

Poster Presentation

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A novel layered aluminophosphate with corner-sharing AlO_6 chains

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The synthesis, Raman spectroscopy and crystal structure of a novel layered aluminophosphate is described. The new phase was derived by the sol-gel method starting from a modified low hydrothermal ALPO4-34 zeolite synthesis procedure[1]. The structure was solved by direct methods using single-crystal X-ray diffraction. The synthesized layered material, with composition $[\text{AlPO}_3(\text{OH})\text{F}(\text{H}_2\text{O})] \cdot (\text{H}_9\text{C}_4\text{ON})$, crystallizes in the monoclinic space group $\text{P}2_1/a$ with $a = 9.2282(5) \text{ \AA}$, $b = 6.9152(4) \text{ \AA}$, $c = 14.4615(9) \text{ \AA}$, $\beta = 101.57(1)^\circ$. Layered aluminophosphates with AlO_6 polyhedra have been previously described [2], although in these compounds Al octahedra share edges. The novel compound has corner sharing $\text{AlO}_4\text{F}(\text{H}_2\text{O})$ chains along [010], where fluorine is at the shared apex, four oxygen atoms are shared with PO_4 tetrahedra and the fifth oxygen is a H_2O group. This kind of aluminophosphate chains is found in nature in tancoite [3]. Chains are linked along [100] through corner sharing with a PO_4 group of the adjacent chain plus hydrogen bonding of the H_2O group. Layers are stacked along c^* through hydrogen bonding with a double layer of morpholine ($\text{H}_9\text{C}_4\text{ON}$) molecules. The chemical stability field of the novel material is strongly dependent from the fluorine/aluminum ratio of the starting gel. At lower fluorine concentrations only ALPO4-34 and/or AlPO_4 (berlinite) are stable depending on the morpholine content. Crystals growth morphology depends on the supersaturation conditions of the starting gel: at low concentrations crystals are well developed hexagonal like plate shaped and are very thin. At higher concentrations they show a more elongated morphology. A treatment with H_2CO_3 leads to a complete morpholine removal, as shown by in situ Raman spectroscopy. Powder X-ray diffraction reveals that after morpholine extraction, the material diffract still coherently in two dimensions while a strong broadening is shown for basal planes.

[1] C. Wang, J. Wu, M. Hu, N. Li, N. Guan, S. Xiang *J. Porous Mater* 2011, 19, 5; 751-759, [2] R.W. Dorner, M. Deifallah, D.S. Coombes, et al. *Chem. Mater.* 2007, 19, 2261-2268., [3] Hawthorne F.C. *Tschermaks Mineralogische und Petrographische Mitteilungen*, 1983, 31 121-135.

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