and their dependence on such synthetic parameters as pH, sulfur content, temperature and aging, the transformations from starting materials. We have done this under real-time hydrothermal conditions using powder diffraction and an IP at beamline X7B. From these results, information on the kinetics of formation, useful to optimize future syntheses, has been obtained.

**PS10.10.13 THE SYNTHESIS AND CRYSTAL STRUCTURES OF ALKALINE EARTH METAL INDIUM PHOSPHATES.** Xuejiao Tang and Abdessadek Lachgar, Chemistry Department, Wake Forest University.

Metal phosphates with open framework structures are well known for their adsorptive, catalytic and ion-exchange properties. Al and Ga phosphates have been widely studied and exhibit great structural variations. In contrast, research on In phosphates has been very limited in scope. As a part of our search for open framework metal phosphates, we have recently been investigating ternary alkali or alkaline earth metal indium phosphates using hydrothermal synthesis techniques. We report the syntheses and crystal structures of alkaline earth metal indium phosphates [\(\text{A}[\text{In}_2\text{(PO}_4)_2\text{(HPO}_4)]\) (A=Ca, Sr or Ba). Ca[\(\text{In}_2\text{(PO}_4)_2\text{(HPO}_4)\] was synthesized hydrothermally from stoichiometric amounts of CaO and InCl\(_3\) in excess H\(_3\text{PO}_4\) and H\(_2\text{O}\). The compound crystallizes in monoclinic symmetry, space group \(\text{P}2_1/\overline{1}\), \(a=6.5708(6), \ b=20.237(2),\ c=6.6572(7)\text{Å}, \beta=91.20(1)^\circ\). The structure contains \(\text{In}_2\text{PO}_4\) dimers built up of two edge-sharing \(\text{In}_2\text{(PO}_3\text{OH})\) octahedra. The dimers connect to each other through \(\text{PO}_2\text{H}_2\text{O}\) tetrahedra by sharing all of their oxo ligands. Cations are located in tunnels of 8-member ring opening running along [001] direction. To our knowledge, this is the first reported indium phosphate containing \(\text{In}_2\text{PO}_4\) dimers. Sr[\(\text{In}_2\text{(PO}_4)_2\text{(HPO}_4)\]] was obtained hydrothermally from Sr(OH)\(_2\) and InCl\(_3\) (1:1) in excess H\(_3\text{PO}_4\) and H\(_2\text{O}\). Space group \(\text{P}2_1/\overline{1}\), \(a=6.615(1), \ b=20.351(3),\ c=6.752(1)\text{Å}, \beta=91.00(1)^\circ\). Its structure is analogue to Ca[\(\text{In}_2\text{(PO}_4)_2\text{(HPO}_4)\]].


The adsorption properties of frameworks with the MFI topology (H-ZSM-5 and its Al-free analogue silicalite-1) have received much attention. There is a general agreement that in low-loaded MFI adsorbent systems the preferred adsorption site is at the intersection of channels. Recently published papers on the localization of naphthalene (nph) in H-ZSM-5 determined by Xray Powder Diffraction (hereafter referred to as XPD1 [Mentzen et al.; Zeolites, 13 (1993) 485]) and XPD2 [Klein et al.; Microporous Materials, 5 (1994) 291]) show inconsistent results. In both papers the structure is described in the orthorhombic space group Pnma. In XPD1 as well as in XPD2 the nph molecules (3.8 and 3.0 mols/u.c., respectively) are at the intersection of channels. However, the inversion of the unit cell axes a and b (a=b=1; the empty orthorhombic HZSM-5 framework has a=b=1), as observed in XPD1, is not reported in XPD2. In addition, the orientation of the nph molecules at the intersection of channels in XPD1 and XPD2 is quite different.

We succeeded in preparing a single crystal of the H-ZSM-5 zeolite loaded with 3.68(2) molecules nph per u.c., large enough to allow a single crystal X-ray diffraction study of the material.

The paper describes the structure of the H-ZSM-5/nph complex, gives the ensuing deformation of the channel pores and compares the orientation of nph as determined from powder and single crystal X-ray diffraction. The inversion of the a and b axes is confirmed and the orientation of nph is yet different from the orientations reported in the XPD-papers.