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.


Keywords: β-rhombohedral boron, crystal structure, chemical bonding