Thermische Isomerisierung eines Silenketazins zum Diazasilacyclopenten: Experimentelle und theoretische Untersuchungen

Thermal Isomerisation of a Sileneketazine to a Diazasilacyclopentene: Experimental and Theoretical Studies

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Lithium-tert-butylmethyldrazonide II, Me₃C(Me)C=N–NHLi, reacts with F₂Si[N(CHMe₂)₂]₂ to give Me₃C(Me)C=N–NH–SiF[N(CHMe₂)₂]₂ 1. The lithium salt of 1, Me₃C(Me)C=N–N(Li)SiF[N(CHMe₂)₂]₂, 1a, prepared in the reaction of 1 with n-C₄H₉Li, is substituted with F₂BN(SiMe₃)₂ forming Me₃C(Me)C=N–NBFN(SiMe₃)₂SiF[N(CHMe₂)₂]₂, 2. Experiments to synthesise the silaketazine, Me₃C(Me)C=N–N=Si[N(CHMe₂)₂], III, via LiF-elimination from 1a lead to the intramolecular formation of an N-functional 1,2-diaza-3-silacyclopentene, H₂C-C(Me₃)=N–NHSi[N(CHMe₂)₂]₂, 3, which is a structural isomer of III. The NH unit of 3 can be lithiated with n-C₄H₉Li. The lithium salt reacts with F₂BN(SiMe₃)₂ forming the substituted ring compound 4. The rearrangement of the silaketazine III to the ring compound 3 is described by density functional calculations predicting a three-step reaction mechanism correlated with the experimental data. The structures of 3 and 4 are discussed in detail.

Key words: Sileneketazine, Diazasilacyclopentene, Reaction Mechanism, Transition States, Density Functional Calculations