Oral Contributions

[MS28 - 02] Thermoresponsive behaviour of interesting phosphate based functional materials. David G. Billing[a]

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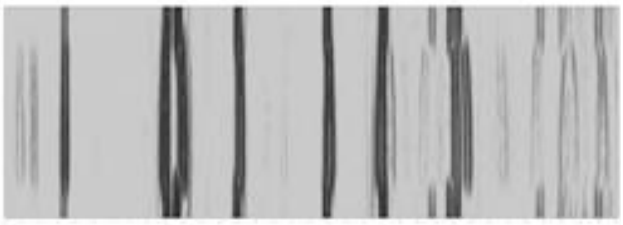
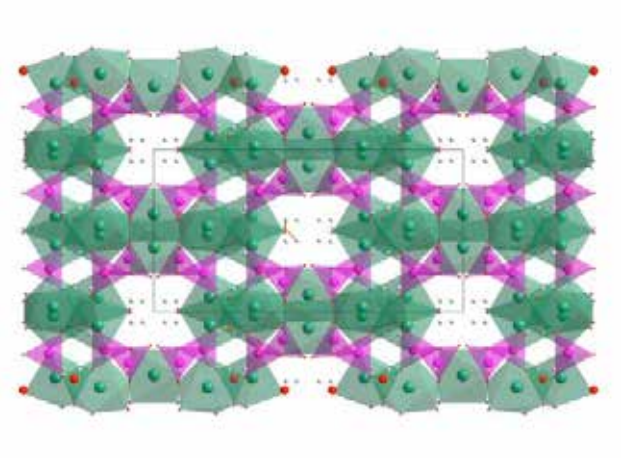
In recent times we have prepared and studied the thermoresponsive behaviour of a number of phosphate or borophosphate based materials. These include a some based on the NaSICON (Na Super Ionic Conductor) structural family with formula $A_xM_yP_3O_{12}$ [$0 \leq x \leq 1$; $1 \leq y \leq 3$] and which crystallize with rhombohedral symmetry [space group R-3c (No. 167)], A series of simple borophophates with the general formula MBPO5 and most recently a number (for example $Sr_{10}[(PO_4)(BO_4)](BO_2)]$) related to the naturally occurring mineral Hureaulite [1]. Whilst work on the preparation of porous borophosphates is ongoing, and focuses on in situ PXRD characterization of the gas-solid interaction phenomena observed. Synthetic strategies employed in the preparation of the materials include traditional solid state, sol-gel and hydrothermal methodologies. In this presentation I will present details of the structural behavior of selected representatives from these families of materials, as studied by variable temperature powder diffraction methods and advanced Rietveld refinement strategies. Results include description of a reversible phase transition identified in $CuSn_2P_3O_{12}$, parametric refinement studies of $MBPO_5$, M = Ca, Sr, Ba and/or Pb, all made via solid state methods, as well as preliminary results on the thermoresponsive behavior of $Sr_{10}[(PO_4)(BO_4)](BO_2)]$ and the potentially porous material H8Mn5P4O20, prepared hydrothermally. In the latter the nature of the bonding between the H2O present within the structure and the main structure framework determines whether or not it is removable in a reversible manner.



Topographical view of PXRD data: $CuSn_2P_3O_{12}$ indicating the presence of a reversible phase transformation.



$H_8Mn_5P_4O_{20}$, showing channels containing H_2O along c axix.

[1] P.M. Moore and T. Araki; Amer. Mineralogist, (1973), 58, 302-307

Keywords: In situ PXRD, Low thermal expansion phosphates, Parametric Rietveld refinement.