Cyclisierung von Di(*tert*-butyl-methyl)ketazin zu 1,2-Diaza-3-bora- und 1,2-Diaza-3-sila-cyclopent-5-enen

Cyclization of Di(*tert*-butyl-methyl)ketazine to 1,2-Diaza-3-bora- and 1,2-Diaza-3-sila-cyclopent-5-enes

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The results of quantum chemical calculations on lithium ketazides suggest mainly four isomeric structures with different modes of lithium coordination (**A** – **D**). A monolithium ketazide thf-adduct (**1**) was isolated supporting the results of the quantum chemical calculations. In reactions of the lithiated di(*tert*-butyl-methyl)ketazine with BCl_3 and Cl_2BPh, 1,2-aza-azonia-3-borata-cyclopent-5-enes (**2**, **3**) were isolated. Substitution of a chlorine atom of **2** and **3** with *t*-BuLi leads to the formation of derivatives **4** and **5**. HCl elimination from **2** with Et_3N gives – *via* a diazaboracyclopentene (**6**) – a bicyclus **7**. In the reaction of the dilithiated ketazine with $F_2BN(SiMe_3)_2$, the diaza-boracyclopentene **8** is obtained while with Cl_4Si, $F_3SiN(SiMe_3)_2$, and Cl_2SiMe_2 the diazasilacyclopentenes **9** – **11** are generated. SiF_4 reacts with the dilithium ketazide to give a spirocyclus (**12**). The monolithium ketazide and Cl_2SiMe_2 react at 30 °C to give a four-membered ring isomer of the substitution product which is formed *via* a 1,3-chlorine shift from silicon to carbon (**13**). A tetrameric silanolate was isolated as a by-product in this reaction. It gives evidence for the structure of lithium ketazide **A**. Crystal structures of **5**, **7**, **10**, and **14** are reported.

Key words: Lithium Ketazides, Quantum Chemical Calculations, Diaza-bora-cyclopentenes, Diaza-sila-cyclopentenes, Aza-silacyclobutane