THF- d_8 solution over a 30–60 min period). However, a 13 C NMR spectrum of **2** in the same solvent at room temperature could not be obtained because of rapid decomposition of the sample. Therefore, a low-temperature study (-30 °C) of a precooled THF- d_8 solution was undertaken in the case of **2**.

A strong low-field shift for the *ipso* carbon atom signal (a narrow signal at 195.6 ppm) was observed in the 13 C NMR spectrum of a THF- d_8 solution of 1, while the low-temperature 13 C NMR spectrum of 2 showed a broad and poorly resolved signal at 201 ppm for the *ipso* carbon atom. It was previously shown⁵ that 13 C chemical shifts of *ipso* carbon atoms of both monomeric and dimeric solvated lithium aryls are in the range 180–200 ppm. We note that the solution structures of 1 and 2 are not clear. However, our 13 C solution NMR spectroscopic investigations indicate that the asymmetric arrangement found in the solid-state structure of complex 1, exhibiting different coordination modes for the two lithium atoms, is not retained in THF solution.

Conclusion

Our results provide more insight into the solid-state structures of two differently aggregated terphenyllithium complexes and demonstrate that the arrangement found in the solid-state structure of THF adducts of terphenyllithium compounds is mostly determined by the nature of the sterically demanding terphenyl ligand. Lower aggregation numbers can be induced by increased crowding at the aryl group, resulting in formation of monomeric aryllithium species: e.g., complex 2. Our work also allows a detailed comparison of the structural data of 1 and 2 with previously reported solvated and unsolvated terphenyllithium salts.

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Supporting Information Available: X-ray crystallographic files in CIF format for the structures of [DppLi]₂(THF) (1) and DnpLi(THF)₂ (2). This material is available free of charge via the Internet at http://pubs.acs.org.

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Additions and Corrections

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