changes of molecular packing, but do not affect the unit cell volume. The thermal hysteresis is connected with changes of weak hydrogen bonds in HS and LS state [5].

[1] P. Gütlich, A. Hauser, H. Spiering, Angew. Chem. Int. Ed. Engl. 1994, 33, 2024. [2] P. Gütlich, H.A. Goodwin (eds.), Top. Curr. Chem. 233, 234, 235, Springer, Berlin, Heidelberg, New York, 2004. [2] Z.J. Zhong, J.Q. Tao, Z. Yu, C.Y. Dun, Y.J. Liu, X.Z. You, J. Chem. Soc., Dalton Trans. 1998, 327. [3] Z. Yu, K. Liu, J.Q. Tao, Z.J. Zhong, X.Z. You, G.G. Siu, Appl. Phys. Lett. 1999, 74, 4029. [5] J. Kusz, M. Zubko, A. Fitch, P. Gütlich, Zeitschrift für Kristallographie, in press.

Keywords: iron(II), spin transition, phase transition

## MS66.P24

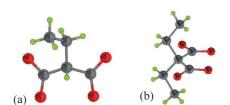
Acta Cryst. (2011) A67, C646

## Novel Compounds Based on Malonate Derivatives and 4,4'-Azobispyridine.

<sup>a</sup>Irene Hernández-Rodríguez, <sup>a</sup> Mariadel Déniz, <sup>a</sup> Jorge Pasán, <sup>a</sup> Oscar Fabelo, <sup>b</sup> Laura Cañadillas-Delgado, <sup>b</sup> Consuelo Yuste, <sup>c</sup> Catalina Ruiz-Pérez<sup>a</sup>. <sup>a</sup>Laboratorio de Rayos X y Materiales Moleculares (MATMOL), Departamento de Física Fundamental II, Facultad de Física, Universidad de La Laguna. <sup>b</sup>Institut Laue Langevin, B.P. 156, 6, Grenoble, France and Instituto de Ciencia de Materiales de Aragón, CSIC-Universidad de Zaragoza, Zaragoza, Spain. <sup>c</sup>Physics Department. CEMDRX Rua Larga, Universidade de Coimbra, P-3004-516, Coimbra, Portugal. Email: i.hdez.rguez@gmail.com

The assembly of inorganic coordination polymers, or metal-organic frameworks (MOFs), have been remarkably developed in recent years due to the combination of the efficience of their synthesis from relatively simple subunits and their potential applications in a wide variety of research fields. Moreover, this kind of complexes exhibits a vast range of supramolecular architectures with different dimensionalities  $-1\mathrm{D}, 2\mathrm{D}$  and  $3\mathrm{D}.$ 

The conformational flexibility of the aliphatic dicarboxylate type ligands is reflected in the diversity of their connecting modes and it is essential for the self-assembly processes. For the other hand, rigid rod-like spacer molecules like 4,4'-azopyridine



**Figure 1.** Aliphatic dicarboxylic acids used as bridging ligands in the different syntheses: (a) Ethylmalonic acid. (b) Diethylmalonic acid.

(azpy) can be used to control topologically the resultant architectures because it can act as pillars between metallic ions to connect one-dimensional or two-dimensional networks, leading to robust structures of bigger dimensionality.

Here we present the synthesis, structural characterization and magnetic properties of a series of novel transition metal compounds based on dicarboxylic acids derived from the malonic acid (such as the ethylmalonic or diethylmalonic acids) and the 4,4'-azobispyridine as bridging ligands.

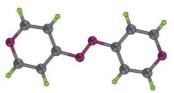


Figure 2. 4,4'-azobispyridine.

Keywords: Crystal Structure, Carboxylic acids, Metal-Organic Frameworks.

## MS66.P25

Acta Cryst. (2011) A67, C646

## Influence of the substituent in the coordination chemistry of R-Malonates.

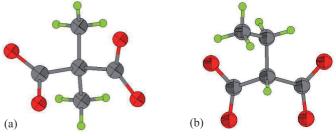
Mariadel Déniz, a Jorge Pasán, a Irene Hernández-Rodríguez, a Oscar Fabelo, b Laura Cañadillas-Delgado, b Miguel Julve, c Catalina Ruiz-Pérez. a Laboratorio de Rayos X y Materiales Moleculares (MATMOL), Departamento de Física Fundamental II, Facultad de Física, Universidad de La Laguna, Avda. Astrofísico Francisco Sánchez s/n, E-38071 La Laguna, Tenerife, Spain. b Present address: Institut Laue Langevin, B.P. 156, 6 Rue J. Horowitz, 38000, Grenoble, France and Instituto de Ciencia de Materiales de Aragón, CSIC-Universidad de Zaragoza, Pedro Cerbuna 12, 50009 Zaragoza, Spain. c Instituto de Ciencia Molecular (ICMol)/Departament de Química Inorgànica, Universitat de València, Polígono La Coma s/n, 46980 Paterna (València), Spain. E-mail: mdeniz@ull.es

Metal-organics frameworks (MOFs) exhibit fascinating structural topologies and potential applications as multifunctional materials, and this is the cause of the rapidly and increasing development of this kind of complexes in recent years.[1] The rational design of MOFs lies in an appropriate choice of the kind of metal ions and the number of coordination modes provided by the organic ligand, such as the rigidity or flexibility of the ligands used.

Polycarboxylic acids are well known due to their flexibility, which gives rise to a great variety of their connecting modes that lead from discrete entities to 3D networks,[2] so they constitute an important family of mutidentate-donor ligands. Specifically, malonic acid is widely used due to its excellent coordination ability. This ligand ocuppies one or two coordination positions of the coordination sphere, neutralizing positive charges of the metal ion. Moreover, modifying this acid, we can increase the degree of control over the intermolecular interactions and improve the structural and physic properties of these compounds.

In the context of molecular magnetism, on the other hand, the study of the magneto-structural correlations allow us to understand the structural and chemical factors that govern the exchange coupling between paramagnetic centres through multiatomic bridges.

We present herein the synthesis, structural characterization and magnetic properties of a series of new copper(II) compounds based on substituted malonate ligands, such as ethylmalonic or dimethylmalonic acid, emphasizing the role of the different intermolecular interactions present in the structures.



**Figure 1.** Some aliphatic dicarboxylic acids used as bridging ligands in the syntheses: (a) Dimethylmalonic acid. (b) Ethylmalonic acid.

[1] F. Lloret, G. De Munno, M. Julve, J. Cano, R. Ruiz, A. Caneschi. *Angew. Chem., Int. Ed.*, **1998**, *37*, 135. J. Pasán, J. Sanchiz, F. Lloret, M. Julve, C. Ruiz-Pérez. *CrystEngComm*, **2007**, *9*, 478-487. C. Janiak. *J. Chem. Soc., Dalton Trans.*, **2003**, 2781. [2] S. I. Stupp, P. V. Braun. *Science*, **1997**, 277, 1242.

Keywords: copper, magnetism, dicarboxylic acids, intermolecular interactions, weak interactions, crystal packing.