Poster Sessions

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

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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(4"Nds)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 30 and 294K. The structures collected at 50, 150 and 294 K are reported here.


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

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

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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.


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