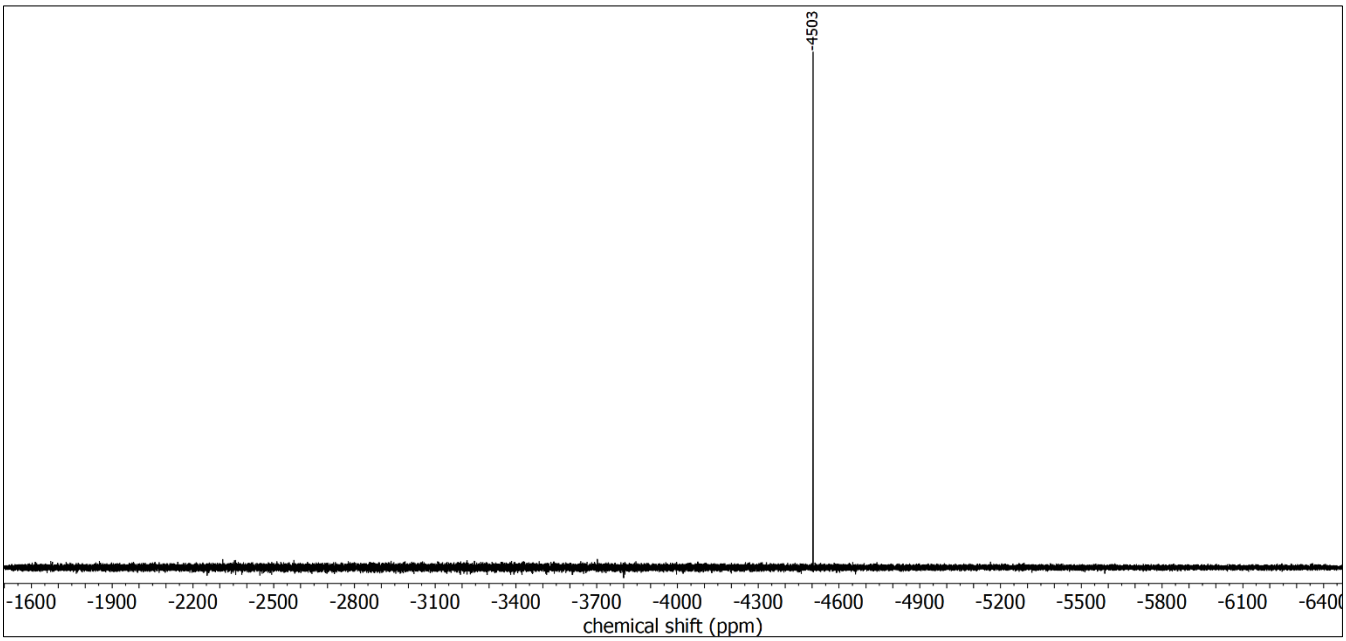

Figure S15. $^{207}Pb\{^{1}H\}$ NMR spectrum (83 MHz, C_6D_6, 294 K) of bis(di-*tert*-butylindenyl)plumbocene, **2c**.

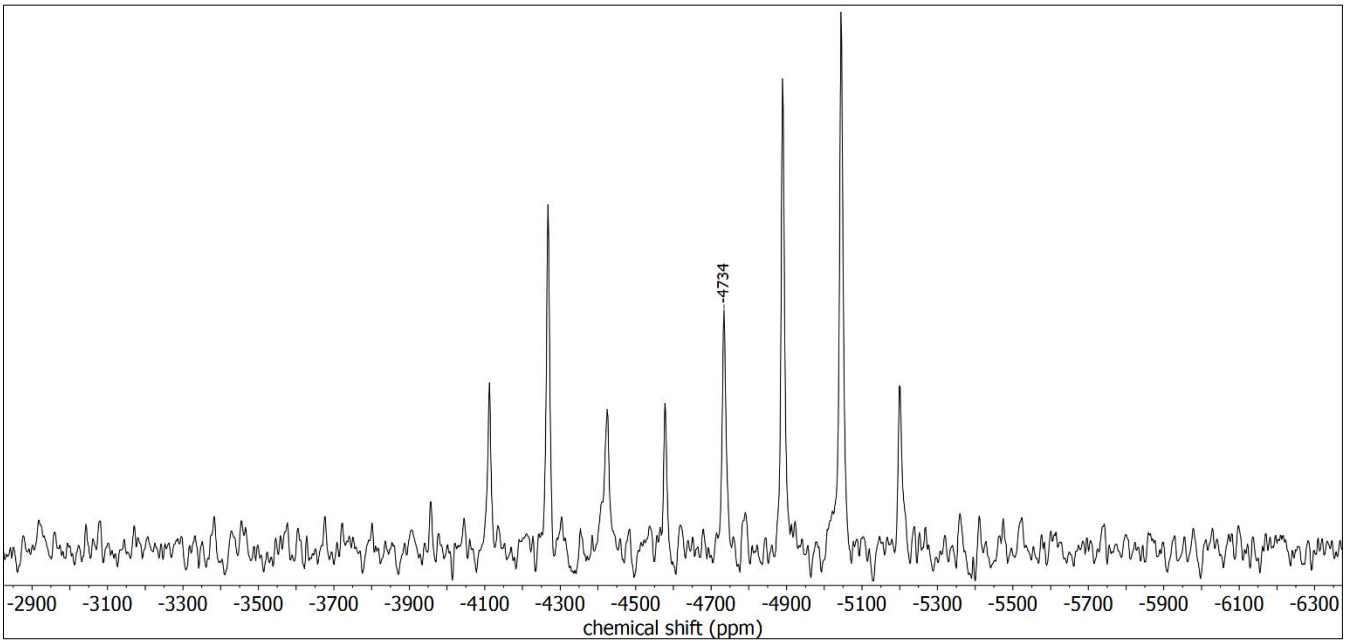

Figure S16. $^{207}Pb\{^{1}H\}$ CP-MAS(13 kHz) NMR spectra (83 MHz) of bis(di-*tert*-butylindenyl)plumbocene, **2c**.

XRD Data

Lithium dimethoxyethane diisopropylindenide, 1a·(dme):

CCDC code	2154213	
Empirical formula	$C_{19}H_{29}LiO_2$	
Formula weight	296.36	
Temperature	133(2) K	
Wavelength	0.71073 Å	
Crystal system	triclinic	
Space group	*P*-1	
Unit cell dimensions	a = 8.1149(10) Å	α = 73.834(4)°
	b = 9.9608(11) Å	β = 74.958(4)°
	c = 12.9882(16) Å	γ = 66.433(4)°
Volume	911.04(19) $Å^3$	
Z	2	
Density (calculated)	1.080 mg/m^3	
Absorption coefficient	0.067 mm^{-1}	
F(000)	324	
Crystal size	0.239 x 0.085 x 0.058 mm^3	
Theta range for data collection	2.537 to 25.675°	
Index ranges	-9<=h<=9, -11<=k<=12, -15<=l<=15	
Reflections collected	24467	
Independent reflections	3309 [R(int) = 0.0728]	
Completeness to theta = 25.242°	96.0%	
Absorption correction	semi-empirical from equivalents	
Max. and min. transmission	0.7455 and 0.6730	
Refinement method	full-matrix least-squares on F^2	
Data / restraints / parameters	3309 / 0 / 208	
Goodness-of-fit on F^2	1.068	
Final R indices [I>2σ(I)]	R1 = 0.0587, wR2 = 0.1505	
R indices (all data)	R1 = 0.0796, wR2 = 0.1645	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.241 and -0.204 $e.Å^{-3}$	

Sodium tris(dimethoxyethane) di-*tert*-butylindenide, 1b·(dme)$_3$:

CCDC code	2154214	
Empirical formula	$C_{29}H_{53}NaO_6$	
Formula weight	520.70	
Temperature	133(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 11.6172(2) Å	α = 90°
	b = 15.9650(3) Å	β = 103.5900(10)°
	c = 17.7264(4) Å	γ = 90°
Volume	3195.64(11) Å^3	
Z	4	
Density (calculated)	1.082 mg/m^3	
Absorption coefficient	0.085 mm^{-1}	
F(000)	1144	
Crystal size	0.309 x 0.249 x 0.138 mm^3	
Theta range for data collection	2.209 to 27.115°	
Index ranges	-14<=h<=14, -20<=k<=20, -22<=l<=22	
Reflections collected	49094	
Independent reflections	7058 [R(int) = 0.0545]	
Completeness to theta = 25.242°	100.0%	
Absorption correction	semi-empirical from equivalents	
Max. and min. transmission	0.7455 and 0.6877	
Refinement method	full-matrix least-squares on F^2	
Data / restraints / parameters	7058 / 0 / 337	
Goodness-of-fit on F^2	1.033	
Final R indices [I>2σ(I)]	R1 = 0.0409, wR2 = 0.0950	
R indices (all data)	R1 = 0.0581, wR2 = 0.1059	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.207 and -0.217 e.Å^{-3}	

Bis(di-*tert*-butylindenyl)germanocene, 2a:

CCDC code	2154217	
Empirical formula	$C_{34}H_{46}Ge$	
Formula weight	527.30	
Temperature	148(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	$P\,2_1/n$	
Unit cell dimensions	a = 10.979(3) Å	α = 90°
	b = 14.731(4) Å	β = 107.306(8)°
	c = 18.973(4) Å	γ = 90°
Volume	2929.7(12) $Å^3$	
Z	4	
Density (calculated)	1.195 Mg/m^3	
Absorption coefficient	1.065 mm^{-1}	
F(000)	1128	
Crystal size	0.254 x 0.202 x 0.088 mm^3	
Theta range for data collection	1.934 to 27.137°.	
Index ranges	-14<=h<=14, -18<=k<=18, -24<=l<=24	
Reflections collected	48002	
Independent reflections	6464 [R(int) = 0.0442]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	semi-empirical from equivalents	
Max. and min. transmission	0.7455 and 0.6975	
Refinement method	full-matrix least-squares on F^2	
Data / restraints / parameters	6464 / 0 / 328	
Goodness-of-fit on F^2	1.027	
Final R indices [I>2σ(I)]	R1 = 0.0262, wR2 = 0.0624	
R indices (all data)	R1 = 0.0334, wR2 = 0.0662	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.312 and -0.294 $e.Å^{-3}$	

Bis(di-*tert*-butylindenyl)stannocene, 2b:

CCDC code	2154215	
Empirical formula	$C_{34}H_{46}Sn$	
Formula weight	573.40	
Temperature	133(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	$P\,2_1/n$	
Unit cell dimensions	a = 11.0857(3) Å	α = 90°
	b = 14.8512(4) Å	β = 105.5710(10)°
	c = 18.8414(5) Å	γ = 90°
Volume	2988.12(14) $Å^3$	
Z	4	
Density (calculated)	1.275 mg/m^3	
Absorption coefficient	0.874 mm^{-1}	
F(000)	1200	
Crystal size	0.234 x 0.201 x 0.137 mm^3	
Theta range for data collection	2.244 to 30.524°	
Index ranges	-15<=h<=15, -21<=k<=21, -26<=l<=25	
Reflections collected	64683	
Independent reflections	9129 [R(int) = 0.0331]	
Completeness to theta = 25.242°	99.9%	
Absorption correction	semi-empirical from equivalents	
Max. and min. transmission	0.7461 and 0.6927	
Refinement method	full-matrix least-squares on F^2	
Data / restraints / parameters	9129 / 0 / 328	
Goodness-of-fit on F^2	1.036	
Final R indices [I>2σ(I)]	R1 = 0.0236, wR2 = 0.0488	
R indices (all data)	R1 = 0.0332, wR2 = 0.0527	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.362 and -0.395 $e.Å^{-3}$	

Bis(di-*tert*-butylindenyl)plumbocene, 2c:

CCDC code	2154216	
Empirical formula	$C_{34}H_{46}Pb$	
Formula weight	661.90	
Temperature	133(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	$P\,2_1/n$	
Unit cell dimensions	a = 11.1603(4) Å	α = 90°
	b = 14.9272(5) Å	β = 106.1980(10)°
	c = 18.8917(7) Å	γ = 90°
Volume	3022.27(19) $Å^3$	
Z	4	
Density (calculated)	1.455 Mg/m^3	
Absorption coefficient	5.601 mm^{-1}	
F(000)	1328	
Crystal size	0.148 x 0.142 x 0.092 mm^3	
Theta range for data collection	2.245 to 28.725°.	
Index ranges	-15<=h<=14, -18<=k<=20, -25<=l<=25	
Reflections collected	50956	
Independent reflections	7815 [R(int) = 0.0351]	
Completeness to theta = 25.242°	100.0%	
Absorption correction	semi-empirical from equivalents	
Max. and min. transmission	0.7458 and 0.6242	
Refinement method	full-matrix least-squares on F^2	
Data / restraints / parameters	7815 / 0 / 328	
Goodness-of-fit on F^2	1.065	
Final R indices [I>2σ(I)]	R1 = 0.0190, wR2 = 0.0377	
R indices (all data)	R1 = 0.0290, wR2 = 0.0408	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.358 and -0.797 $e.Å^{-3}$	

Computational Details

All calculations were performed using the Gaussian 16, Revision C.01 package of programs[1]. Geometry optimizations have been carried out at the PBE0-D3/def2-TZVP[2] level of theory. The optimized structure was confirmed to be a minimum on the potential energy surface by a subsequent frequency analysis (all positive eigenvalues).

xyz coordinates of optimized geometry of bis(di-*tert*-butylindenyl)germanocene, 2a:

Ge	-0.00000100	-0.00001000	0.03965300
C	2.20394700	0.41307700	1.10172700
C	-2.20397100	-0.41306300	1.10169800
C	2.12343500	-0.99340700	0.91732600
C	2.43422300	0.96495400	-0.20864400
C	2.34975000	1.12808200	2.42936900
C	-2.12343800	0.99341600	0.91728200
C	-2.43422600	-0.96495300	-0.20867100
C	-2.34980900	-1.12805300	2.42934400
H	1.97954200	-1.70163500	1.71961900
C	2.16591400	-1.33720800	-0.44542100
C	2.67715100	2.27936200	-0.65930500
C	2.39963500	-0.11275900	-1.15993800
C	3.78580200	1.65470200	2.55554000
C	2.09273600	0.16817700	3.58857000
C	1.36616800	2.29553500	2.54738800
H	-1.97955700	1.70165100	1.71957100
C	-2.16589000	1.33720500	-0.44546900
C	-2.39961200	0.11274900	-1.15997600
C	-2.67715000	-2.27936500	-0.65932100
C	-1.36621200	-2.29548800	2.54741200
C	-2.09285900	-0.16813000	3.58854500
C	-3.78585700	-1.65469500	2.55547200
C	2.10134500	-2.73657600	-1.01684100
H	2.72282500	3.10484400	0.03971200
C	2.87218900	2.51239700	-1.99614500
C	2.58937200	0.16968500	-2.52887700
H	3.92564200	2.15112200	3.52029700
H	4.50272800	0.83330600	2.48582500
H	4.02443400	2.37069800	1.76778100
H	2.16125900	0.70393700	4.53859200
H	1.09675800	-0.27708200	3.52791700
H	2.82667100	-0.64083000	3.60866000
H	1.52570000	2.83735900	3.48397400
H	1.47177800	3.00618500	1.72711400
H	0.33536200	1.93230100	2.53801200
C	-2.10130300	2.73656600	-1.01690000
C	-2.58932900	-0.16970900	-2.52891600
C	-2.87216600	-2.51241500	-1.99616100
H	-2.72283800	-3.10483900	0.03970500
H	-1.52578500	-2.83732100	3.48398600
H	-1.47176300	-3.00613300	1.72712600
H	-0.33541400	-1.93223400	2.53809600
H	-2.16141400	-0.70388200	4.53857000
H	-1.09688700	0.27714800	3.52793800
H	-2.82680900	0.64086400	3.60859600
H	-3.92572500	-2.15109500	3.52023500
H	-4.50279500	-0.83331300	2.48571000
H	-4.02444900	-2.37071300	1.76772100
C	3.46321000	-3.08953800	-1.62930400
C	1.78776000	-3.75012000	0.08144100
C	1.00969700	-2.84974400	-2.08683800
H	3.06812500	3.52119600	-2.34151800
C	2.82433600	1.45893800	-2.93085700
H	2.56779600	-0.62475000	-3.26370900
C	-1.00963200	2.84972000	-2.08687500
C	-1.78773800	3.75012000	0.08138000
C	-3.46315400	3.08953100	-1.62939300
H	-2.56773300	0.62471500	-3.26375700
C	-2.82429300	-1.45896700	-2.93088400
H	-3.06809900	-3.52121800	-2.34152600
H	3.44390000	-4.10315300	-2.04015600
H	3.73346800	-2.40341700	-2.43359900
H	4.25023900	-3.04097300	-0.87286800
H	1.72445500	-4.75347200	-0.34692500
H	2.56397200	-3.76520800	0.85073900
H	0.83061300	-3.52937300	0.56180900
H	1.01576100	-3.85180400	-2.52604000
H	0.02036800	-2.67589800	-1.65656400
H	1.14504000	-2.13006100	-2.89425400
H	2.98185100	1.67350100	-3.98169100
H	-1.01568900	3.85177200	-2.52609500
H	-0.02031400	2.67588500	-1.65657400
H	-1.14495500	2.13002200	-2.89428100
H	-1.72441800	4.75346700	-0.34699500
H	-2.56396800	3.76521900	0.85065900
H	-0.83060400	3.52937400	0.56177400
H	-3.44382900	4.10314200	-2.04025400
H	-3.73340000	2.40340500	-2.43368800
H	-4.25019900	3.04097800	-0.87297400
H	-2.98179200	-1.67354100	-3.98171900

References

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