

**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

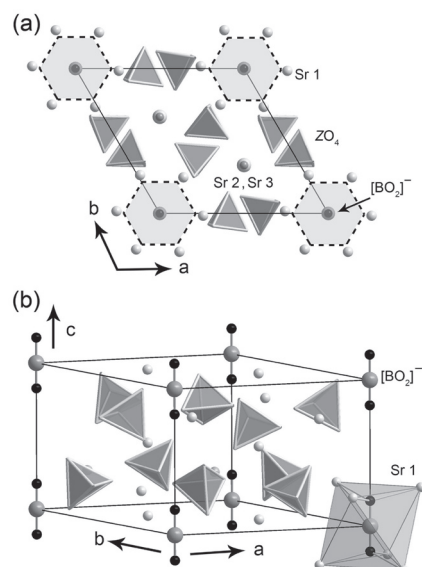
[1] Huang Y.-X.; Ewald B.; Schnelle W.; Prots Yu.; Kniep R., *Inorg Chem.* **2006**, 45, 7578

**Keywords:** borophosphates; hydrothermal growth; solid solutions

#### FA2-MS01-P20

**$Sr_{10}(PO_4)_{5.5}(BO_4)_{0.5}(BO_2)$ : A Strontium Borate-Phosphate Closely Related to the Apatite Crystal Structure.** Shuang Chen<sup>ab</sup>, Stefan Hoffmann<sup>a</sup>, Wilder Carrillo-Cabrera<sup>a</sup>, Lev G. Akselrud<sup>c</sup>, Yurii Prots<sup>a</sup>, Jing-Tai Zhao<sup>b</sup>, Rüdiger Kniep<sup>a</sup>. <sup>a</sup>Max-Planck-Institut für Chemische Physik fester Stoffe. <sup>b</sup>Shanghai Institute of Ceramics, Chinese Academy of Sciences. <sup>c</sup>Department of Inorganic Chemistry, Lviv State University. E-mail: [shuang.chen@cpfs.mpg.de](mailto:shuang.chen@cpfs.mpg.de)

Strontium borate-phosphate  $Sr_{10}(PO_4)_{5.5}(BO_4)_{0.5}(BO_2)$  was prepared from  $SrCO_3$ ,  $NH_4H_2PO_4$  and  $H_3BO_3$  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,  $V = 607.29(10)$  Å<sup>3</sup>,  $Z = 1$ ).  $Sr_{10}(PO_4)_{5.5}(BO_4)_{0.5}(BO_2)$  is a derivative of the apatite crystal structure. Strontium sites are found to be fully occupied while  $[PO_4]^{3-}$  tetrahedra are partly replaced by  $[BO_4]^{5-}$  groups. The crystal structure contains Sr cations occupying the 6g (Sr1) and 2d (Sr2, Sr3) sites, isolated tetrahedral  $[PO_4]^{3-}/[BO_4]^{5-}$  groups, and linear  $[BO_2]^-$  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  $[PO_4]^{3-}/[BO_4]^{5-}$  tetrahedra destroys the mirror plane characteristic for the apatite crystal structure ( $P6_3/m$ ) [1].



**Figure. 1** Crystal structure of  $Sr_{10}(PO_4)_{5.5}(BO_4)_{0.5}(BO_2)$ : (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  $[BO_2]^-$  groups and the corresponding trigonal antiprism formed by Sr1.

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

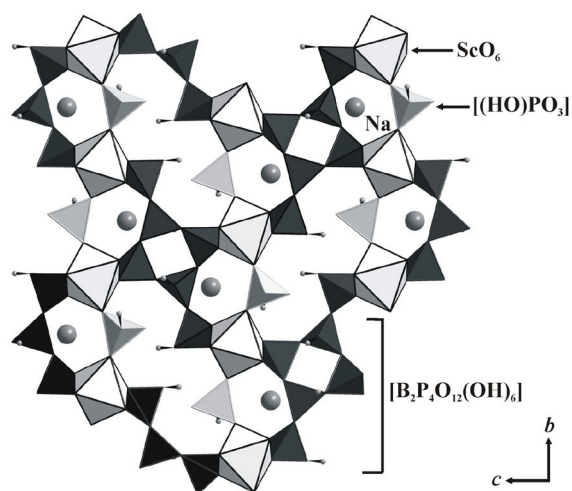
**Keywords:** apatite; strontium borate-phosphate; crystal structure

#### FA2-MS01-P21

**$NaSc[BP_2O_6(OH)_3] [(HO)PO_3]$ : Synthesis and Crystal Structure of the First Alkali Metal Scandium Borophosphate Hydrogenphosphate.** Stefan Hoffmann<sup>a</sup>, Prashanth Wilfred Menezes<sup>a</sup>, Yurii Prots<sup>a</sup>, Rüdiger Kniep<sup>a</sup>. <sup>a</sup>Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden, Germany. E-mail: [hoffmann@cpfs.mpg.de](mailto: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,  $NaSc[BP_2O_6(OH)_3] [(HO)PO_3]$ , 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,  $\beta = 94.201(4)^\circ$ ,  $V = 981.41(11)$  Å<sup>3</sup> and  $Z = 2$ . The anionic partial structure of  $NaSc[BP_2O_6(OH)_3] [(HO)PO_3]$  contains isolated

borophosphate oligomers (open-branched four membered rings,  $[B_2P_4O_{12}(OH)_6]^{4-}$ ) and isolated hydrogenphosphate groups ( $[(HO)PO_3]^{2-}$ ) which are interconnected by  $ScO_6$  coordination octahedra by sharing common oxygen corners. The resulting three-dimensional framework is characterized by channels running along  $[100]$  (Figure 1) formed by an arrangement of twelve-, six- and four-membered rings. Sodium ions reside within the six-membered rings.



**Figure 1.** 3D arrangement of polyhedra in the crystal structure of  $NaSc[BP_2O_6(OH)_3][(HO)PO_3]$  viewed along  $[100]$ .

[1] Cheetham A.K., Férey G., Loiseau T., *Angew. Chem. Int. Ed.*, **1999**, 38, 3268. [2] Ewald B., Huang Y.-X., Kniep R., *Z. Anorg. Allg. Chem.*, **2007**, 633, 1517.

**Keywords:** borophosphate; alkali metal; scandium