

MS14-P30 | INSIGHT INTO THE CRYSTALLIZATION AND STRUCTURAL FEATURES OF CAESIUM-BEARING CHAIN-TYPE BOROPHOSPHATES

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Three borophosphates, CsBP₂O₆(OH)₂ (I), CsMn[BP₂O₈(OH)] (II) and Cs_{0.54}Mn_{1.17}BP₂O₈(H₂O)_{2.32} (III), were grown under hydrothermal conditions. Their crystal structures were solved using single crystal X-ray diffraction: (I)-monoclinic, *I*2/a, *a*=14.5329(3) Å, *b*=7.4869(2) Å, *c*=13.4002(3) Å, β=90.059(2)°, *V*=1458.03(6) Å³, *Z*=8; (II)-monoclinic, *P*2₁/*c*, *a*=9.1446(2) Å, *b*=8.6946(1) Å, *c*=9.6361(2) Å, β=100.139(2)°, *V*=754.19(2) Å³, *Z*=4; (III)-hexagonal, *P*6₁22, *a*=9.6292(3) Å, *c*=15.8051(3) Å, β=100.139(2)°, *V*=754.19(2) Å³, *Z*=6. The crystal architecture of (I) presents a unique structural type, whereas (II) and (III) are novel cesium-manganese representatives of known families. The structural features of (I)-(III) are infinite anionic chains with tB:tP ratio of 1:2 as main structural building blocks. The chains of (II) consist of alternating corner sharing tetrahedral BO₃(OH) borate and PO₄ phosphate groups with an additional branched phosphate tetrahedron. In the case of (I) and (III) the borate and phosphate tetrahedra share oxygen vertices to form four-ring chains with identical topology. These chains are extended along [010] direction in the crystal structure of (I) and are twisted along 6₁ axes in the structure of (III). The influence of different crystallization conditions on the structure formation of obtained caesium borophosphates will be discussed. The work was supported by the RFBR (№18-03-00908).