

Poster Presentations

[MS20-P09] Thermoresponsive behaviour of CaBPO₅, SrBPO₅ and H₈Mn₅O₂₀P₄.
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Metal borophosphates and phosphates have been the focus of intensive research activity in the past few years owing to their diverse crystal structures. The three-dimensional open framework structures of metal borophosphates and phosphates have had technological importance in shape-selective catalysis and ion exchange applications. [1] The two dimensional linear structures have been used in electronic applications, heat engine components and even dentalware. [2] However these applications are all nullified if the material loses dimensional integrity and develops microcracks at high operational temperatures. In this work we present the thermal expansion behaviour of borophosphates CaBPO₅ [3] and SrBPO₅ [4] determined by variable temperature powder x-ray diffraction (VT-PXRD) and manganese phosphate H₈Mn₅O₂₀P₄ determined by differential scanning calorimetry (DSC). VT-PXRD patterns for both CaBPO₅ and SrBPO₅ were collected from room temperature to 900 °C at 25 °C intervals. The evolution of the lattice parameters were determined by the sequential and parametric refinement protocols. Both materials crystallize in the trigonal system (space group P3121) at room temperature to 900 °C. Whereas the lattice parameters were set as refinable in the sequential method, the individual cell parameters were described using an empirically derived function in the parametric method. [3] Both refinement protocols model a near linear anisotropic increase in the *a/b* and *c* lattice parameters as a function of temperature. Low positive thermal expansion behaviour at 900 °C is reported (parametric method) along

the *a/b* (0.193 ppm.K⁻¹) and *c* (0.336 ppm.K⁻¹) directions for CaBPO₅ and *a/b* (0.625 ppm.K⁻¹) and *c* (0.625 ppm.K⁻¹) directions for SrBPO₅. This corresponds to a 1.43% and 1.36% increase in the bulk volume of the lattice for CaBPO₅ and SrBPO₅, respectively. In terms of relating the low thermal expansion behaviour of these materials to their composition and structure, one could envision that the rigid and strongly bonded BO₄ and PO₄ polyhedra in conjunction with the lattice spacing (open structure) play a role in limiting the large structural fluctuations as a function of temperature. The three-dimensional open framework H₈Mn₅O₂₀P₄ crystallises in the monoclinic system (space group C2/c) with *a* = 17.5790(4), *b* = 9.1091(2), *c* = 9.4866(2). The compound was characterised by single crystal x-ray diffraction studies. The structure is composed of connections between MnO₆ octahedra and PO₄ and PO₃(OH) tetrahedral forming channels along the [001] direction. The channels are occupied by water molecules bonded to the manganese atoms. DSC thermograms reveal that the compound decomposes at 340 °C with double endotherms with maxima at 122 °C and 213 °C corresponding to dehydration processes of this material. Work in progress involves investigating the thermoresponsive behaviour of the isostructural phases (Ba, Pb)BPO₅ and H₈Mn₅O₂₀P₄, and related new materials.

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