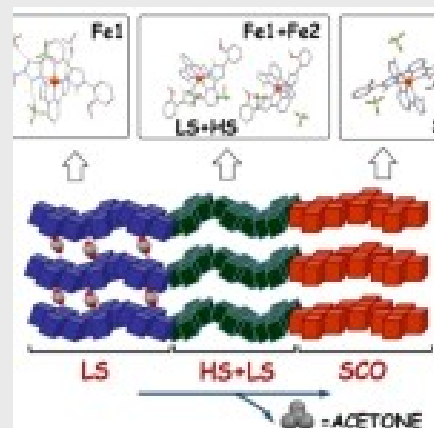


Crystallographic Transitions Coupled to Spin Crossover in Molecular Complexes

Date: Friday 13 February, 12h00, 2015.

Place: Department of Theoretical Condensed Matter Physics, Facultad Ciencias, Module 5, Seminar Room (5th Floor).

Speaker: Guillem Aromí, Group of Magnetism and Functional Molecules (GMMF) Universitat de Barcelona, Barcelona, Spain.



Abstract:

Spin crossover (SCO) is a switch of spin states that may be seen in some octahedral d4 to d7 transition metals, triggered by external stimuli, also involving changes to other properties. In the case of Fe(II), it causes dramatic variations in bond distances to the metal and other parameters. Thus, when the spin active species lay connected by intermolecular interactions within a crystal, long range effects may induce cooperativity to this transition and often, a hysteresis loop, which is the signature of bistability. The intimate relation between structure and spin, very often results in intricate coupled crystallographic/magnetic transitions during SCO. In order to unveil the details of such coupling, we have designed ligands for the preparation of Fe(II) SCO complexes with dense arrays of intermolecular interactions [1-4]. This work has uncovered intriguing correlations spin state / crystallographic order [1,3] and in particular, reversible solvent desorption processes involving spin transitions and drastic crystallographic changes, as shown by single crystal X-ray crystallography.[5] Remarkably, these transitions occur through an intermediate spin and crystallographically ordered phase, also fully characterized. Astonishingly, several combinations of these three phases have been demonstrated by single crystal X-ray diffraction to coexist within one single crystal.

References:

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