

Lithium-Nitrogen Bonds in Lithium Pyrrole Amides

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Secondary Lithium amides are a frequently used reagent in inorganic and organic synthesis. Their reactivity is determined by their structure and aggregation.[1] *Brown et al.* investigated the aggregation of $\text{Li}[\text{N}(\text{SiMe}_3)]$ in liquid phase by NMR Spectroscopy concluding that there is equilibrium between a dimeric and a monomeric form.[2] In 1986 *Snaith et al.* compared the aggregation behaviour of lithium amides and alkyl lithium compounds.[3] They stated that Li_2N_2 four membered rings act as building blocks of ladder or cube like higher aggregates. The aggregation behavior of these lithium amides became, in the following years, a major subject in coordination chemistry. Theoretical calculations by *Silvi et al.* suggested a sp^3 rather than a sp^2 hybridization at the nitrogen atom.[4] This however is in contradiction to the bond geometry in lithium amides being aggregated as dimers or higher aggregates. To contribute to the clarification of the bonding situation in this type of compound we decided to perform an experimental charge density study on compound (1) depicted in Figure 1.[5] Therein the amidic nitrogen atoms N(1) and N(4) are included in an aromatic five membered ring and therefore are anticipated to be sp^2 hybridized. Within the molecule there are also four sp^3 hybridized amine nitrogen atoms that can be seen as an internal comparison. This makes the chosen compound an ideal candidate to investigate the differences from a charge density point of view.

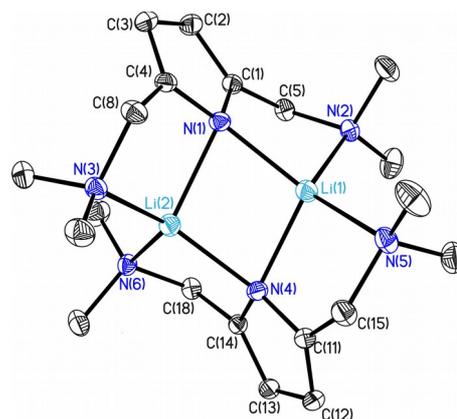


Figure 1 Crystal structure of investigated lithium pyrrole amide (1)

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