Poster Presentation

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Intermolecular interaction studies of complexes with N_4O_2 coordination sphere

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The Spin-Crossover (SCO) phenomenon implicates a switchable between a low-spin (LS) diamagnetic state, which is stable at low temperatures and a paramagnetic high-spin state (HS), which is stable at higher temperatures. This transition is generated by an external perturbation such as temperature, pressure or light. In general, the switching process in solid-state systems is controlled by cooperative intermolecular interactions. The correlation of structure with physical properties is crucial to the identification of these interactions and ultimately the understanding of the complex processes that control the SCO phenomenon[1]. Since the last decade, different research groups have studied the structural, optical and magnetic properties of complexes with N_2O_4 coordination sphere, containing Schiff Base ligands.[2]
With the aim of understanding the relationship between the intermolecular interactions and the magnetic properties, we carried out the syntheses and crystal structure analysis of a series of Fe(III) and Mn (III) complexes with N_2O_4 coordination sphere.

The Schiff base ligands were synthesised from condensation reaction between 5-subsituted-salicylaldehyde and 1,2-bis(3-aminopropylamino)ethane and the complexes were formed using differents Fe(III) and Mn(III) salts with different counterions(ClO_4^-, NO_3^-, BF_4^-, $CF_3SO_3^-$). The crystal structures show the metal centres are hexacoordinated (MN_4O_2) and the coordination polyhedron can be described as a distorted octahedron formed by the 4 N atoms of the tetraamine fragment and 2 hydroxyl O atoms from the salicylaldehyde in a trans configuration (see Figure).
Finally, we studied the intermolecular interactions using Crystal Explorer Software[3] between the complexes, the counterion or the solvating molecule, the most remarkable features observed are type II halogen···halogen intermolecular interactions or O-H···O hydrogen bond interactions, these interactions could stabilise the high spin and the SCO state.

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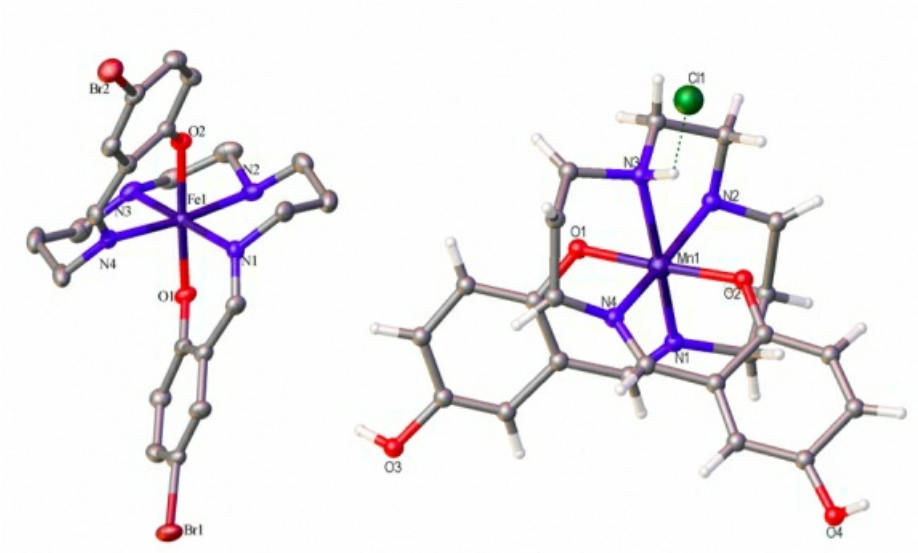

ORTEP of Fe(III) complex (left) and Mn(III) complex (right)

Keywords: Schiff base ligands, Iron(III) complexes, Mn(III) complexes