Electronic Supplementary Information for Dalton Transactions

Supporting information

for

Synthesis and theoretical studies on rare three-coordinate lead complexes

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Figure S1. Thermal ellipsoid plot (30%) of 3. H atoms omitted for clarity.

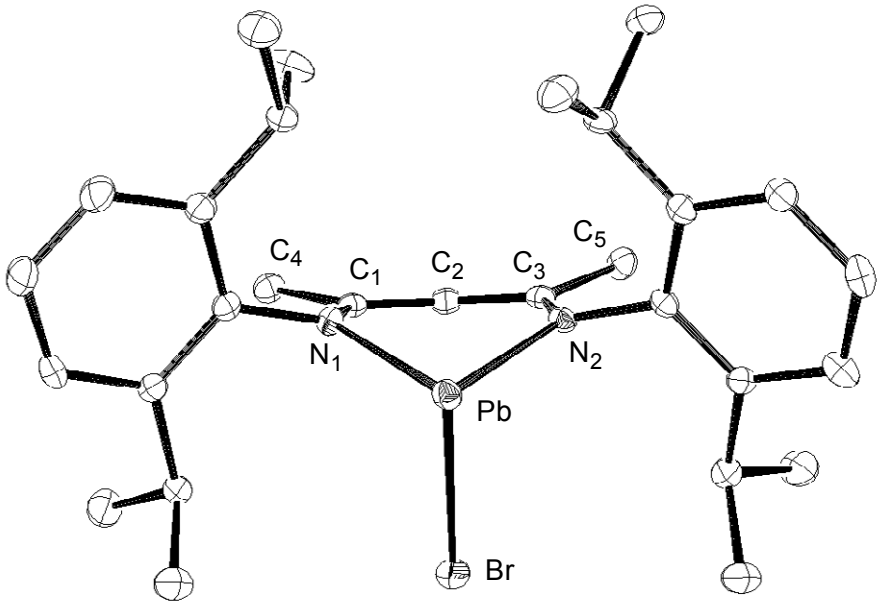

Figure S2. Temperature dependent NMR spectra of **5** showing the change in resonances corresponding to the (NSiMe3) protons.

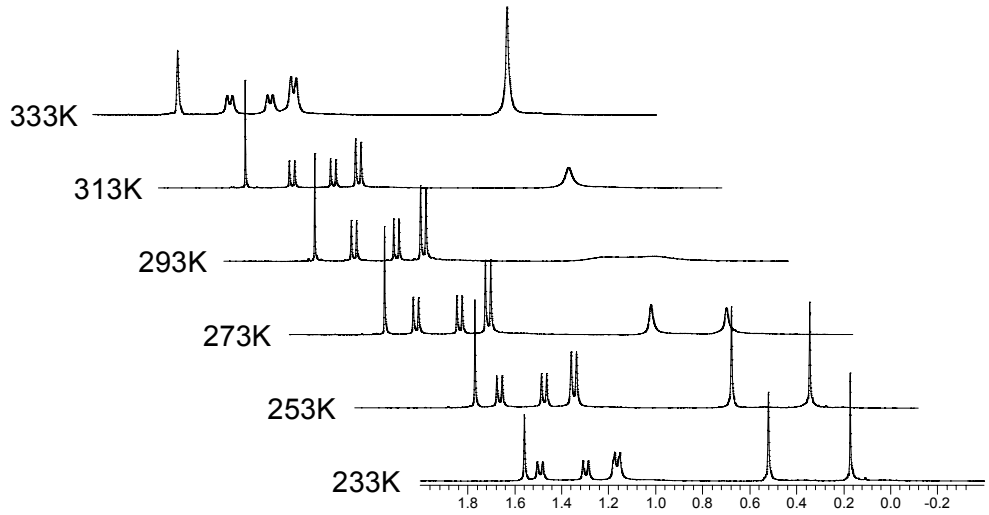

Table S1. Distance between Pb and the C_3N_2 plane as determined using DFT calculations (see text) for both [{N(Me)C(Me)}$_2$CH]PbX and [{N(C_6H_5)C(Me)}$_2$CH]PbX (X = Cl, Br, I).

	[{N(Me)C(Me)}$_2$CH]$^-$			[{N(C_6H_5)C(Me)}$_2$CH]$^-$		
	LPbCl	LPbBr	LPbI	LPbCl	LPbBr	LPbI
Pb-C_3N_2 plane	0.042	0.078	0.025	0.221	0.307	0.473

Figure S3. Optimised geometry for [{N(Me)C(Me)}$_2$CH]PbCl. H atoms omitted for clarity.

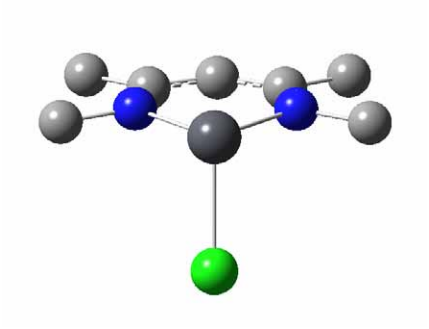

Figure S4. Optimised geometry for [{N(Me)C(Me)}$_2$CH]PbBr. H atoms omitted for clarity.

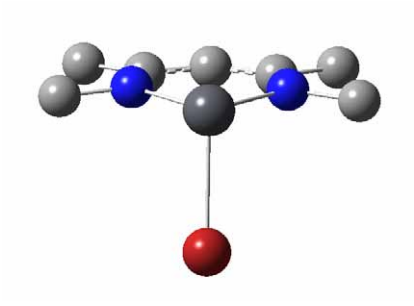

Figure S5. Optimised geometry for [{N(Me)C(Me)}$_2$CH]PbI. H atoms omitted for clarity.

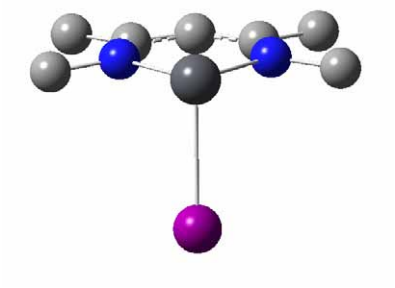

Figure S6. Optimised geometry for [{N(C_6H_5)C(Me)}$_2$CH]PbCl. H atoms omitted for clarity.

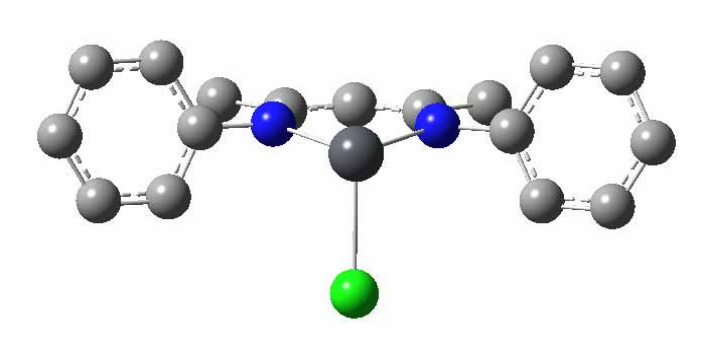

Figure S7. Optimised geometry for [{N(C_6H_5)C(Me)}$_2$CH]PbBr. H atoms omitted for clarity.

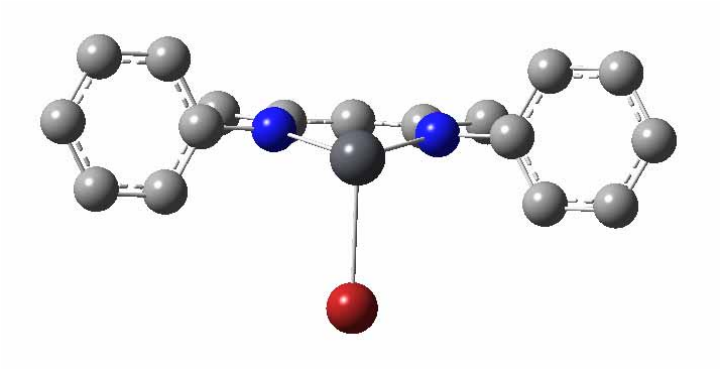

Figure S8. Optimised geometry for [{N(C_6H_5)C(Me)}$_2$CH]PbI. H atoms omitted for clarity.

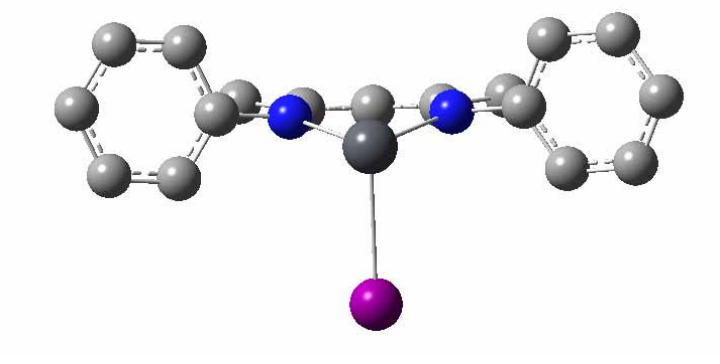

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Figure S9. ^{1}H NMR spectrum of compound **1**

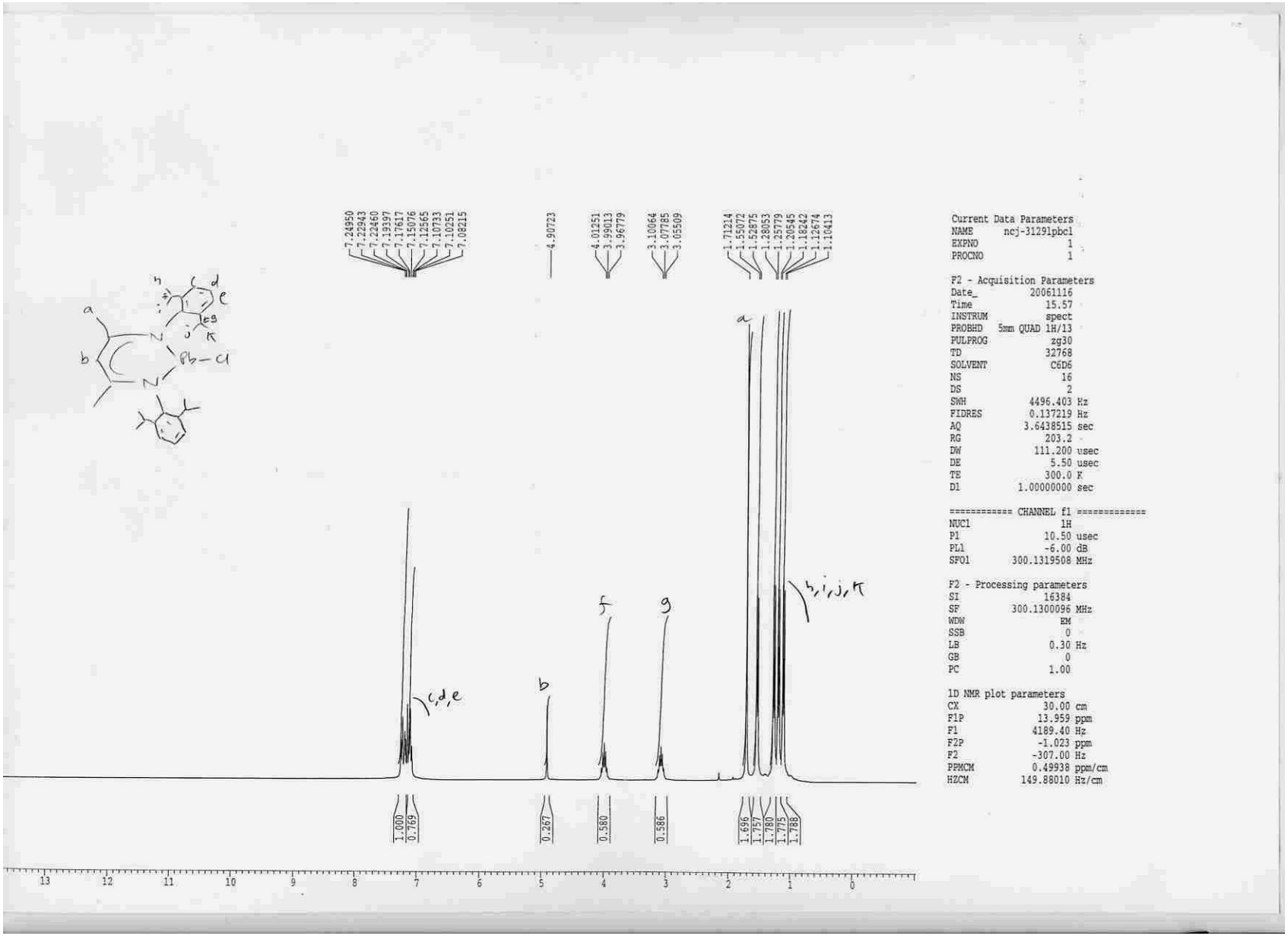
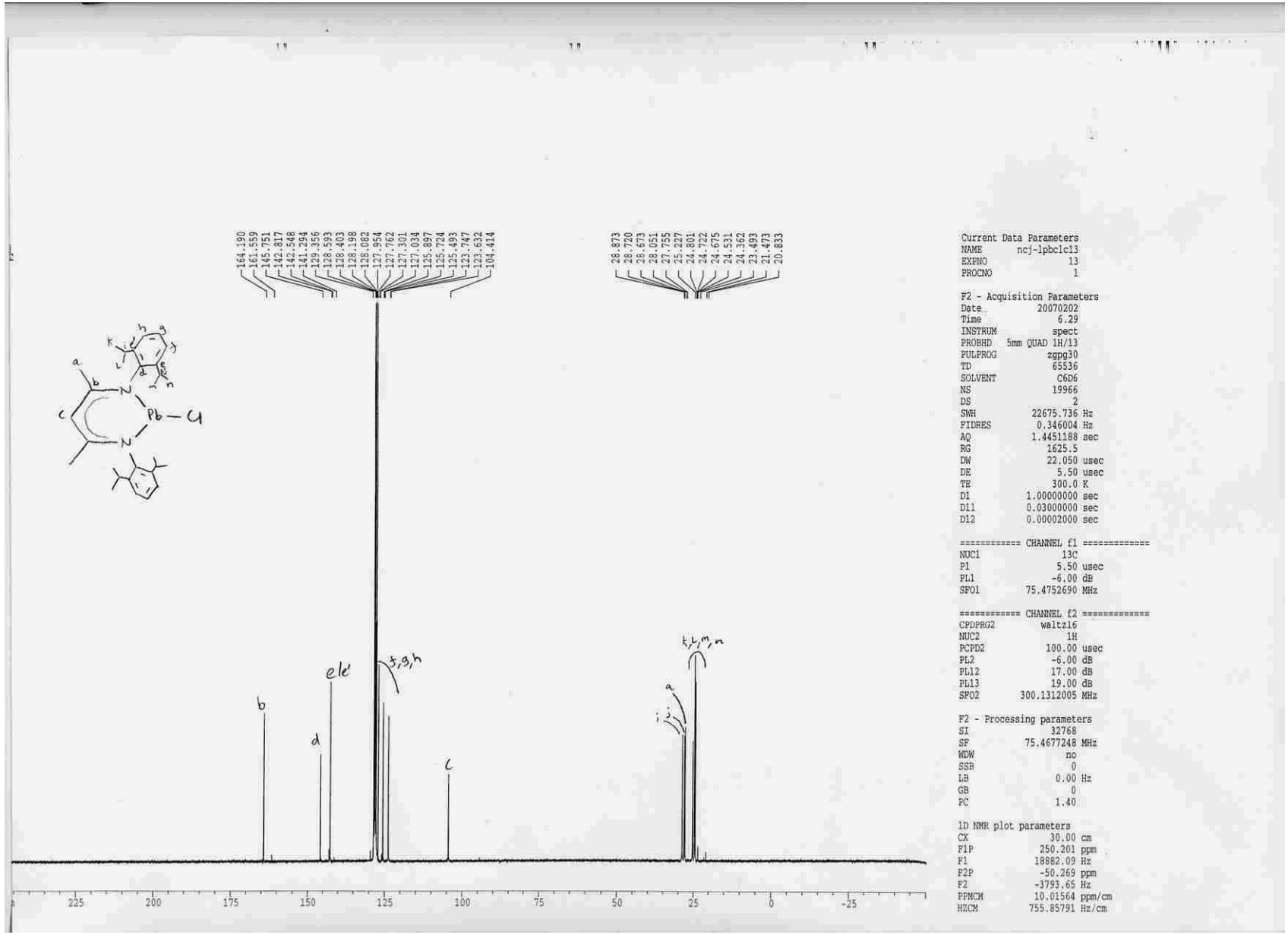


Figure S10. ^{13}C NMR spectrum of compound **1**



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PROCNO 1

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FIDRES 0.346004 Hz
AQ 1.4451188 sec
RG 1625.5
DW 22.050 usec
DE 5.50 usec
TE 300.0 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec

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P1 5.50 usec
PL1 -6.00 dB
SFO1 75.4752690 MHz

============ CHANNEL f2 =============
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PL12 17.00 dB
PL13 19.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
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GB 0
PC 1.40

1D NMR plot parameters
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F2 -3793.65 Hz
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HZCM 755.85791 Hz/cm