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# Expanding the Sr–B–N–H system with the compound Sr<sub>13</sub>(BN<sub>2</sub>)<sub>6</sub>H<sub>8</sub> 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<sup>2+</sup> luminescence.[1] On the other hand, the compound class of nitridoborate hydrides is with only two known compounds, namely Ca<sub>2</sub>BN<sub>2</sub>H and Sr<sub>2</sub>BN<sub>2</sub>H, only little explored so far.[2,3] We hereby present a new member of this group, Sr<sub>13</sub>(BN<sub>2</sub>)<sub>6</sub>H<sub>8</sub>. The compound crystallizes in the hexagonal space group P6<sub>3</sub>/m (no. 176) and reveals trigonal planar and distorted tetrahedrally coordinated hydride ions as well as slightly bent [N–B–N]<sub>3</sub><sup>–</sup> 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 <sup>1</sup>H and <sup>11</sup>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 Sr<sub>13</sub>(BN<sub>2</sub>)<sub>6</sub>H<sub>8</sub>.

[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.

**Primary author:** WANDEL, Sophia Lena

**Co-authors:** MUTSCHKE, Alexander; Dr KHALYAVIN, Dmitry; Prof. SCHNICK, Wolfgang

**Presenter:** WANDEL, Sophia Lena

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