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Expanding the Sr–B–N–H system with the compound $\text{Sr}_{13}(\text{BN}_2)_6\text{H}_8$ validated by X-ray and neutron powder diffraction

Tuesday 21 March 2023 16:00 (2 hours)

Multianionic compounds containing hydrides built a large variety of compounds, e. g. hydride fluorides, hydride oxides or hydride nitrides, which can act as functional materials such as hydride ionic conductors or host lattices for Eu^{2+} luminescence.[1] On the other hand, the compound class of nitridoborate hydrides is with only two known compounds, namely $\text{Ca}_2\text{BN}_2\text{H}$ and $\text{Sr}_2\text{BN}_2\text{H}$, only little explored so far.[2,3] We hereby present a new member of this group, $\text{Sr}_{13}(\text{BN}_2)_6\text{H}_8$. The compound crystallizes in the hexagonal space group $P6_3/m$ (no. 176) and reveals trigonal planar and distorted tetrahedrally coordinated hydride ions as well as slightly bent $[\text{N}–\text{B}–\text{N}]^{3-}$ units coordinated by strontium atoms. The structure was partially solved by X-ray powder diffraction and corroborated with neutron powder diffraction of the corresponding deuterated compound. Further analytics such as ^1H and ^{11}B MAS NMR, FTIR and Raman spectroscopy confirm the proposed structure model and the presence of anionic hydrogen. DFT calculations further validate the experimental outcome and reveal the electronic structure of $\text{Sr}_{13}(\text{BN}_2)_6\text{H}_8$.

[1] H. Kageyama et al., *Nat. Commun.* **2018**, 9, 772.

[2] M. Somer et al., *Z. Allg. Anorg. Chem.* **2004**, 630, 1068.

[3] S. Wandelt et al., *Inorg. Chem.* **2022**, 61, 12685.

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