Figure 1. a) Unit cell volume $V$ versus nominal manganese content $x$ in the system $\text{Mn}_x\text{Co}_{1-x}\text{BP}_2\text{O}_6(\text{OH})_3$. b) Edge-sharing $M^6\text{O}_6$-octahedra wound around a 3, screw axis.

Keywords: borophosphates; hydrothermal growth; solid solutions

FA2-MS01-P20

Sr$_{10}$(PO$_4$)$_5$(BO$_4$)$_{0.5}$(BO$_2$): A Strontium Borate-Phosphate Closely Related to the Apatite Crystal Structure. Shuang Chen$^{ab}$, Stefan Hoffmann$^{a}$, Wilder Carrillo-Cabrera$^b$, Lev G. Akselrud$^b$, Yuriy Prots$^b$, Jing-Tai Zhao$^b$, Rüdiger Kniep$^b$, Max-Planck-Institut für Chemische Physik fester Stoffe$^b$, Shanghai Institute of Ceramics, Chinese Academy of Sciences$^c$, Department of Inorganic Chemistry, Lviv State University.

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Strontium borate-phosphate $\text{Sr}_{10}(\text{PO}_4)_{5}\text{(BO}_4)_{0.5}\text{(BO}_2)$ was prepared from $\text{SrCO}_3$, $\text{NH}_2\text{H}_2\text{PO}_4$ and $\text{H}_2\text{BO}_3$ 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 $P\overline{3}$ No.147; $a = 9.7973(8)$ Å, $c = 7.3056(8)$ Å, $V = 607.29(10)$ Å$^3$, $Z = 1$). Sr$_{10}$(PO$_4$)$_5$(BO$_4$)$_{0.5}$(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 $P\overline{3}$ because the orientation of the $[\text{PO}_4]^{3-}/[\text{BO}_4]^{-}$ tetrahedra destroys the mirror plane characteristic for the apatite crystal structure ($P\overline{6}_3/m$) [1].

Figure 1 Crystal structure of Sr$_{10}$(PO$_4$)$_5$(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 $[\text{BO}_2]^{-}$ groups and the corresponding trigonal antiprisma formed by Sr1.

Keywords: apatite; strontium borate-phosphate; crystal structure

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NaSc[BP$_2$O$_6$(OH)$_3$][(HO)PO$_3$]: Synthesis and Crystal Structure of the First Alkali Metal Scandium Borophosphate Hydrogenphosphate. Stefan Hoffmann$^a$, Prashanth Wilfred Menezes$^a$, Yuriy Prots$^b$, Rüdiger Kniep$^b$. Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden, Germany.

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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$_2$O$_6$(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$^3$ and $Z = 2$. The anionic partial structure of NaSc[BP$_2$O$_6$(OH)$_3$][(HO)PO$_3$] contains isolated
borophosphate oligomers (open–branched four membered rings, $[\text{B}_2\text{P}_4\text{O}_{12}(\text{OH})_6]^{4-}$) and isolated hydrogenphosphate groups ($[(\text{HO})\text{PO}_3]^{2-}$) 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$_2$O$_6$(OH)$_3$][(HO)PO$_3$] viewed along [100].


Keywords: borophosphate; alkali metal; scandium