Poster Presentation

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Single-crystal X-ray diffraction investigation of β-rhombohedral boron

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The crystal structure of β-rhombohedral boron and its chemical bonding are still a matter of debate [1]. The most widely accepted structure model of β-rhombohedral boron is the one published by Slack et al. in 1988 [2].
According to Slack's model β-boron crystallizes in space group R-3m and comprises 320 atoms per hexagonal unit cell. Building blocks of B_12 icosahedra and triply-fused icosahedra (B_28 units) make up a complex three-dimensional framework
including 15 crystallographically independent boron atoms. Additional interstitial sites, which are all only partially occupied, and vacancies in the framework cause distortions from the ideal icosahedral geometry [2].
These numerous intrinsic defects give rise to the striking thermodynamic stability of β-boron at ambient pressure in all temperatures areas below the melting [1].
We have reinvestigated β-boron by high-resolution X-Ray diffraction at 100 K in order to establish a more detailed structure model, in particular with respect to the partial occupied sites (POS). The purpose is a more comprehensive concept of the (POS) in between the β-boron framework as well as a topological analysis of its chemical bonds.
[1] Ogitsu, T. et al. (2013). Chem. Rev. 113, 3425-3449.
[2] Slack, G. A. et al. (1988). J. Solid State Chem. 76, 52-63.
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