MS31- The role of supramolecular interactions in polymorphs and co-crystals

Chairs: Dr. Laszlo Fabian, Prof. Mino R. Caira

MS31-P01

Polymorphism in a 2D Copper(I) coordination polymer based on a flexible ligand

Olaya Gómez-Paz[1], Rosa Carballo[1], Ezequiel M. Vázquez-López[1], Ana B. Lago[2]

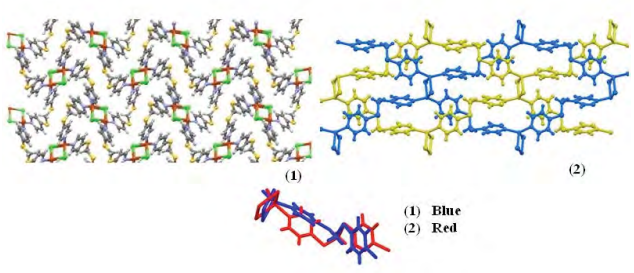
1. Departamento de Química Inorgánica, Instituto de Investigación Sanitaria Galicia Sur (IISGS) - Universidade de Vigo, E-36310 Vigo, Galicia, Spain
2. Laboratorio de Rayos X y Materiales Moleculares, Departamento de Física Fundamental - Universidad de La Laguna., E-38204 La Laguna, Tenerife, Spain

email: olgomez@uvigo.es

Coordination polymers (CPs) based on organic flexible ligands are promising materials due to their potential dynamic behaviour. In addition, the use of such kind of ligands allows the formation of polymorphic isomers which can be isolated in certain synthetic and crystallization conditions.

In this work, we describe two polymorphic forms (**1** $P2_1/c$ and **2** $C2/c$) for the 2D coordination polymer $^{2}_{\infty}$[CuCl(4bpytm)] containing the spacer bis(4-pyridylthio)methane (4bpytm) which has proven its conformational flexibility in other coordination polymers [1]. Both Cu(I) compounds are obtained by a hydrothermal procedure from Cu(II) precursors. Crystals of **1** are isolated from a reaction using busulfan or procainamide hydrochloride and crystals of **2** results from a direct reaction between the ligand and the Cu(II) salt. It is interesting to note that the type of arrangement observed here have been only scarcely observed for this ligand [2,3].

The two compounds are 2D networks achieved by the bridging role of 4bpytm ligand and the Cu_2Cl_2 core. The ligand in the two compounds shows very different torsion angles and this fact lets that (**2**) have got interpenetration in its laminar structure whereas in (**1**) the sheets are parallel stacked.



References:

[1] A. Amoedo-Portela, R. Carballo, J.S. Casas, E. García-Martínez, A. B. Lago-Blanco, A. Sánchez-González, J. Sordo, E. M. Vázquez-López. Z. Anorg. Allg. Chem. 2005, 631, 2241-2246.
[2] L. Hou, W.-J. Shi, Y.-Y. Wang, B. Liu, W.-H. Huang, Q.-Z. Shi. CrystEngComm, 2010, 12, 4365-4371.
[3] L. Zang, H.-Y. Xie, W.-J. Shi. Acta Cyst, 2008, C64, m76-m78.

Keywords: copper(I) complexes, coordination polymers, crystal structures, metallosupramolecular chemistry.