

The experiments we have carried out with these compounds in gel media demonstrate the formation of different and new structures, even in the same U-tube (see Figure). This kind of experiment shows the possibility to tune the conditions to prepare new phases of these coordination polymers.

[1] L. Carlucci, G. Ciani, J.M. García-Ruiz, M. Moret, D.M. Proserpio, S. Rizzato, *Crystal Growth & Design* **2009**, *9* (12), 5024–5034. [2] C. Daiguebonne, A. Deluzet, M. Camara, K. Boubekeur, N. Audebrand, Y. Gérault, C. Baux, O. Guillou, *Crystal Growth & Design* **2003**, *3* (6), 1015–1020. [3] L.-P. Hsu, J.-Y. Wu, K.-L. Lu, *J.Inorg.Organomet.Polym.Mater.* **2007**, *17* (1), 259-265. [4] F. A. Almeida Paz, Y.Z. Khimyak, J. Klinowski, *Acta Cryst.* **2003**, *E59*, m8-m10.

**Keywords:** gel media, crystal growth, coordination polymers.

## MS24.P70

*Acta Cryst.* (2011) **A67**, C384

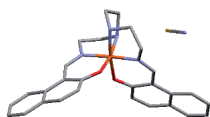
### New iron (III) two-step spin crossover compounds

Isabel C. Santos, Bruno J.C. Vieira, Laura C.J. Pereira, Vasco Gama, *Dep. Química, ITN/CFMC-UL, 2686-953 Sacavém, (Portugal)*. E-mail: icsantos@itn.pt

In recent years researcher's developed an effort to obtain molecular-based functional materials exhibiting properties of technological interest. Spin Crossover (SCO) emerges as a very powerful tool to be employed in such research.

In octahedral ligand fields, transition metal ions with d4-d7 configuration can assume a high-spin (HS) or a low-spin (LS) electronic arrangement, depending if the crystal field energy is lower or higher than the main spin pairing energy. In some of these cases bistability can take place, i.e. LS-HS transitions occur at different temperatures, they can be gradual or occur abruptly, eventually with an hysteresis loop. These materials possess increased interest in view of their possible application as display, memory and switching devices [1,2].

The two-step spin crossover of a new iron(III) compound [Fe<sup>III</sup>(Nst)]SCN is studied by magnetic and crystallographic methods revealing two spin transitions with an ordered intermediate phase built by the repetition of the [HS–LS] motif. Crystallographic data were collected on a single crystal temperatures between ; 50 and 294K. The structures collected at 50, 150 and 294 K are reported here.



[1] P. Gütllich, A. Hauser, H.C. Spiering, *Angew. Chem. Int. Ed.* **1994**, *33*, 2024. [2] J.A. Real, A.B. Gaspar, M.C. Munoz, *J Chem. Soc. Dalton Trans.* **2005**, 2062 .

**Keywords:** spin crossover, X-ray diffraction

## MS24.P71

*Acta Cryst.* (2011) **A67**, C384

### Solid-state synthesis and structure solution of chiral co-crystals and salts

Laura Chelazzi, Fabrizia Grepioni, Dario Braga, *Department of Chemistry "G. Ciamician", University of Bologna, (Italy)*. E-mail: laura.chelazzi@unibo.it

Co-crystallization provides a new strategy for altering the chemical and physical properties of molecular solid forms. The possibility of co-crystallization has to take into account the competition with kinetic factors associated with the nucleation stage of the crystallization processes. A way to overcome the thermodynamic-kinetic dualism is the “solvent-free” condition. It has also been shown that, in some systems, chiral recognition can affect solid state reactions just as it does in solution chemistry, and that products of grinding and solution experiments can be different [1],[2].

In the present work we make use of solution experiments and mechano-chemical techniques to obtain co-crystals or salts of chiral compounds [3]. For this purpose, serine(-), serine(+), serine-/+ and dicarboxylic acids were chosen as starting materials. Salts and co-crystals obtained were studied by single-crystal and powder X-ray diffraction methods, showing the formation of different polymorphs depending on the synthetic method (crystallization from solution, grinding or kneading). The new salts were also studied by thermal analysis (DSC, TG) and variable-temperature X-ray powder diffraction to check their thermal stability.

[1] R. Kuroda, Y. Imai and T. Sato, *Chirality* **2001**, *13*, 588; [2] S. Chen, H. Xi, R. F. Henry, I. Marsden and G. G. Z. Zhang, *CrystEngComm* **2009**, *11*,427; [3] D. Braga, F. Grepioni and G. I. Lampronti, *CrystEngComm* **2011**, Advance Article DOI: 10.1039/C0CE00576B

**Keywords:** polymorphism, X-ray, amino acids

## MS24.P72

*Acta Cryst.* (2011) **A67**, C384-C385

### Single-crystal to single-crystal transformations of a flexible porous Zn(II) framework

Ilne Grobler, Vincent J. Smith, Prashant Bhatt, Leonard J. Barbour, *Department of Chemistry, Stellenbosch University (South Africa)*. E-mail: ilne@sun.ac.za

Host-guest complexation by metal-organic frameworks (MOF's) is a highly topical area of research owing to applications in storage, separation and delivery of guest molecules. In particular, dynamic frameworks with guest responsive properties are essential for improved selectivity and controlled uptake and storage purposes [1]. Guest removal and exchange processes often result in collapse of a host framework and/or loss of the single-crystal quality of the material. In exceptional cases, these processes occur as single-crystal to single-crystal transformations that can be studied directly using single crystal X-ray diffraction.

Our investigation centers on the permanent porosity and exchange of guest molecules, by a three-dimensional Zn(II) MOF ([Zn(L)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>]CH<sub>3</sub>OH, see Fig. 1) that has well-defined one-dimensional, square-shaped channels. Significant structural changes occur when the host framework accommodates different guest molecules whilst retaining its single crystal-nature.

The MOF consists of two-dimensional layers or nets stacked on top of one another and interconnected by polymeric metal-water-metal coordination. The as-synthesized framework includes methanol molecules hydrogen bonded to the framework. The crystals are remarkably robust and remain transparent following removal of the methanol molecules at 150°C under reduced pressure. A series of exchange experiments were carried out, all of which occurred *via* a single-crystal to single-crystal process.