Electronic Supplementary Information

Lithium Heterocuprates: The Influence of the Amido Group on Organoamidocuprate Structure

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2D $^{1}H,^{7}Li$ HOESY NMR spectrum of 4

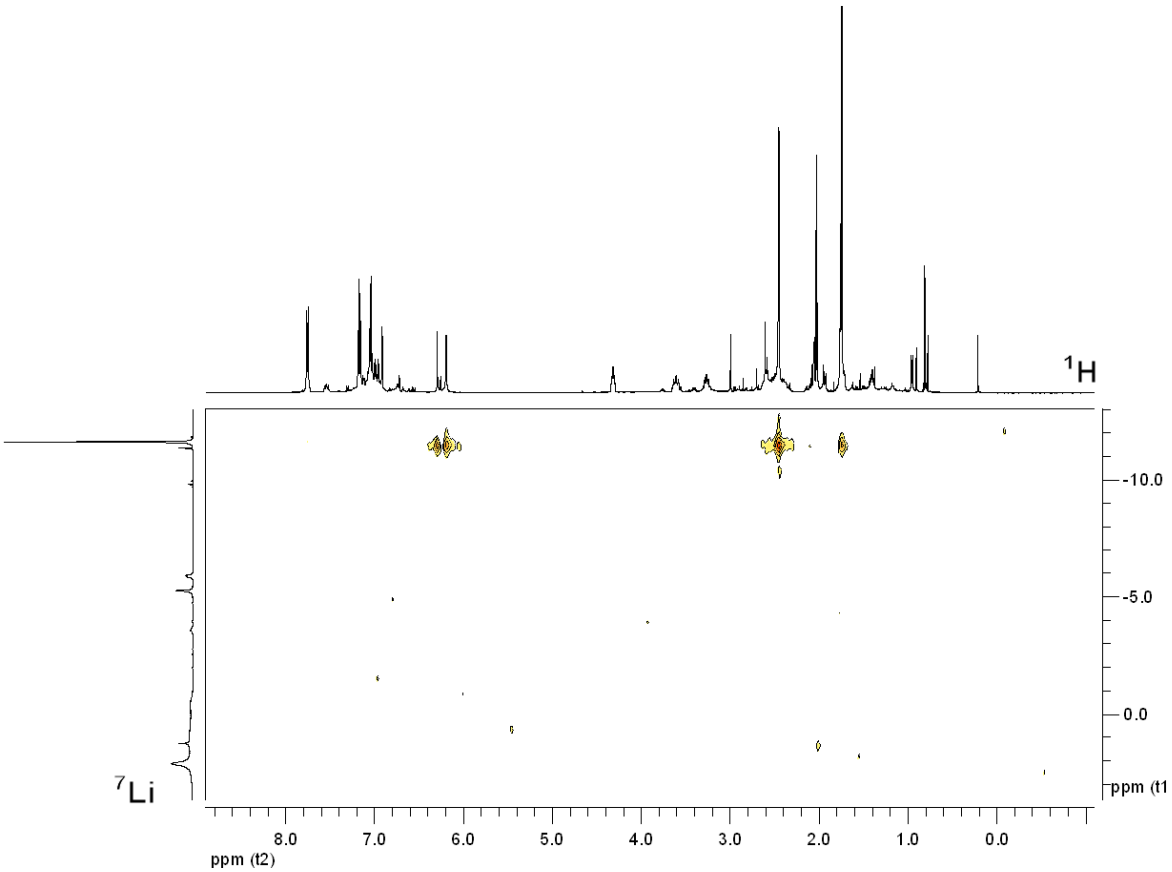

Figure S1. PFG inverse-detected 2D $^{1}H,^{7}Li$ HOESY NMR spectrum of $[Cu_2Li_2Mes_2(N(\textit{R}\text{-}CH(Ph)Me)(CH_2CF_3))_2]$ (4)

The ^{7}Li resonance at 2.11 ppm shows cross-correlations to ^{1}H NMR $\delta = 2.01$ (amido methyl group) and the ^{7}Li resonance at -11.63 ppm exhibits cross-correlations to ^{1}H NMR $\delta = 1.75$ (*para*-CH_3), 2.46 (*ortho*-CH_3), 6.19, 6.30 (Ar-H).

Addition comments of the X-ray crystal structure of 3

Refinements of the structure of **3** revealed a pair of *ca*. 4.1 eÅ^{-3} residual electron density peaks, separated by approximately 2.8 Å, situated *ca*. 1.8 Å from the C(43) and C(63) methyl groups. These are chemically unrealistic positions, and given that the separation between the two peaks is very similar to the Cu(1)···Cu(2) separation seen in the complex, these peaks were interpreted as being the copper atoms of a small occupancy twin component (the lighter atoms would not be apparent). Careful inspection of the original diffraction images clearly showed the crystal to be twinned, possibly multiply so. Efforts to handle this twinning at the data processing stage were unsuccessful; though numerous attempts were made to model various overlapping orientations of the lattice, none of these approaches gave better final results than just processing the data without acknowledging the presence of any twinning.