Figure 1: Anisotropic displacement parameters of \([\text{PhC(NBu)}_2\text{SiH(BH}_3\text{)}]^{-}\) is the first silicon(II) monohydride, containing a central silicon atom. A covalent, shared interaction to a sp\(^3\) hybridized boron atom stabilizes the hydride. The positively charged H-Si-BH\(_3\) moiety is coordinated by the lone-pairs of the benzamidinate ligand. These non-shared interactions allow a highly flexible coordination geometry at the silicon atom \(\text{II}\) compared to covalently bound ligands.

**Lewis acid-base stabilized silicon**

Group 14 hydrides are of steadily growing practical interest since they are widely used in synthetic chemistry, as alloys for electronic devices, and as precursors for high purity elements. Silicon can be envisaged as the sister element of carbon and several silicon hydrides derived from Si(IV) are known. Although GeH\(_3\) and PbH\(_2\) are readily available, the corresponding stable Si(III) compound of oxidation state \(\text{II}\) is elusive to date. Unstable species have been studied at high or at very low temperatures, the later stabilized in a matrix. However, Si(II) hydrides have not been stabilized at room temperature, so far. Recently, we reported the synthesis of the stable Lewis acid-base stabilized silicon(II) monohydride \([\text{PhNC(NBu)}_2\text{SiH(BH}_3\text{)}]^{-}\) in good yield. The target hydride was obtained from the reaction of the corresponding silicon(II) chloride \([\text{PhNC(NBu)}_2\text{SiCl}]^{-}\) with potassium trifluoromethyl borohydride \([\text{KBF}_3\text{H}]^{-}\).

**First silicon(II) monohydride**

Based on charge density investigations from a high-resolution, low-temperature diffraction experiment \([1]\) it looks like there is only one consistent interpretation of the electronic structure of \([\text{PhNC(NBu)}_2\text{SiH(BH}_3\text{)}]^{-}\). It should be pointed out that \(\text{LiSiH(BH}_3\text{)}\) is the first silicon(II) monohydride, containing a central silicon atom. A covalent, shared interaction to a sp\(^3\) hybridized boron atom stabilizes the hydride. The positively charged H-Si-BH\(_3\) moiety is coordinated by the lone-pairs of the benzamidinate ligand. These non-shared interactions allow a highly flexible coordination geometry at the silicon atom \(\text{II}\) compared to covalently bound ligands.

**Details from X-ray analysis**

The structure determination of such unprecedented species is far from routine. A combination of advanced hardware and powerful software is essential to get the high quality data needed for a successful multipole refinement that is essential to the experimental charge density investigation. Here Bruker’s TURBO X-RAY SOURCE equipped with HELIOS X-ray optics and the sensitive APEX II detector were combined with the flexible integration engine SAINT - part of the APEX2 software suite. We collected data up to \(\theta = 100^\circ\) with an impressive completeness of 92.4 %.

**Application Note SC-XRD #393**

**Charge density investigation of Stable Silicon(II) Monohydride**

**References**


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