

Supporting Information

Loss of chirality through facile Lewis base mediated aza-enolate formation in Na and K (*S*)-*N*-(α -methylbenzyl)methallylamides

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Table S1 Summary of crystallographic data for compounds **1** and **2**

Compound	1	2
Chemical formula	C ₇₂ H ₉₀ Li ₁₂ N ₆	C ₂₄ H ₃₂ N ₂ Na ₂
Formula mass (g/mol)	1122.78	394.50
Crystal system	Trigonal	Monoclinic
<i>a</i> (Å)	25.7286(5)	11.4543(6)
<i>b</i> (Å)	25.7286(5)	11.3694(7)
<i>c</i> (Å)	8.9644(2)	8.8489(5)
α (°)	90	90
β (°)	90	103.044(4)
γ (°)	120	90
Unit cell volume (Å ³)	5139.06(18)	1122.64(11)
Temperature (K)	123(2)	123(2)
Space group	R3	P2 ₁ /c
No. of formula units per unit cell, <i>Z</i>	3	2
No. of reflections measured	18469	10457
No. of independent reflections	4001	3178
R _{int}	0.0274	0.0175
Final R ₁ values (<i>I</i> >2σ(<i>I</i>))	0.0305	0.0413
Final wR(<i>F</i> ²) values (<i>I</i> >2σ(<i>I</i>))	0.0812	0.1096
Final R ₁ values (all data)	0.0314	0.0461
Final wR(<i>F</i> ²) values (all data)	0.0821	0.1137

1 [PhCH(CH₃)N(CH₂C{CH₃}=CHLi)Li]₆**2** [PhC(=CH₂)N(CH₂CH{CH₃}₂)Na].._∞

Compound 1 - [PhCH(CH₃)N(CH₂C{CH₃}=CHLi)Li]₆

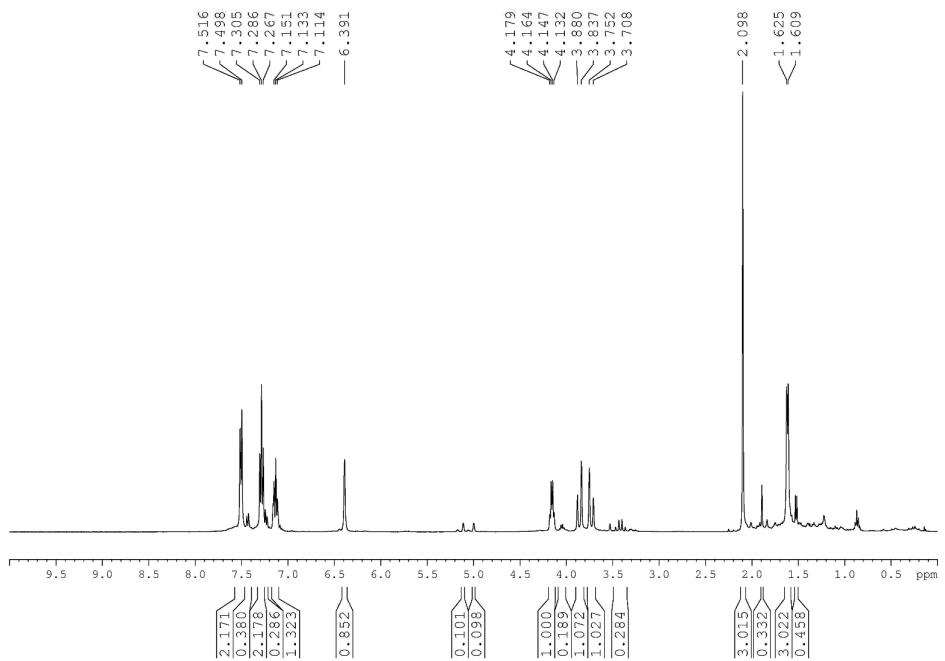


Figure S1 ¹H NMR spectrum of compound 1

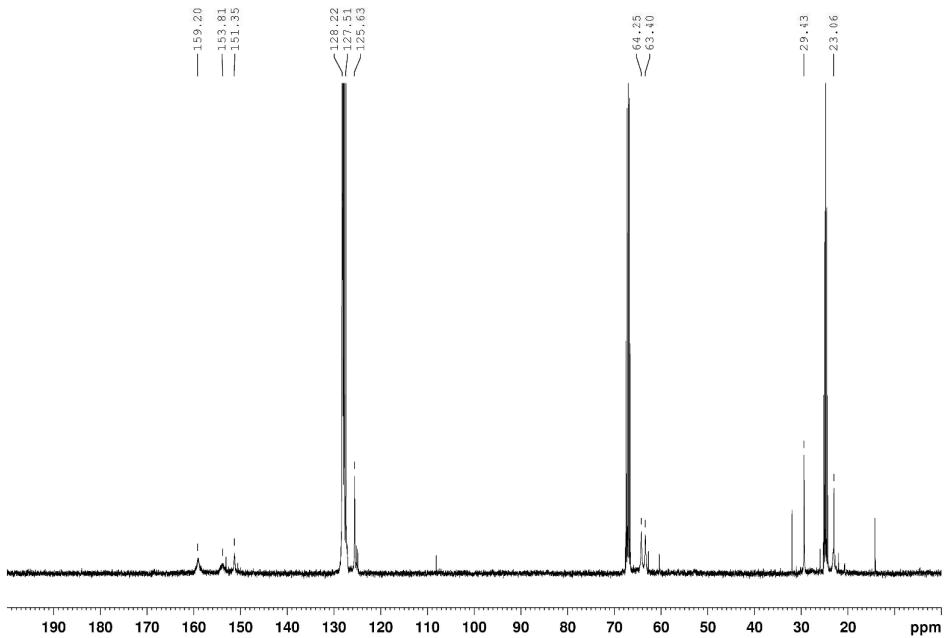


Figure S2 ¹³C NMR spectrum of compound 1

Compound 2 - [PhC(=CH₂)N(CH₂CH{CH₃}₂)Na]_∞

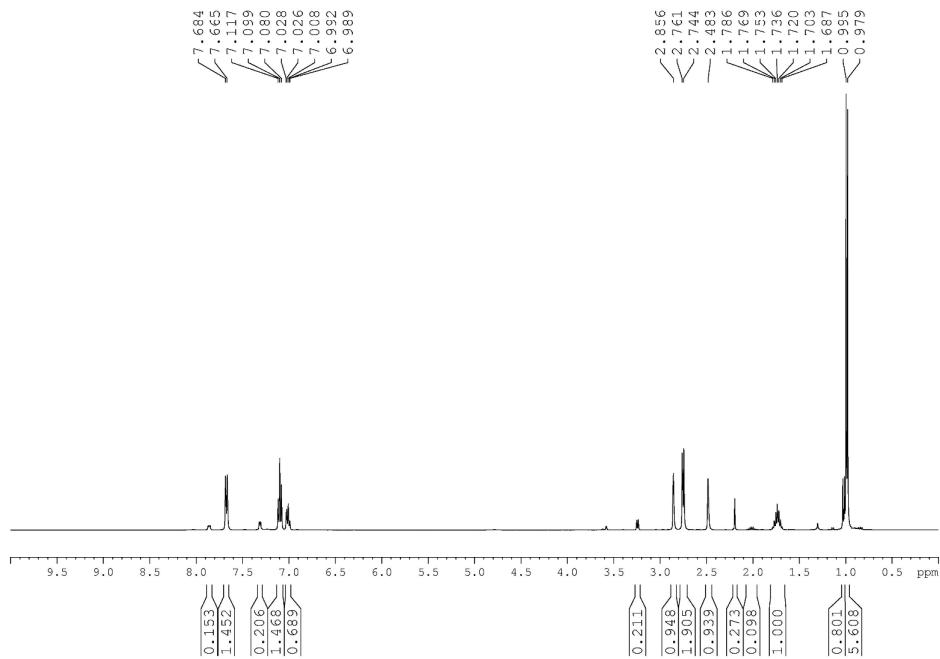


Figure S3 ¹H NMR spectrum of compound 2

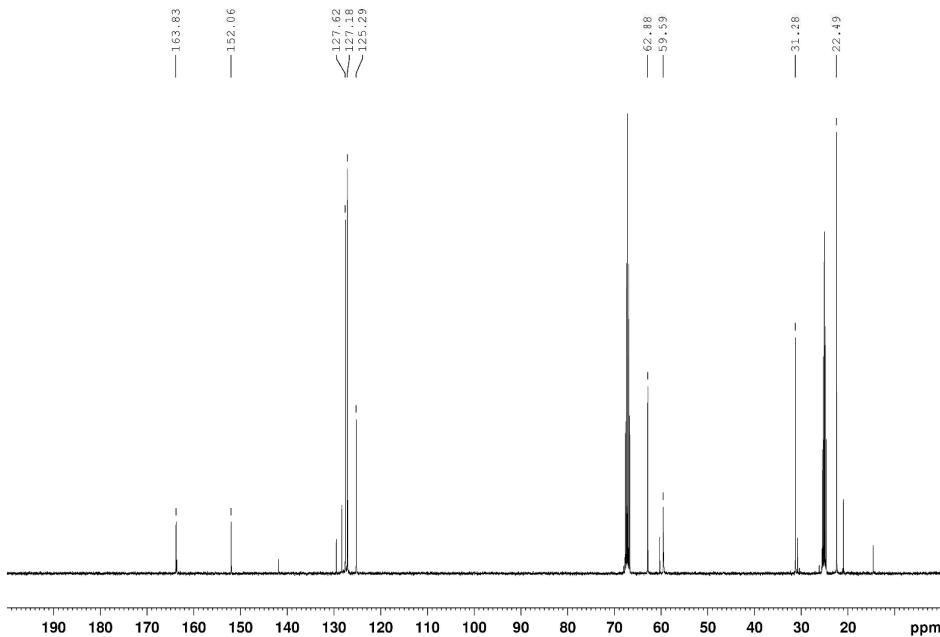


Figure S4 ¹³C NMR spectrum of compound 2

Compound 3 - $[\text{PhC}(=\text{CH}_2)\text{N}(\text{CH}_2\text{CH}\{\text{CH}_3\}_2)\text{Na}\cdot\text{TMEDA}]_n$

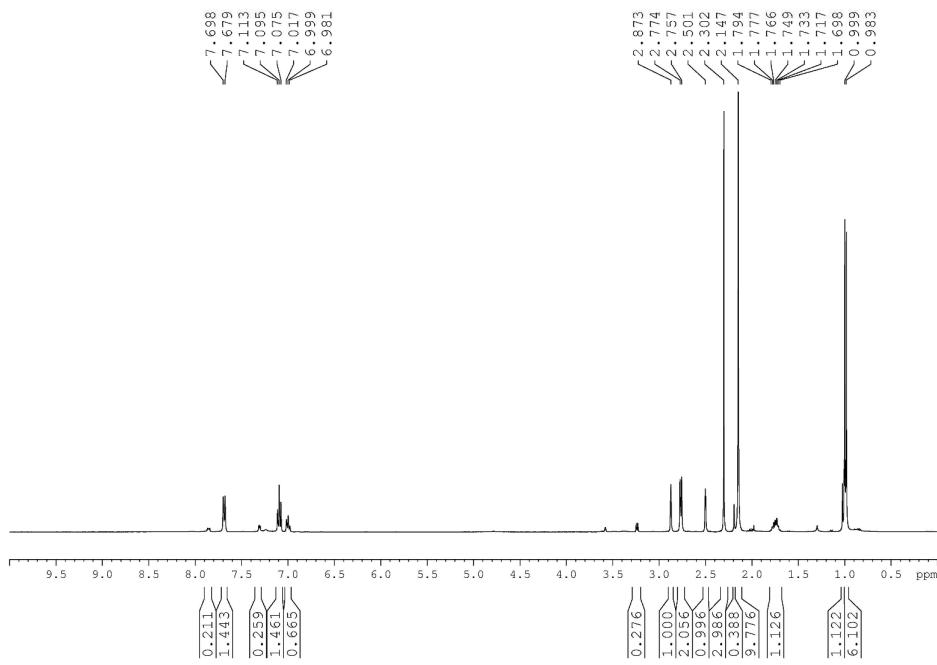


Figure S5 ^1H NMR spectrum of compound 3

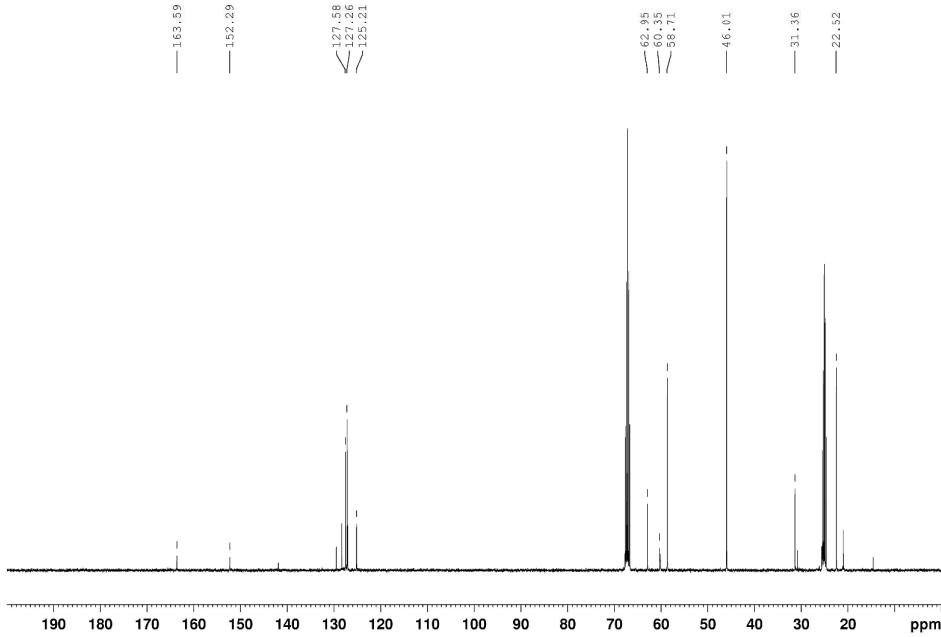


Figure S6 ^{13}C NMR spectrum of compound 3

Compound 4 - [PhC(=CH₂)N(CH₂CH{CH₃}₂)Na·PMDETA]_n

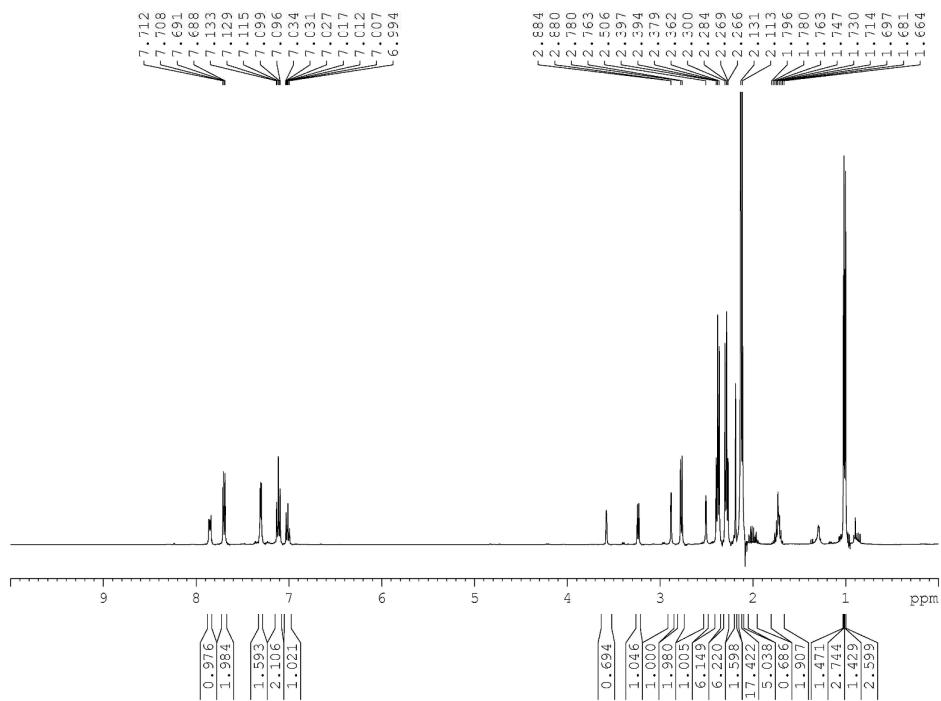


Figure S7 ^1H NMR spectrum of compound 4

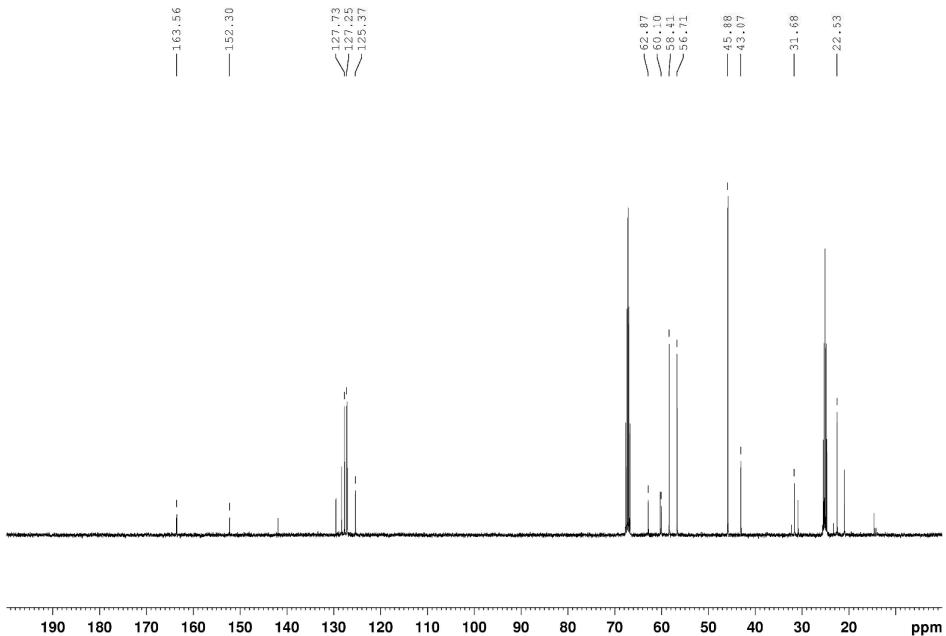


Figure S8 ^{13}C NMR spectrum of compound 4

Compound 5 - $[\text{PhC}(=\text{CH}_2)\text{N}(\text{CH}_2\text{CH}\{\text{CH}_3\}_2)\text{K}]_n$

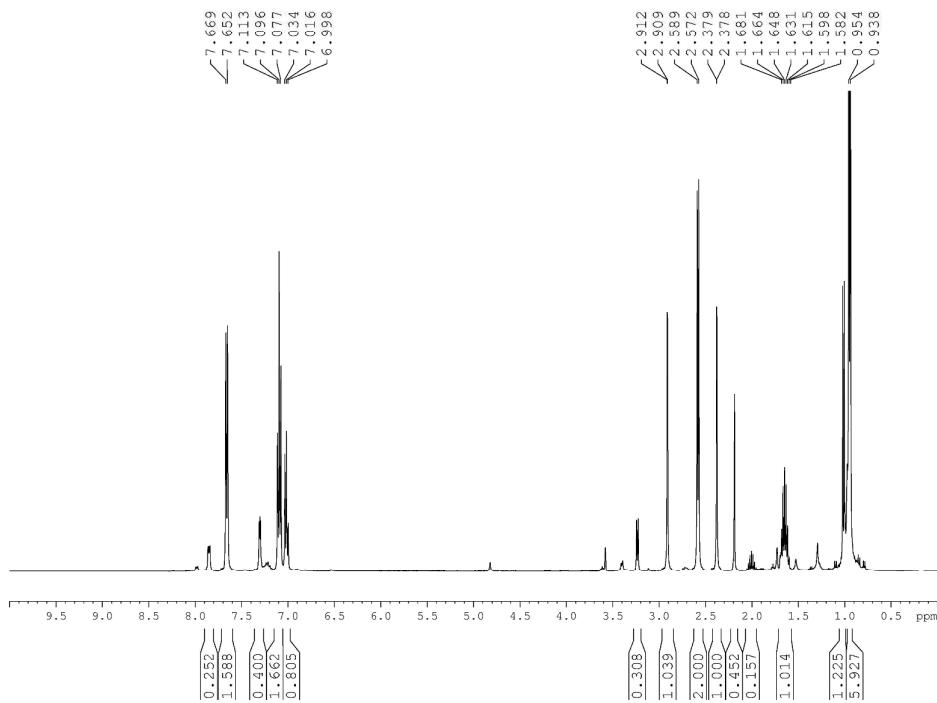


Figure S9 ^1H NMR spectrum of compound 5

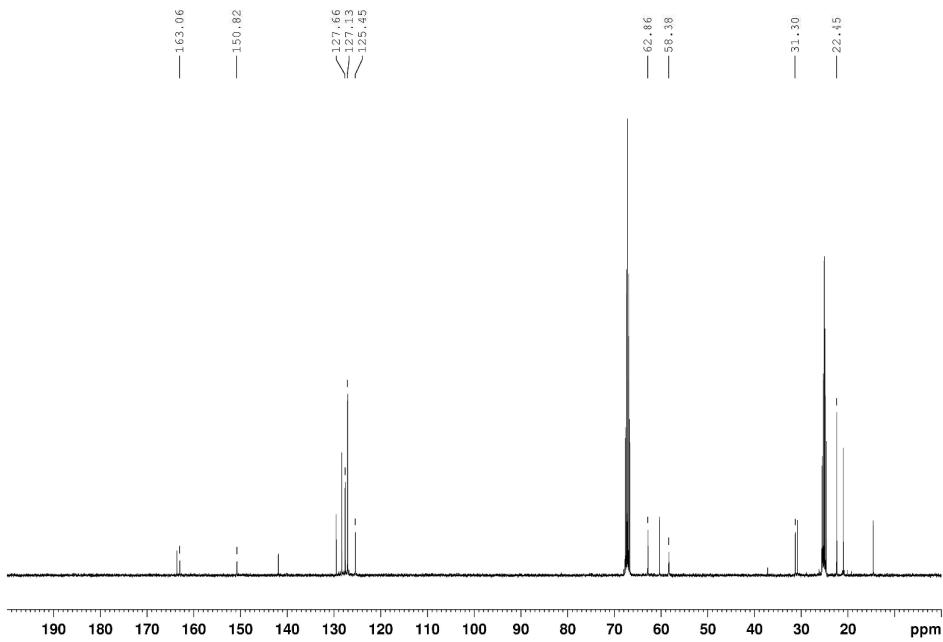


Figure S10 ^{13}C NMR spectrum of compound 5

Compound 6 - [PhCH(CH₃)N(CH=C{CH₃}₂)Na]_n

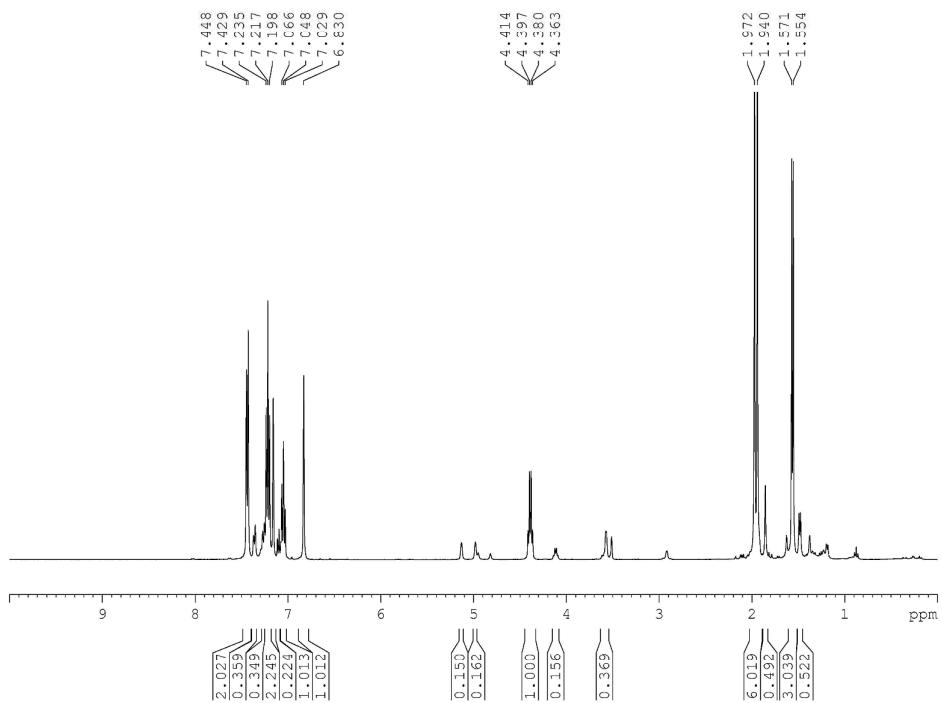


Figure S11 ¹H NMR spectrum of compound 6

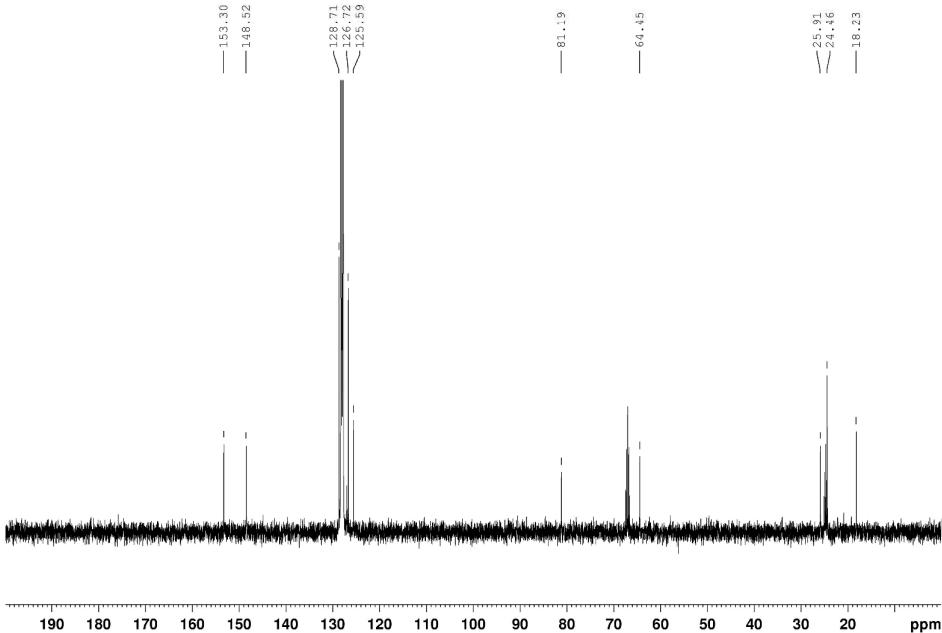


Figure S12 ¹³C NMR spectrum of compound 6

Compound 7 - [PhCH(CH₃)N(CH=C(CH₃)₂)K]_n

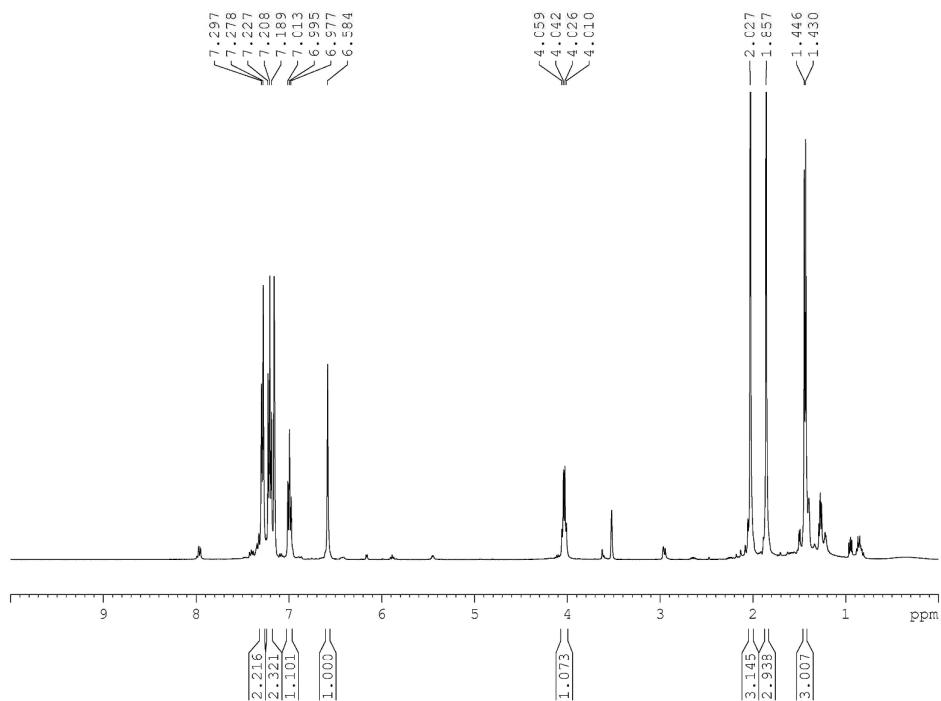


Figure S13 ^1H NMR spectrum of compound 7

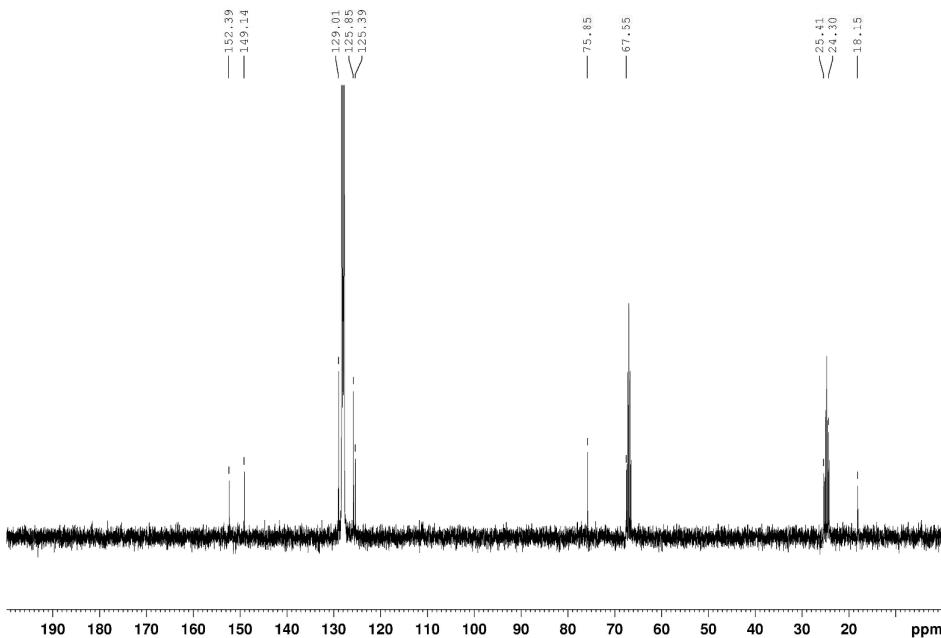


Figure S14 ^{13}C NMR spectrum of compound 7

Compound 8 - [PhC(CH₃)N(=CHCH{CH₃}₂)K]_n

The relevant signals are outlined in black.

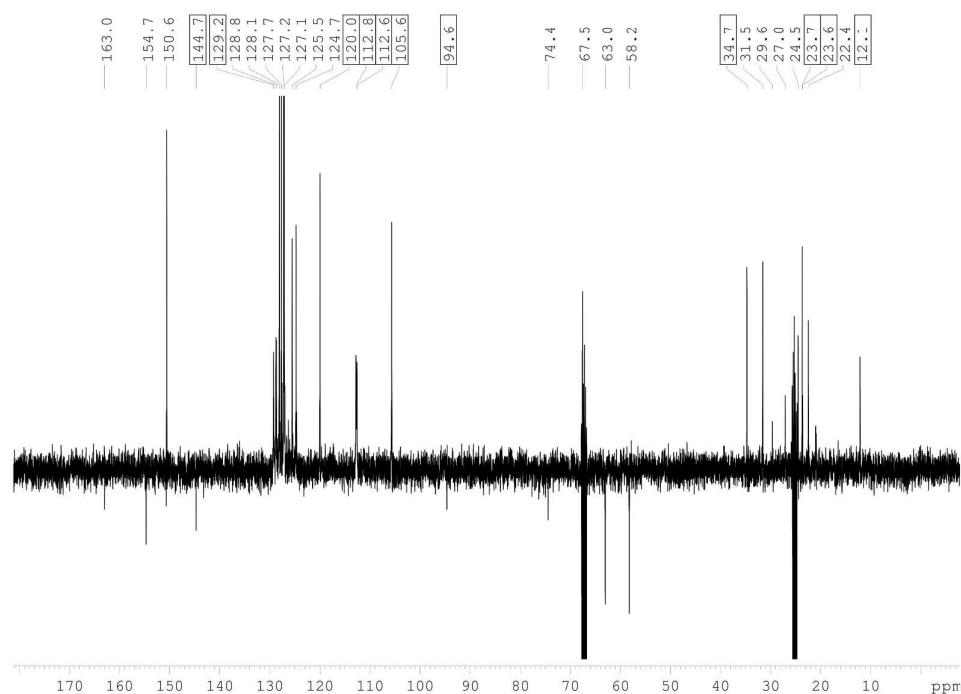


Figure S15 ¹H NMR spectrum of compound 8

Table S2 Summary of ¹H NMR spectral data for compounds 2 – 5

Compound	para-H	meta-H	ortho-H	=CH ₂	N-CH ₂ -	-CH-	-(CH ₃) ₂
2	7.01	7.10	7.68	2.86 2.48	2.75	1.74	0.99
3	7.00	7.09	7.69	2.87 2.50	2.77	1.75	0.99
4	7.01	7.11	7.70	2.88 2.51	2.77	1.73	1.01
5	7.02	7.10	7.66	2.91 2.38	2.58	1.65	0.95

- 2** [PhC(=CH₂)N(CH₂CH{CH₃}₂)Na]_∞
3 [PhC(=CH₂)N(CH₂CH{CH₃}₂Na)·TMEDA]_n
4 [PhC(=CH₂)N(CH₂CH{CH₃}₂Na)·PMDETA]_n
5 [PhC(=CH₂)N(CH₂CH{CH₃}₂)K]_n