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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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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 °C). 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 3 . This reciprocal space analysis also revealed the presence of positional disorder via large refined MSDs. The crystal structure consists of a helical anionic framework, ∞[BP2O8] 3-, 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.

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