

**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  $M^6O_6$ -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

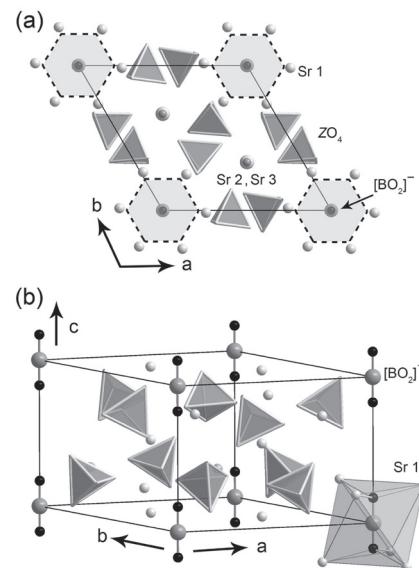
**Keywords:** borophosphates; hydrothermal growth; solid solutions

#### FA2-MS01-P20

**Sr<sub>10</sub>(PO<sub>4</sub>)<sub>5.5</sub>(BO<sub>4</sub>)<sub>0.5</sub>(BO<sub>2</sub>): A Strontium Borate-Phosphate Closely Related to the Apatite Crystal Structure.** Shuang Chen<sup>a,b</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

Strontium borate-phosphate  $\text{Sr}_{10}(\text{PO}_4)_{5.5}(\text{BO}_4)_{0.5}(\text{BO}_2)$  was prepared from  $\text{SrCO}_3$ ,  $\text{NH}_4\text{H}_2\text{PO}_4$  and  $\text{H}_3\text{BO}_3$  at high temperature ( $1150 - 1550^\circ\text{C}$ ) 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>,  $Z = 1$ ).  $\text{Sr}_{10}(\text{PO}_4)_{5.5}(\text{BO}_4)_{0.5}(\text{BO}_2)$  is a derivative of the apatite crystal structure. Strontium sites are found to be fully occupied while  $[\text{PO}_4]^{3-}$  tetrahedra are partly replaced by  $[\text{BO}_4]^{3-}$  groups. The crystal structure contains Sr cations occupying the 6g (Sr1) and 2d (Sr2, Sr3) sites, isolated tetrahedral  $[\text{PO}_4]^{3-}/[\text{BO}_4]^{3-}$  groups, and linear  $[\text{BO}_2]^-$  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  $[\text{PO}_4]/[\text{BO}_4]$  tetrahedra destroys the mirror plane characteristic for the apatite crystal structure ( $P6_3/m$ ) [1].



**Figure 1** Crystal structure of  $\text{Sr}_{10}(\text{PO}_4)_{5.5}(\text{BO}_4)_{0.5}(\text{BO}_2)$ : (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  $[\text{BO}_2]^-$  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<sub>2</sub>O<sub>6</sub>(OH)<sub>3</sub>]<sub>2</sub>[(HO)PO<sub>3</sub>]: 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

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,  $\text{NaSc[BP}_2\text{O}_6(\text{OH})_3\text{]}_2[(\text{HO})\text{PO}_3]$ , 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  $\text{NaSc[BP}_2\text{O}_6(\text{OH})_3\text{]}_2[(\text{HO})\text{PO}_3]$  contains isolated