Electronic Supplementary Information

Alkali metal salts of ditopic carbanionic carbenes as

reagents for the synthesis of novel complexes of group 12

and 14 metals

Jordan B. Waters and Jose M. Goicoechea*

Department of Chemistry, University of Oxford, Chemistry Research Laboratory, Mansfield

Road, Oxford OX1 3TA, U.K.

CONTENTS

1. NMR spectra

2. ESI-MS spectra

1. NMR data

¹ H NMR data (ppm)	KIPr	1	2	3	4
$C_6\underline{H}_3\{CH(CH_3)\}_2$	7.13 (1H)	7.21 (1H)	7.21 (1H)	7.20 (1H)	7.21 (1H)
	7.09 (2H)	7.13 (2H)	7.14 (3H)	7.14 (2H)	7.14 (2H)
	7.05 (3H)	7.11 (3H)	7.10 (2H)	7.11 (3H)	7.11 (3H)
NCC <u>H</u> N	6.07 (1H)	6.92 (1H)	7.01 (1H)	6.83 (1H)	7.00 (1H)
$C_6H_3\{C\underline{H}(CH_3)\}_2$	3.28 (2H)	3.23 (2H)	3.26 (2H)	3.48 (2H)	3.19 (2H)
	3.04 (2H)	3.03 (2H)	3.06 (2H)	3.08 (2H)	3.06 (2H)
$C_6H_3\{CH(C\underline{H}_3)\}_2$	1.12 (6H)	1.28 (6H)	1.30 (6H)	1.32 (6H)	1.30 (6H)
	1.10 (6H)	1.16 (6H)	1.17 (6H)	1.16 (6H)	1.17 (6H)
	1.08 (12H)	1.10 (12H)	1.10 (6H)	1.12 (6H)	1.11 (12H)
			1.09 (6H)	1.06 (6H)	
$N{Si(C\underline{H}_3)_3}_2$	N.A.	-0.08 (36H)	0.04 (36H)	0.03 (36H)	0.12 (36H)
¹³ C NMR data (ppm)					
<u><u>C</u>N₂</u>	215.1	219.9	218.7	219.7	216.1
N <u>C</u> CHN	176.3	152.6	163.2	157.1	143.4
$\underline{\mathbf{C}}_{6}\mathrm{H}_{3}\mathrm{\{CH(CH_{3})\}_{2}}$	149.5	147.5	147.5	147.5	147.6
	143.8	146.6	147.1	147.1	147.2
	147.2	142.0	143.7	142.9	127.9
	146.8	133.2	141.7	142.0	127.6
	126.5	127.8	130.4	128.3	123.4
	125.7	126.9	127.8	127.8	123.3
	123.0	123.4	123.4	123.3	
	122.7	123.3	123.2	123.2	
NC <u>C</u> HN	126.8	145.4	127.3	127.0	135.4
$C_6H_3\{\underline{C}H(CH_3)\}_2$	28.7	29.1	29.5	29.9	29.1
	28.6	28.7	28.6	28.7	28.6
$C_6H_3\{CH(\underline{C}H_3)\}_2$	25.5	27.1	27.3	27.8	26.9
	25.4	25.2	25.5	25.5	25.6
	24.5	24.7	24.8	24.6	24.8
	24.0	23.5	23.3	22.8	24.1
$N{Si(\underline{C}H_3)_3}_2$		7.1	7.6	7.5	7.8

Table S1. Comparison of ¹H and ¹³C{¹H} NMR data for **KIPr** and compounds 1–4.



Figure S1. ¹H NMR spectrum of KIPr in d_8 -THF.



Figure S2. ¹³C NMR spectrum of KIPr in d_8 -THF.



Figure S3. ¹H NMR spectrum of [K(2,2,2-crypt)][1] in d_8 -THF.



Figure S4. ¹³C NMR spectrum of [K(2,2,2-crypt)][1] in d_8 -THF.



Figure S5. ¹H NMR spectrum of [K(18-crown-6)][2] in d_8 -THF.



Figure S6. ¹³C NMR spectrum of [K(18-crown-6)][2] in d_8 -THF.



Figure S7. ¹H NMR spectrum of [K(18-crown-6)][3] in d_8 -THF.



Figure S8. ¹³C NMR spectrum of [K(18-crown-6)][3] in d_8 -THF.



Figure S9. ¹H NMR spectrum of [K(18-crown-6)][4] in d_8 -THF.



Figure S10. ¹³C NMR spectrum of [K(18-crown-6)][4] in d_8 -THF.



Figure S11. ¹H NMR spectrum of [K(18-crown-6)][5] in d_8 -THF.



Figure S12. ¹³C NMR spectrum of [K(18-crown-6)][5] in d_8 -THF.



Figure S11. ¹H NMR spectrum of [K(18-crown-6)][6] in d_8 -THF.



Figure S12. ¹³C NMR spectrum of [K(18-crown-6)][6] in d_8 -THF.

2. ESI-MS data



Figure S13. Negative ion-mode ESI-MS spectrum for **KIPr** run in THF. Experimental (red) and calculated (blue) isotopic distributions pictured in the inset.



Figure S14. Negative ion-mode ESI-MS spectrum for [K(2,2,2-crypt)][1] run in THF. Experimental (red) and calculated (blue) isotopic distributions pictured in the insets.



Figure S15. Negative ion-mode ESI-MS spectrum for [K(18-crown-6)][**2**] run in THF. Experimental (red) and calculated (blue) isotopic distributions pictured in the inset.



Figure S16. Negative ion-mode ESI-MS spectrum for [K(18-crown-6)][**3**] run in THF. Experimental (red) and calculated (blue) isotopic distributions pictured in the insets.



Figure S17. Negative ion-mode ESI-MS spectrum for [K(18-crown-6)][4] run in THF. Experimental (red) and calculated (blue) isotopic distributions pictured in the insets.



Figure S17. Negative ion-mode ESI-MS spectrum for [K(18-crown-6)][**5**] run in THF. Experimental (red) and calculated (blue) isotopic distributions pictured in the inset.



Figure S18. Negative ion-mode ESI-MS spectrum for [K(18-crown-6)][6] run in THF. Experimental (red) and calculated (blue) isotopic distributions pictured in the inset.