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Thermoresponsive behaviour of (NH4)0.5Co1.25(H2O)2[BP2O8].(H2O)0.5 with CZP framework topology

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Theme: Crystal Engineering and Structural Chemistry
Four CZP (chiral zincophosphate) zeolite topology compounds [1] with the general formula MIMII (H2O)2[BP2O8].yH2O (MI = Na, NH4 and MII = Mn, Co, y = 0.5, 1) have been prepared under mild hydrothermal conditions (at 180 ℃). Such microporous compounds with aesthetically interesting crystal structures can have interests in fields such as catalysis, storage, separation and ion-exchange. One compound of this family, (NH4)0.5Co1.25(H2O)2[BP2O8].(H2O)0.5, has been studied by variable temperature high resolution powder X-ray diffraction
experiments carried out from 298 to
1073 K. Complete Rietveld
refinements were achieved by
combining stereochemical restraints
with the powder diffraction data. At
room temperature, this compound
crystallizes in the P65 (No. 170)
space group with Z = 4 belonging to
the hexagonal system. The unit cell
parameters obtained were: a = 9.4330(2) Å, c = 15.5203(2) Å, V = 1196.01(5) Å
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reciprocal space analysis also revealed the presence of positional disorder via large refined MSDs. The crystal structure consists of a helical anionic framework, ∞[BP2O8]
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, composed of
corner sharing BO4 and PO4 tetrahedra. Water and ammonia molecules are found within the helical channels running along the [001] direction. This compound undergoes a series of dehydration, de-ammoniation (analysis augmented by thermogravimetric experiments and Fourier analysis) and finally long range structural decomposition into an amorphous phase. Total scattering analysis [2] was applied for the first time coupled to the above conventional structural refinement approach to map the identified positional disorder into real space, and to further unravel the gaseous dissociation and subsequent decomposition pathway of the rigid host structure.

Primary author: Dr MOGODI, Mashikoane (European Synchrotron Radiation Facility (ESRF))

Presenter: Dr MOGODI, Mashikoane (European Synchrotron Radiation Facility (ESRF))

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