Solid State Transformations: A Gate to Polymorphism or Multi-stability in SCO Coordination Complexes

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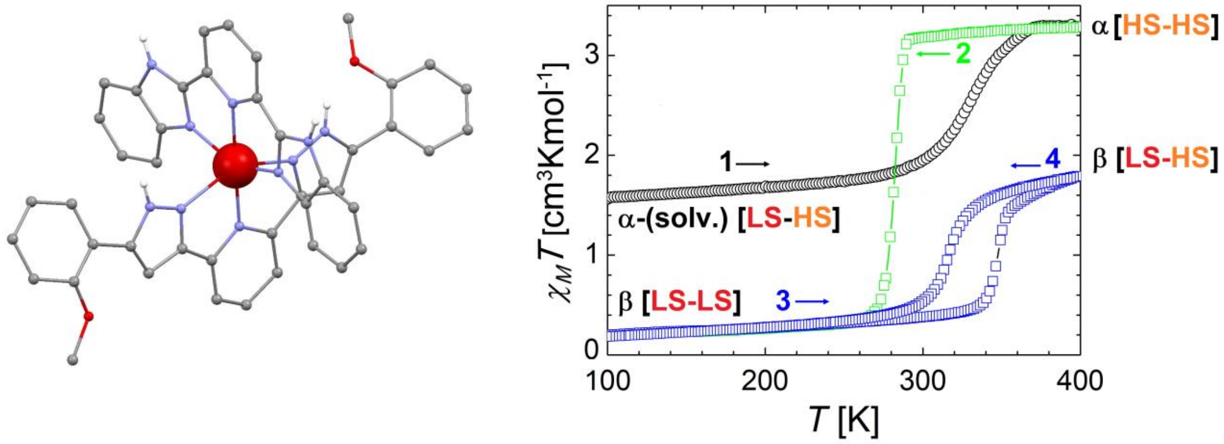
Spin Crossover (SCO) coordination complexes are a rich source of molecular switchable materials for potential spintronic applications. In the solid state, the SCO often couples with crystallographic transitions and/or changes to the composition of the crystal lattice. When such transformations occur in a single-crystal-to-single-crystal (SCSC) manner, X-ray diffraction constitutes a valuable window of information to exploit these solid-state reactions. This rarely happens with materials made of discrete molecules, where the intermolecular interactions may not suffice to preserve the integrity of the single crystals. We have developed a series of Fe(II) SCO complexes with crystal lattices flexible enough to allow a great variety of solid state transformations, while sufficiently robust to maintain single crystal integrity.[1] Some of these compounds have unveiled unique features of solid-state transformations coupled to SCO processes. These include, i) the formation of intermediate phases within a single crystal during the reaction,[2] solid-state pathways to reach polymorphs of SCO compounds,[3] a succession of irreversible phase transitions delineating four different thermal pathways providing four possible magnetic responses, depending on the thermal history of the sample (Figure).



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2 G. Aromí, C. Beavers, J. S. Costa, G. Craig, O. Roubeau, *et al.Chem. Sci*., **2016**, *7*, 2907
3 C. Bartual, C. Codina, O. Roubeau, G. Aromí, *Chem., Eur. J.* **2016**, *22,* 12767.