

Although from the same family, the two phosphates adopt two different crystal structures.  $\text{Rb}_2\text{MnP}_2\text{O}_7 \cdot \text{H}_2\text{O}$  crystallizes in the monoclinic  $P2_1/c$  space group with lattice parameters  $a = 5.3845(5) \text{ \AA}$ ,  $b = 10.241(1) \text{ \AA}$ ,  $c = 15.566(2) \text{ \AA}$ ,  $\beta = 93.15(1)^\circ$ ,  $Z = 4$ ,  $V = 857,00(4) \text{ \AA}^3$ .  $\text{Cs}_2\text{MnP}_2\text{O}_7$  crystallizes in the orthorhombic  $Pnma$  ( $n^\circ 62$ ) space group and the unit cell parameters are  $a = 16.3398(3) \text{ \AA}$ ,  $b = 5.3872(1) \text{ \AA}$ ,  $c = 9.8872(2) \text{ \AA}$ ,  $Z = 4$ ,  $V = 870,33(3) \text{ \AA}^3$ . Both structures are however closely related. They can be described by a single axis stacking of undulating  $[\text{MnP}_2\text{O}_{10}]_\infty$  layers; alkaline cations occupy the interlayer spaces. The water molecule in  $\text{Rb}_2\text{MnP}_2\text{O}_7 \cdot \text{H}_2\text{O}$  is positioned also between the  $[\text{MnP}_2\text{O}_{10}]_\infty$  layers. Its presence is confirmed by the  $1607\text{cm}^{-1}$ ,  $3173\text{cm}^{-1}$  and  $3545\text{cm}^{-1}$  absorption bands observed in the infrared spectrum.

Some parallel can be made between the structures of  $\text{Rb}_2\text{MnP}_2\text{O}_7 \cdot \text{H}_2\text{O}$  /  $\text{Cs}_2\text{MnP}_2\text{O}_7$  [1] and some phosphates of the enlarged  $\text{A}_2\text{MP}_2\text{O}_7$  family like  $\text{K}_2\text{CuP}_2\text{O}_7$  [2]. On the other hand, within the entire  $\text{A}_2\text{MnP}_2\text{O}_7$  ( $A = \text{Li, Na, K, Rb, Cs}$ ) family itself, every phosphate adopts a different crystal structure with either layered or 3D  $[\text{MnP}_2\text{O}_7]$  framework and various Mn coordination [1, 3 - 5].

[1] S. Kaoua, S. Péchev, S. Krimi, P. Gravereau, J-P. Chaminade<sup>a</sup>, A. El Jazouli (submitted). [2] A. ElMaadi, A. Boukhari, E.M. Holt, *Journal of Alloys and Compounds* **1995**, 223, 13. [3] L. Adam, A. Guesdon, B. Raveau, *J. Solid State Chem.* **2008**, 181, 3110-3115. [4] A. ElMaadi, A. Boukhari, E.M. Holt and S. Flandrois, *CR.Acad. Sci. Paris, Set. II*, **1994**, 318,765. [5] N.K.Lokanath, M.A. Sridhar, J. Shashidara Prasad, G.S. Gopalakrishnan, K.G. Ashamanjari, *Bulletin of Materials Science (Bangalore)* **2000**, 23(3), 175-178

**Keywords:** phosphate, structure, layered

## MS25.P18

*Acta Cryst.* (2011) **A67**, C399

### Three-dimensional lanthanide MOF based on a linear ditopic dicarboxylate

Ander C. Arias,<sup>a</sup> Pau Diaz Gallifa,<sup>a</sup> Carla Martínez-Benito,<sup>a</sup> Irene Hernandez-Rodriguez,<sup>a</sup> Jorge Pasán,<sup>a</sup> Catalina Ruiz-Perez,<sup>a</sup> <sup>a</sup>Laboratorio de Rayos X y Materiales Moleculares (MatMol), Dpto. Física Fundamental II, Facultad de Física, Universidad de La Laguna, La Laguna (Spain). E-mail: achapar@ull.es

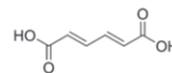
Since its first appearance, the MOF-type materials (Metal-Organic Frameworks) has shown a promising future into the materials science, due to their big applications in all fields, from structural materials (giving light and resilient structures), to their magnetic properties (opening a new field of research in the information store devices.)

For the last ten years, our research group has centered its attention upon the field of MOF-type materials, with special interest into the magnetic properties. In the preparation of these materials our strategy has been based on carboxylic ligands, using transition metal and lanthanide ions as paramagnetic centres and organic molecules containing this substituent as ligands.

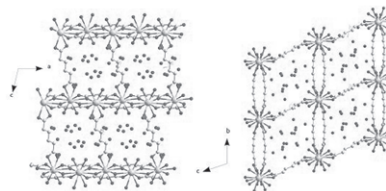
We have selected the *trans,trans*-muconic acid (**Figure 1**,  $\text{H}_2\text{ttmuc}$ ) because it is a linear, ditopic ligand with a rigid rod-like configuration. This ligand has two connection sites at both extremes, giving as a result a ligand which can act as edges in three-dimensional MOFs where the formation of cavities is favoured. The muconic acid is a dicarboxylic acid. The double unsaturated muconic acid has three isomeric forms, designated *trans,trans*-muconic acid, *cis,trans*-muconic acid, and *cis,cis*-muconic acid, which differ by the geometry around the double bonds.

Previous results of this ligand include the preparation of transition metal complexes, such as Fe[1], Cu[1], Ni[2] and Co[3], to form networks of different dimensionalities. However, the use of lanthanides remains unexplored, and thus here in we present the preliminary results

on the crystal structure of the praseodymium(III) compound (**Figures 2a & 2b**), that show that the MOF formed is three-dimensional with cavities where water molecules are hosted.



**Figure 1.** *trans,trans*-Muconic Acid ( $\text{H}_2\text{ttmuc}$ )



**Figure 2a & 2b.** Crystalline structure of  $\text{Pr}[\text{tt-muc}] \cdot \text{a.c}$

[1] C.Serre, F.Millange, S.Surble, G.Ferey, *Angew.Chem.,Int.Ed.* **2004**, 43, 6286. [2] M.H.Mir, Li Wang, Ming Wah Wong, J.J.Vittal; *Chem.Commun.* **2009**, 4539. [3] K.Yoneda, M.Ohba, T.Shiga, H.Oshio, S.Kitagawa; *Chem.Lett.* **2007**, 36, 1184.

**Keywords:** muconic acid, mof-type materials.

## MS26.P01

*Acta Cryst.* (2011) **A67**, C399-C400

### Formation of LC-phase in concentrated solutions of mono-carboxylic acids by SANS

Viktor I. Petrenko,<sup>a,b</sup> Mikhail V. Avdeev,<sup>a</sup> Vasil M. Garamus,<sup>c</sup> Viktor L. Aksenov,<sup>d,a</sup> Lászlo Rosta,<sup>c</sup> Leonid A. Bulavin,<sup>b</sup> <sup>a</sup>Joint Institute for Nuclear Research, Dubna, (Russia). <sup>b</sup>Kyiv Taras Shevchenko National University, (Ukraine). <sup>c</sup>Helmholtz-Zentrum Geesthacht, (Germany). <sup>d</sup>National Research Centre "Kurchatov Institute", Moscow, (Russia). <sup>e</sup>Research Institute for Solid State Physics and Optics, Budapest, (Hungary). E-mail: vip@nf.jinr.ru

Mono-carboxylic acids (bent non-saturated oleic acid (OA) and strictly linear saturated stearic (SA) and myristic (MA) acids) show different efficiency in stabilization of ferrofluids, in particular, regarding nano-magnetite in organic non-polar carriers [1]. The difference can be related to the interaction between acid molecules in organic non-polar solutions added to stabilized ferrofluids at the preparation stage. To clarify this point we study the concentration effects in pure solutions of OA, MA, SA based on deuterated benzene and decalin by means of small-angle neutron scattering (SANS). The behavior of the studied acids in the two solvents is quite similar. The increase in the concentration of MA and SA results in vigorous growth of solution viscosity followed by the formation of a new jelly-like phase. We associate this effect with the transition into the liquid crystalline (LC) state, which is well-known in the thermodynamics of stiff rod-like polymers. At the same time, such transition is not observed in the OA solutions.

The characteristic size of the acid molecules (2 nm) is close to the resolution limit of the SANS method. This means that only the Guinier region of the scattering curves can be reliably treated in the case of diluted isotropic solutions [2]. The important feature of the used analysis is that the dependence of the forward scattering intensity on the solute concentration is determined only by the isotropic part of the particle interaction potential [3]. The excluded volume repulsion is found to dominate over the attraction (presumably van der Waals forces) for OA and MA. In its turn, for SA the attractive component is higher than the repulsive one. This results in a shift of the transition into the liquid