

Figure 1. a) Unit cell volume V versus nominal manganese content x in the system $Mn_xCo_{1-x}[BPO_4(OH)_2]$ b) Edge-sharing $M^{II}O_6$ -octahedra wound around a 3_1 screw axis

[1] Huang Y.-X.; Ewald B.; Schnelle W.; Prots Yu.; Kniep R., *Inorg Chem.* **2006**, 45, 7578

Keywords: borophosphates; hydrothermal growth; solid solutions

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Sr₁₀(PO₄)_{5.5}(BO₄)_{0.5}(BO₂): A Strontium Borate-Phosphate Closely Related to the Apatite Crystal Structure. Shuang Chen^{ab}, Stefan Hoffmann^a, Wilder Carrillo-Cabrera^a, Lev G. Akselrud^c, Yurii Prots^a, Jing-Tai Zhao^b, Rüdiger Kniep^a. ^aMax-Planck-Institut für Chemische Physik fester Stoffe. ^bShanghai Institute of Ceramics, Chinese Academy of Sciences. ^cDepartment of Inorganic Chemistry, Lviv State University. E-mail: shuang.chen@cpfs.mpg.de

Strontium borate-phosphate Sr₁₀(PO₄)_{5.5}(BO₄)_{0.5}(BO₂) was prepared from SrCO₃, NH₄H₂PO₄ and H₃BO₃ at high temperature (1150 – 1550 °C) and was found to be free of alkali metal compounds. X-ray structure determination was carried out on a single crystal obtained from the melt (space group $P\bar{3}$ No.147; $a = 9.7973(8)$ Å, $c = 7.3056(8)$ Å, $V = 607.29(10)$ Å³, $Z = 1$). Sr₁₀(PO₄)_{5.5}(BO₄)_{0.5}(BO₂) is a derivative of the apatite crystal structure. Strontium sites are found to be fully occupied while [PO₄]³⁻ tetrahedra are partly replaced by [BO₄]⁵⁻ groups. The crystal structure contains Sr cations occupying the 6g (Sr1) and 2d (Sr2, Sr3) sites, isolated tetrahedral [PO₄]³⁻/[BO₄]⁵⁻ groups, and linear [BO₂]⁻ groups located in the hexagonally shaped (trigonal antiprismatic) channels formed by Sr1 atoms and running along [001] (Figure 1). The space group of the present compound is reduced to $P\bar{3}$ because the orientation of the [PO₄]/[BO₄] tetrahedra destroys the mirror plane characteristic for the apatite crystal structure ($P6_3/m$) [1].

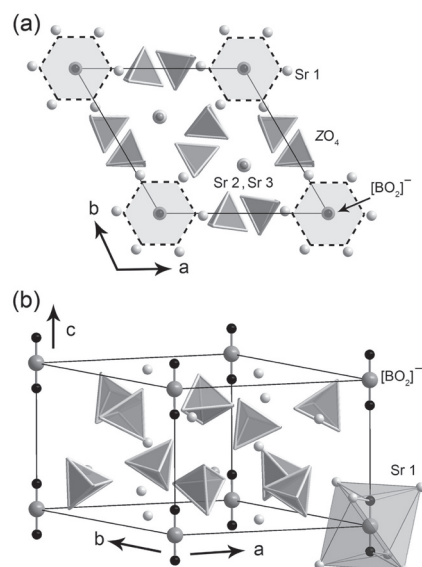


Figure. 1 Crystal structure of Sr₁₀(PO₄)_{5.5}(BO₄)_{0.5}(BO₂): (a) Projection along [001] showing the hexagonally shaped channels formed by Sr1 around the three-fold inversion axis ($Z = P_{0.95}B_{0.05}$). (b) Side view emphasizing the linear [BO₂]⁻ groups and the corresponding trigonal antiprism formed by Sr1.

[1] Calvo C., Faggiani R., Krishnamurthy N., *Acta Crystallogr.* **1975**, 31 B, 188.

Keywords: apatite; strontium borate-phosphate; crystal structure

FA2-MS01-P21

NaSc[BP₂O₆(OH)₃][(HO)PO₃]: Synthesis and Crystal Structure of the First Alkali Metal Scandium Borophosphate Hydrogenphosphate. Stefan Hoffmann^a, Prashanth Wilfred Menezes^a, Yurii Prots^a, Rüdiger Kniep^a. ^aMax-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden, Germany. E-mail: hoffmann@cpfs.mpg.de

Metal phosphates and borophosphates have received much attention because of their fascinating structural architectures and potential applications [1-2]. The combination of complex borophosphate anions together with (hydrogen) phosphate groups is rather rare and may generate a new class of materials with novel properties. The first alkali metal scandium borophosphate hydrogenphosphate, NaSc[BP₂O₆(OH)₃][(HO)PO₃], was synthesized under mild hydrothermal conditions in the course of our investigations in alkali metal containing scandium borophosphates. The crystal structure was determined from single crystal X-ray data: monoclinic, space group $P2_1/c$ (No. 14), $a = 5.0010(4)$ Å, $b = 12.4271(9)$ Å, $c = 15.8340(14)$ Å, $\beta = 94.201(4)^\circ$, $V = 981.41(11)$ Å³ and $Z = 2$. The anionic partial structure of NaSc[BP₂O₆(OH)₃][(HO)PO₃] contains isolated