

**P.09.03.12***Acta Cryst.* (2005). A61, C358**Characterization of a Novel Quaternary Dielectric Crystallographic Family**Ricardo Rodríguez-Mijangos, *Centro de Investigación en Física, Universidad de Sonora. A. P. 5-88., Hermosillo, Sonora, México.* E-mail: mijangos@cajeme.cifus.uson.mx.

In this work is reported the growth and characterization of a novel family of alkali halide crystals, produced for the mixing of four ionic salts. These quaternary crystals imply the existence of four ternary crystals [1] and six known binary crystals. The characterization is applied to two crystals with different component concentration, one of these with a Europium impurity. It was obtained the lattice constant by X ray diffractometry. The optical absorption spectra of irradiated crystals shown a single F band. The Generalized Vegard's law, applied to the novel ternary system recently studied [2], was extended to the quaternary crystal. Good agreement with the experimental results was obtained.

[1] Mijangos R. R., Cordero-Borboa A., Camarillo E., Riveros H., Castaño V., *Physics Letters A*, 1998, **245**, 123. [2] Mijangos R. R., Cordero-Borboa A., Alvarez E., Cervantes M., *Physics Letters A*, 2001, **282**, 512.

**Keywords:** solid solutions, accurate lattice parameters measurements, absorption spectroscopy experimental

**P.09.03.13***Acta Cryst.* (2005). A61, C358**Co(II) *n*-alkyl Phosphonates: Examples of Hybrid Organic-inorganic Compounds**

Elvira M. Bauer<sup>a</sup>, Carlo Bellitto<sup>a</sup>, Marcello Colapietro<sup>b</sup>, Said A. Ibrahim<sup>c</sup>, Mohamed R. Mahmoud<sup>d</sup>, Gustavo Portalone<sup>b</sup>, Guido Rigini<sup>a</sup>, <sup>a</sup>*DISM-CNR, Monterotondo, Italy.* <sup>b</sup>*Department of Chemistry, University of Rome "La Sapienza", Rome, Italy.* <sup>c</sup>*Department of Chemistry, University of Assiut, Assiut, Egypt.* E-mail: Elvira.Bauer@ism.cnr.it

Organic-inorganic hybrids like metal alkyl phosphonates are very flexible systems because of the possibility of designing the organic moiety [1]. In this work we present our studies on the synthesis and single crystal structure determination of two new Co(II) *n*-alkyl phosphonates, i.e. Co(II) *methyl*-phosphonate, Co[(CH<sub>3</sub>PO<sub>3</sub>)(H<sub>2</sub>O)], and Co(II) *ethyl*-phosphonate, Co[(C<sub>2</sub>H<sub>5</sub>PO<sub>3</sub>)(H<sub>2</sub>O)]. Cobalt(II) *methyl*-phosphonate, crystallizes in the orthorhombic space group *Pna*2<sub>1</sub> with *a*=17.408(6)Å, *b*=4.790(3)Å, *c*=5.652(1)Å. Cobalt(II) *ethyl*-phosphonate crystallizes in the monoclinic space group *Pn*, with the following unit-cell parameters: *a*=4.806(2)Å, *b*=10.243(3)Å, *c*=5.674(1)Å and β=90.56(3)°. An hybrid layered structure made of alternation of inorganic and organic layers was found for both Co alkyl phosphonates. In both cases the inorganic layer is based on distorted [CoO<sub>6</sub>] chromophores with five oxygens from the [PO<sub>3</sub>]<sup>2-</sup> group and one from the water molecule. The organic layer is composed by the alkyl groups of the adjacent ligands with van der Waals contacts between them.

[1] See for example "Functional Hybrid Materials" P. Gomez-Romero & C. Sanchez Eds., Wiley&VCH, 2004.

**Keywords:** crystal engineering, organic hybrid materials, metal phosphonates

**P.09.04.1***Acta Cryst.* (2005). A61, C358**Crystal Packing in Co(II) Pyromellitate Complexes tuning the Water Aggregation**

Oscar Fabelo<sup>a</sup>, Laura Cañadillas-Delgado<sup>a</sup>, Fernando S. Delgado<sup>a</sup>, María Laz<sup>a</sup>, María Hernández-Molina<sup>a</sup>, Catalina Ruiz-Pérez<sup>a</sup>, Francesc Lloret<sup>b</sup>, Miguel Julve<sup>b</sup>, <sup>a</sup>*Laboratorio de Rayos X y Materiales Moleculares, Universidad de La Laguna, Spain.* <sup>b</sup>*ICMOL/Departament de Química Inorgànica, Universitat de València, Spain.* E-mail: caruiz@ull.es ; orfabelo@ull.es

Three different polymeric complexes were designed and synthesized from Co(II) and 1,2,4,5-benzenetetracarboxylic acid (H4-

bt). These complexes exhibit a zeolite-like structure; which cavities are suitable to host water molecules. The dimensionality and crystal packing depend on the syntheses methods. Closer packed structures are obtained from gels to hydrothermal method synthesis.

The clusters of water play an important role in the stabilization of supramolecular systems [1], their structural study is important for understanding the behavior of biological systems. A great number of metal-organic frameworks (MOF) have been reported to accommodate clusters and chains of water [2]. We present herein three cobalt(II) MOF's where the crystal packing controls and templates the formation of different kinds of water aggregation (discrete clusters or nanowires).

Stabilization of guest molecules is due to weak directional intermolecular forces such as hydrogen bonds. Special attention has been paid to these interactions for understanding the anchoring between host-guest molecules.

[1] Ludwig R., *Angew. Chem. Int.*, 2001, **40**, 1808-1827. [2] Yaghi O. M., O'keeffe M., Ockwig N.W., Chae H. D., Eddaoudi M., Kim J., *Nature*, 2003, **432**, 705-714.

**Keywords:** hydrothermal method, gels, water structure

**P.09.04.2***Acta Cryst.* (2005). A61, C358**Alkali-Templated Malonate Copper(II) Complexes**

Fernando S. Delgado<sup>a</sup>, Joaquín Sanchiz<sup>a</sup>, Catalina Ruiz-Pérez<sup>a</sup>, Francesc Lloret<sup>b</sup>, Miguel Julve<sup>b</sup>, <sup>a</sup>*Laboratorio de Rayos X y Materiales Moleculares, Universidad de La Laguna, Spain.* <sup>b</sup>*ICMOL/Departamento de Química Inorgànica, Universitat de València, Spain.* E-mail: caruiz@ull.es; fersdt@ull.es

In the context of our copper(II) malonate complexes studies [1,2], we have synthesized and characterized the compounds of formula {[A(H<sub>2</sub>O)<sub>n</sub>]<sub>2</sub>[Cu(mal)<sub>2</sub>(H<sub>2</sub>O)<sub>m</sub>]} (A = Li, Na, K, Rb, Cs).

The structure of these compounds consists of [Cu(mal)<sub>2</sub>(H<sub>2</sub>O)<sub>m</sub>]<sup>2-</sup> anions and [A(H<sub>2</sub>O)<sub>n</sub>]<sup>+</sup> cations that are held together by means of carboxylate bridges and water molecules leading to three-dimensional networks.

We want to show how the size of alkali metal ion can control the malonate-bridged copper(II) structure, so we have analyzed the networks that both cationic and anionic units build up.

First, the [A(H<sub>2</sub>O)<sub>n</sub>]<sup>+</sup> units are connected through μ-oxo bridges affording thus, different cationic structures: dimmers (Li), single chains (Na, K), double helical chains (Rb) and layers (Cs).

Depending on the alkali metal ion the [Cu(mal)<sub>2</sub>(H<sub>2</sub>O)<sub>m</sub>]<sup>2-</sup> units are linked to other ones through malonate carboxylate bridges to give anionic networks exhibiting different topologies: monomers (Li, Cs), chains (Rb) and layers (Na, K).

We have also studied the magnetic properties of these compounds. The behaviour being ferromagnetic when the copper(II) units are connected through *anti-anti* carboxylate bridges (Na, K, Rb).

[1] Pasán J., Delgado F.S., Rodríguez-Martín Y., Ruiz-Pérez C., Sanchiz J., Lloret F., Julve M., *Polyhedron*, 2003, **22**, 2143. [2] Delgado F.S., Ruiz-Pérez C., Sanchiz J., Lloret F., Julve M., *Cryst.Eng.Comm.*, 2004, **6**, 443.

**Keywords:** carboxylic acids, alkali metal anionic salts, crystal engineering

**P.09.04.3***Acta Cryst.* (2005). A61, C358-C359**(4,4)-Metal-Organic Framework Templated by 1,2,3,4-Butanetetracarboxylic Acid**

Laura Cañadillas-Delgado<sup>a</sup>, Óscar Fabelo<sup>a</sup>, Fernando S. Delgado<sup>a</sup>, Catalina Ruiz-Pérez<sup>a</sup>, Francesc Lloret<sup>b</sup>, Miguel Julve<sup>b</sup>, <sup>a</sup>*Laboratorio de Rayos-X y Materiales Moleculares, Universidad de La Laguna, Spain.* <sup>b</sup>*ICMOL/Departament de Química Inorgànica, Universitat de València, Spain.* E-mail: caruiz@ull.es; ldelgado@ull.es

The design or selection of a suitable ligand containing certain features, such as flexibility, versatile binding modes and ability to form hydrogen bonds are crucial in the building of polymeric complexes. In this line we have chosen a new ligand, known as 1,2,3,4-butanetetracarboxylic acid, which possesses several