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Crystal structure and thermoresponsive studies of porous and non-porous borophosphates.

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In this work we present the synthesis and structure-property investigation of anhydrous non-porous borophosphates BPO_4 and hydrated porous $(\text{NH}_4)_0.5\text{Co}_1.25(\text{H}_2\text{O})_2(\text{BP}_2\text{O}_8)(\text{H}_2\text{O})_x$ phases. Cristobalite-type BPO_4 crystallizes in the tetragonal lattice, space group I-4 (No. 82) [1]. Variable-Temperature Powder X-ray diffraction (VT-PXRD) patterns of this material were analysed by the sequential Rietveld refinement protocol. This method was used to determine the temperature dependency of the lattice parameters and linear thermal expansion coefficient. The refinement reveals significant anisotropy along the a- and c- crystallographic axes as a function of temperature, with thermal expansion coefficients of $10.6 \times 10^{-6} /^\circ\text{C}$ and $2.83 \times 10^{-6} /^\circ\text{C}$, respectively. Structural changes accompanying this thermoresponsive behaviour will be discussed, including the variation of the interatomic distances and P-O-B (inter-polyhedral angle) with temperature. The open framework borophosphate $(\text{NH}_4)_0.5\text{Co}_1.25(\text{H}_2\text{O})_2(\text{BP}_2\text{O}_8)(\text{H}_2\text{O})_x$ was synthesized under mild hydrothermal conditions at 180°C . The crystal structure was refined in the hexagonal lattice, space group P65 (no. 170) [2]. The compound is composed of NH_4^+ and H_2O molecules located within the helical channels running along the [001] direction. Thermoresponsive investigation conducted by TGA analysis reveal a four step mass loss process, with the final step observed at $500\text{-}700^\circ\text{C}$ range. Preliminary VT-PXRD results of this compound will also be presented.

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