

**Lithium, sodium and potassium picolyl complexes: syntheses, structures
and bonding**

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SUPPORTING INFORMATION

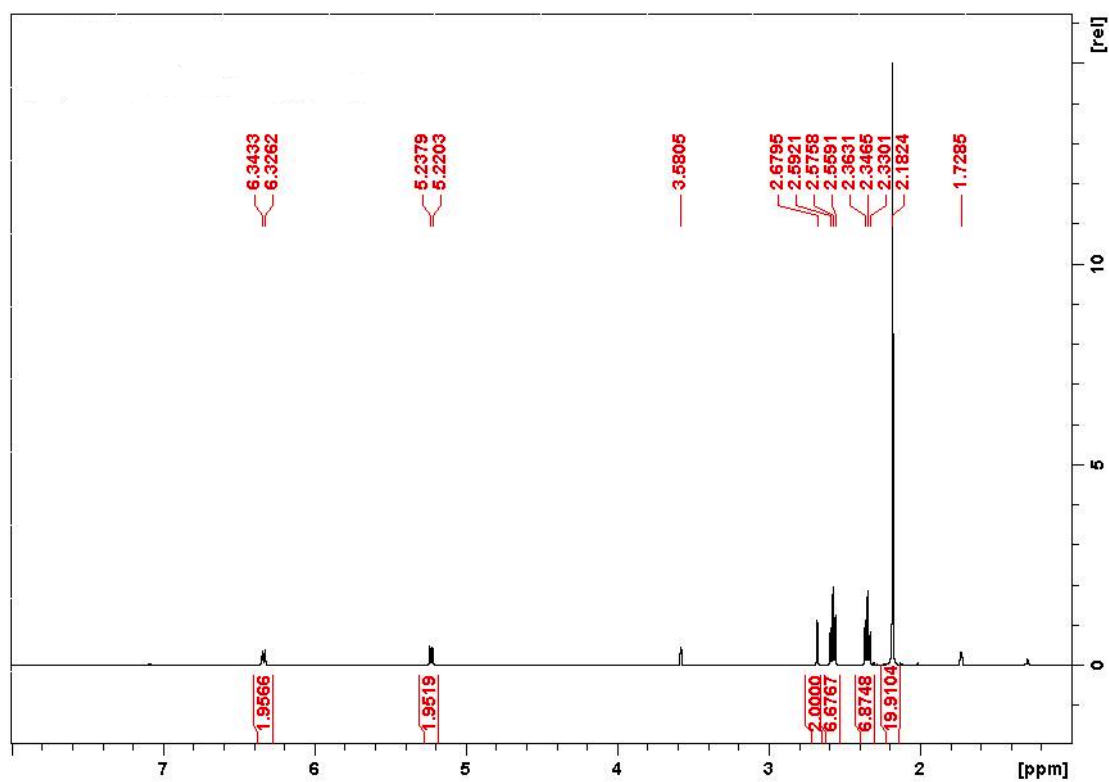


Fig S1 ^1H NMR spectrum of complex **1** in $\text{d}_8\text{-THF}$

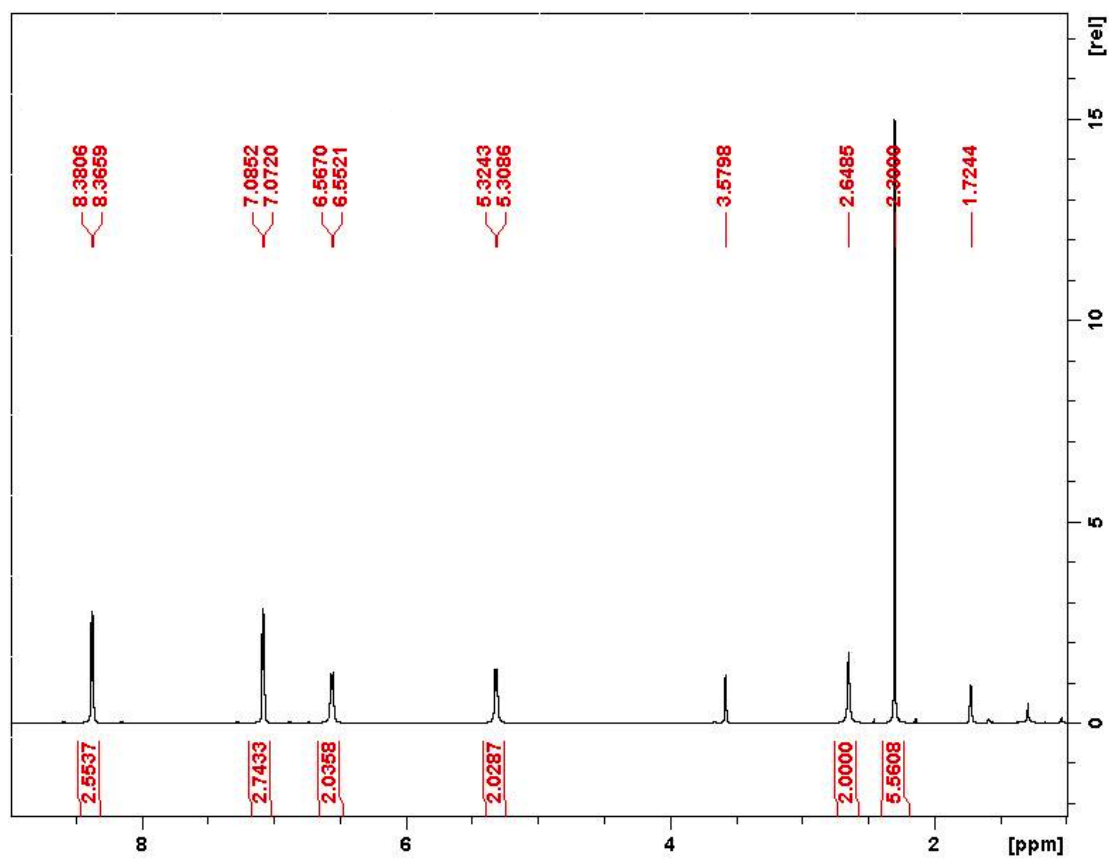


Fig S2 ^1H NMR spectrum of complex **3** in $\text{d}_8\text{-THF}$

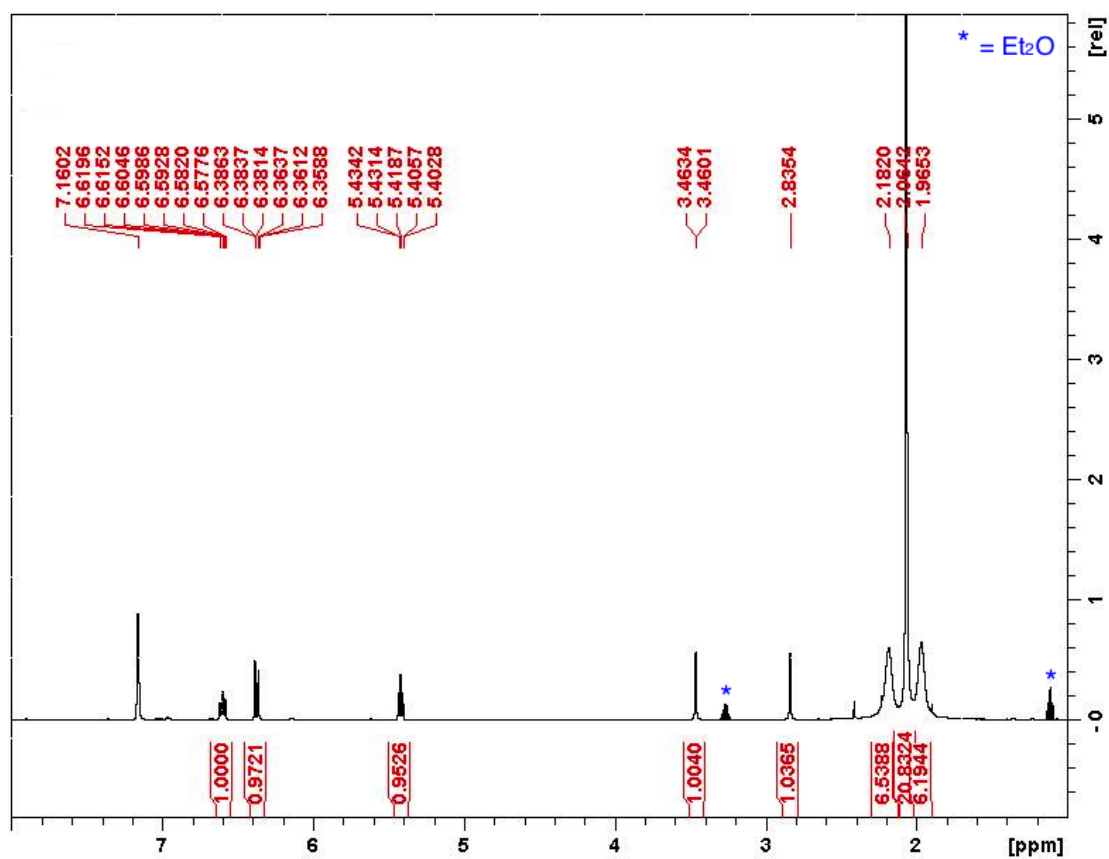


Fig S3 ¹H NMR spectrum of complex 4 in C₆D₆

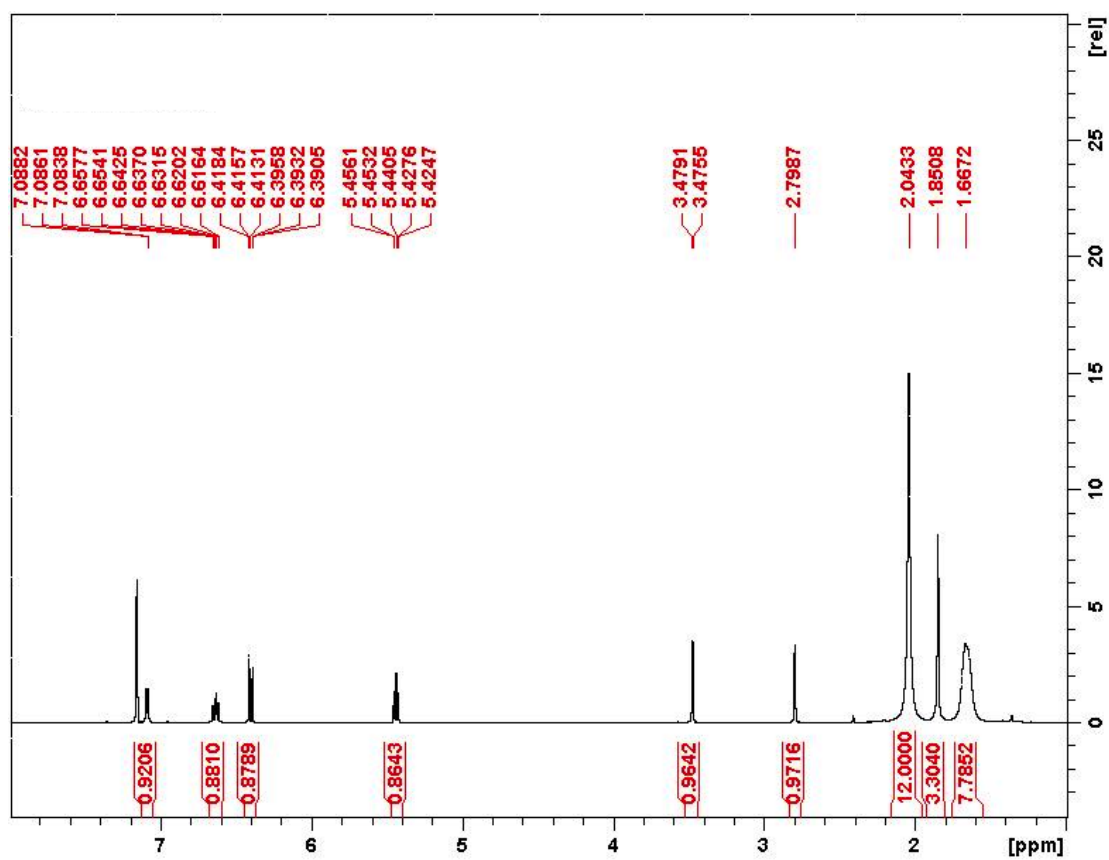


Fig S4 ¹H NMR spectrum of complex 4' in C₆D₆

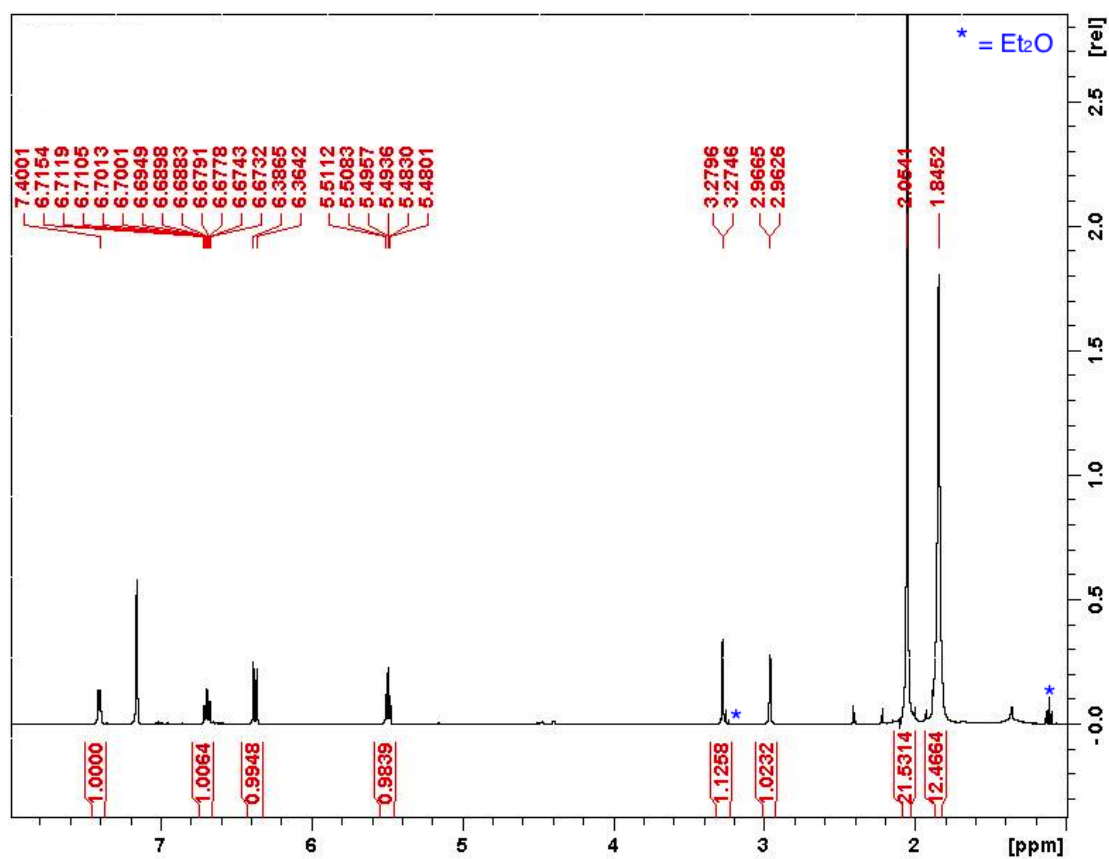


Fig S5 ^1H NMR spectrum of complex **5** in C_6D_6

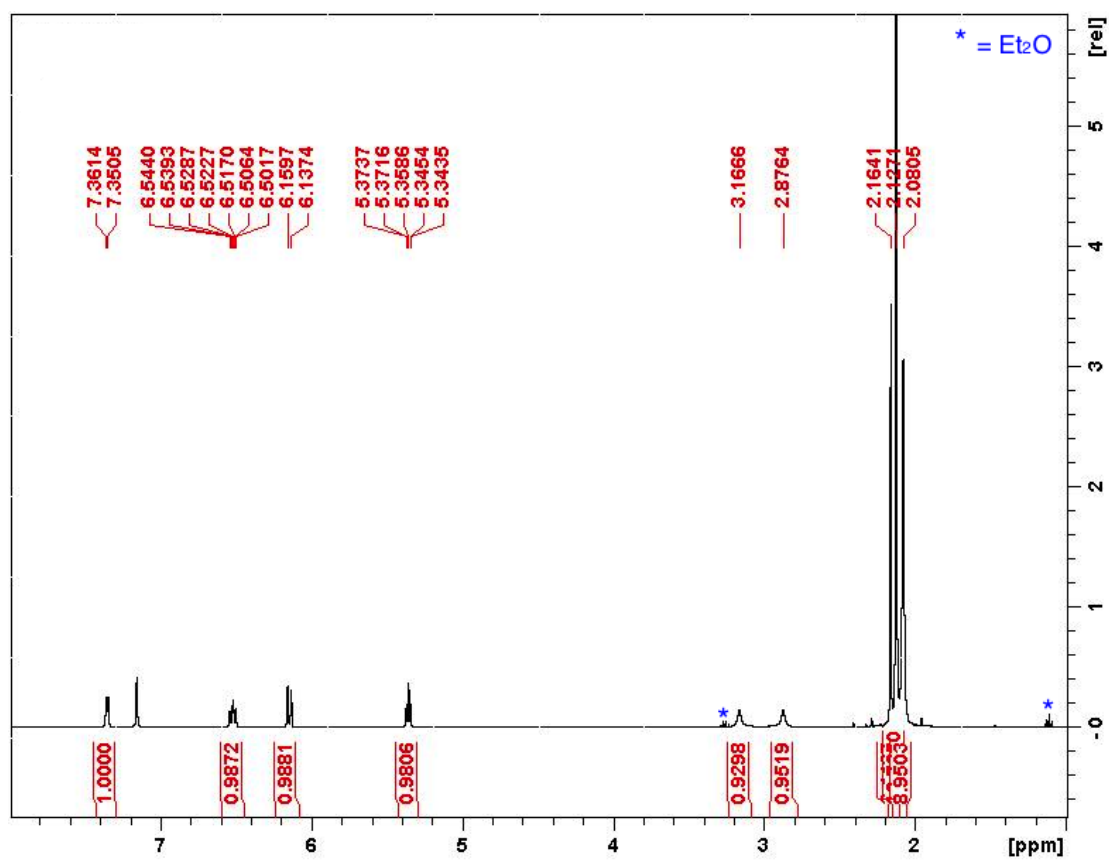


Fig S6 ^1H NMR spectrum of complex **6** in C_6D_6

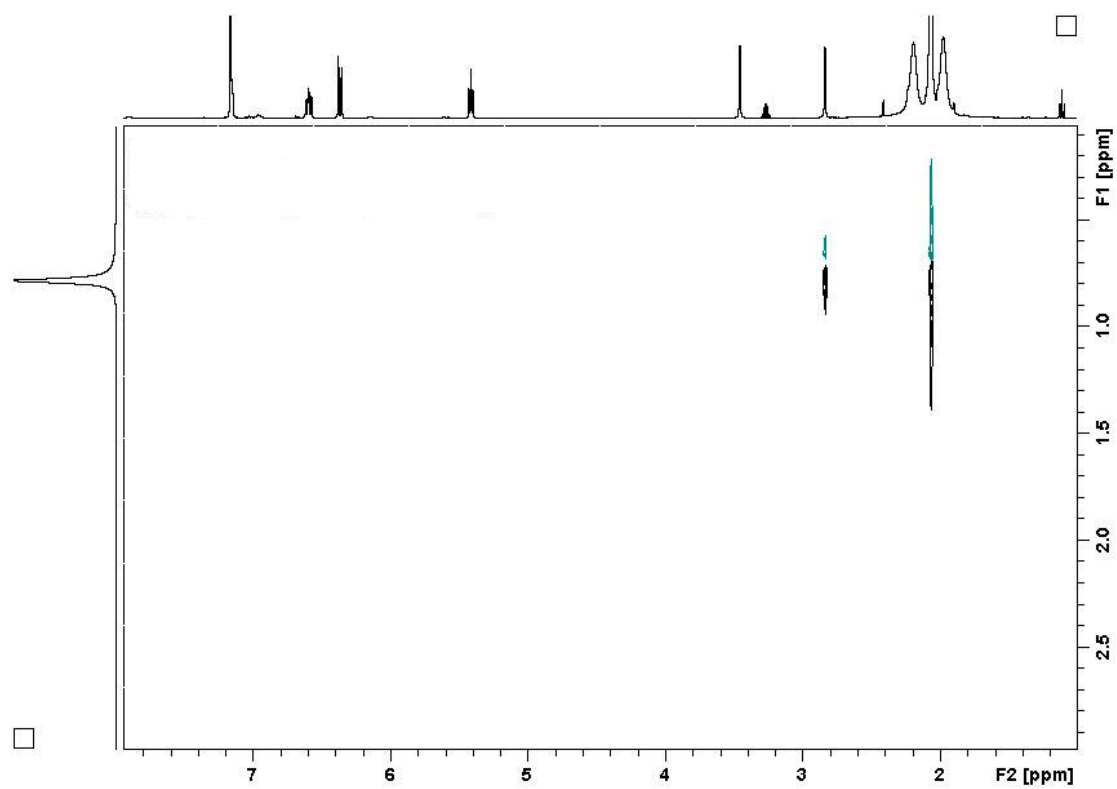


Fig S7 ^1H - ^7Li HOESY NMR spectrum of complex **4** in C_6D_6

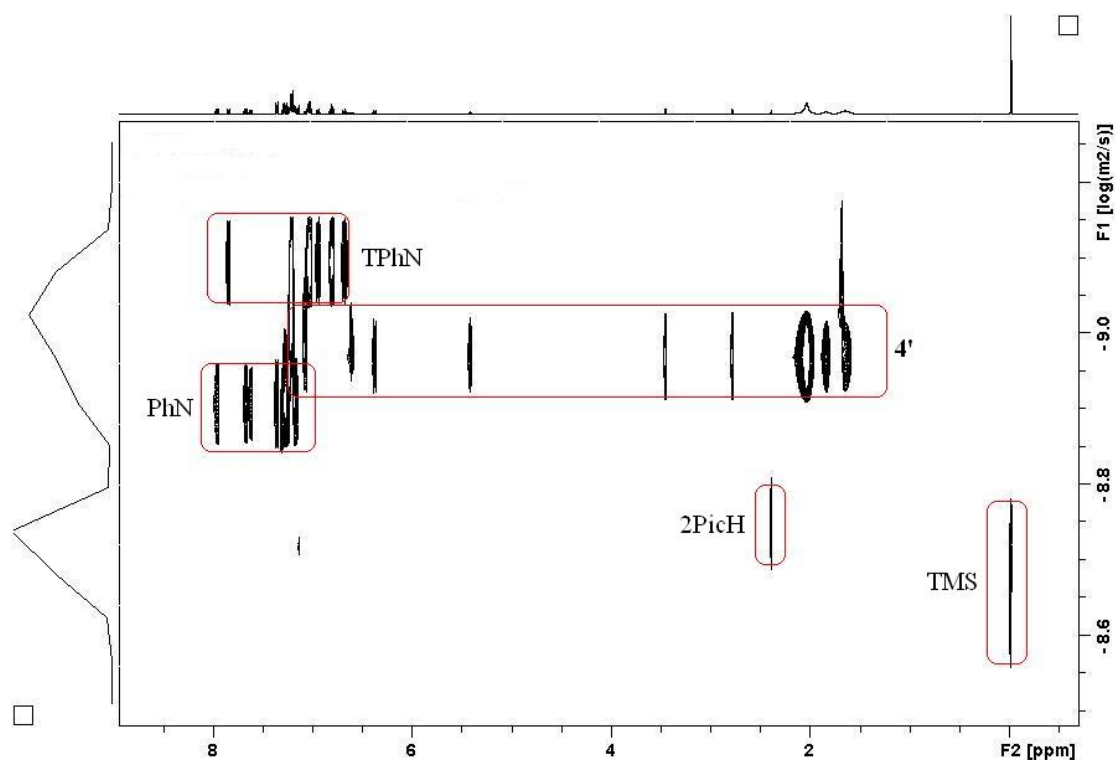


Figure S8 ^1H DOSY NMR spectrum of complex **4'** in C_6D_6 solution at 300 K in the presence of inert standards 1,2,3,4-tetraphenylnaphthalene (TPhN), 1-phenylnaphthalene (PhN) and tetramethylsilane (TMS).

Graph S1 Plot of $\log D$ versus $\log FW$ from the ^1H DOSY NMR data obtained for the mixture of **4'** and the inert standards TPhN, PhN and TMS in C_6D_6 solution at 300K

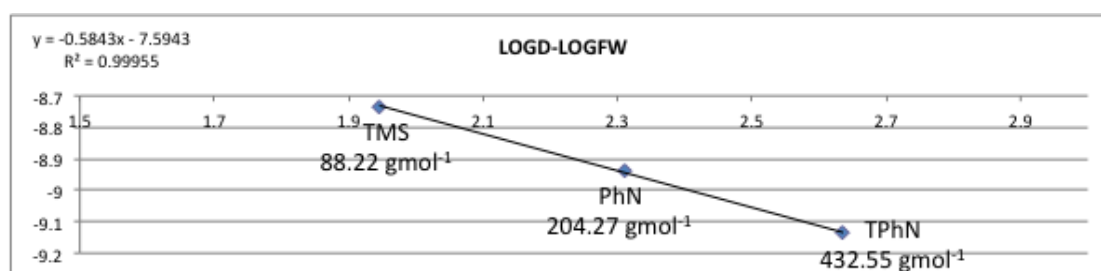


Table S1 D-FW analysis from the ^1H DOSY NMR data obtained for the mixture of **4'** and the standards TPhN, PhN and TMS in C_6D_6 solution at 300K

Compound	D_{Av} ($\times 10^{-10} \text{ m}^2\text{s}^{-1}$)	$\text{Log } D_{\text{Av}}$	FW (gmol^{-1})	Log FW
TPhN	7.29	-9.137272	432.55 ^a	2.636036
PhN	11.50	-8.939302	204.27 ^a	2.310204
TMS	18.47	-8.733533	88.22 ^a	1.945567
4'	9.72	-9.012378	267.28 ^b	2.426970

^a Real FW ^b FW calculated from [$\log D = -0.5843 \cdot \log \text{FW} - 7.5943$ ($r^2 = 0.9995$)]

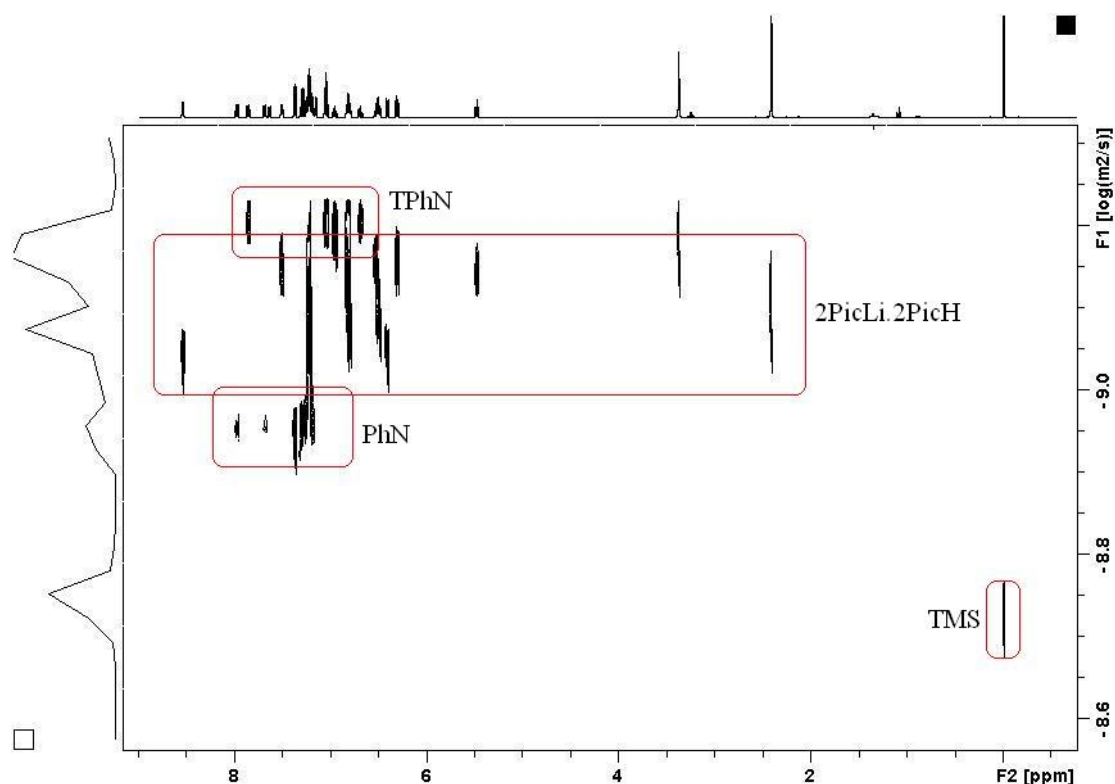


Figure S9 ^1H DOSY NMR spectrum of complex 2-picLi•2-picH in C_6D_6 solution at 300 K in the presence of inert standards 1,2,3,4-tetraphenylnaphthalene (TPhN), 1-phenylnaphthalene (PhN) and tetramethylsilane (TMS).

Graph S2 Plot of $\log D$ versus $\log FW$ from the ^1H DOSY NMR data obtained for the mixture of 2-picLi•2-picH and the inert standards TPhN, PhN and TMS in C_6D_6 solution at 300K

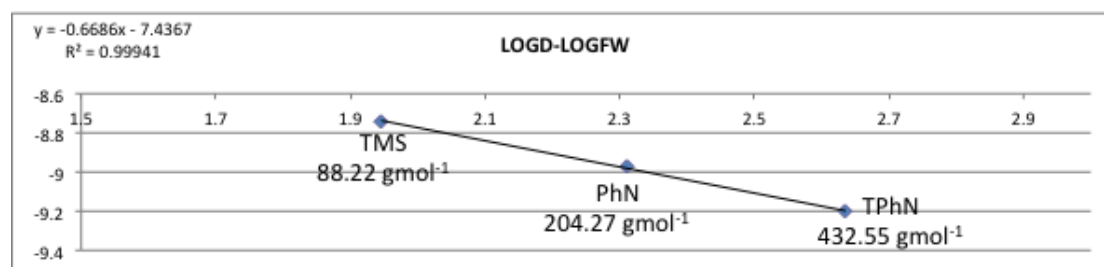


Table S3 D-FW analysis from the ^1H DOSY NMR data obtained for the mixture of 2-picLi•2-picH and the standards TPhN, PhN and TMS in C_6D_6 solution at 300K

Compound	D_{Av} ($\times 10^{-10} \text{ m}^2\text{s}^{-1}$)	$\text{Log } D_{\text{Av}}$	FW (gmol^{-1})	Log FW
TPhN	6.27	-9.202681	432.55 ^a	2.636036
PhN	10.59	-8.974899	204.27 ^a	2.310204
TMS	18.17	-8.740645	88.22 ^a	1.945567
2-picLi•2-picH	6.81	-9.166874	387.04 ^b	2.587757

^a Real FW ^b FW calculated from [$\text{log } D = -0.6686 \cdot \text{logFW} - 7.4367$ ($r^2 = 0.9994$)]