

Poster Presentation

MS83.P04

Structural Studies of Iron(III) Complexes with N4O2 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]. With the aim of developing new SCO materials, we carried out the syntheses and crystal structure analysis of seven iron(III) complexes, mixing 5-bromo-salicylaldehyde or 5-chloro-salicylaldehyde and ethylenediamine with iron(III) chloride and/or ammonium hexafluorophosphate solutions by slow diffusion or reflux in methanol or 2-propanol (figure 1). The crystal structures show the iron(III) centre is hexacoordinated (FeN4O2) and the coordination polyhedron can be described as a distorted octahedron formed by the 4 N atoms of the ethylenediamine fragment and 2 hydroxyl O atoms from the salicylaldehyde fragment, this distortion was evaluated at 120 and 298 K, the major distortion were observed in complexes [2]⁺ PF₆⁻ MeOH, [2]⁺ PF₆⁻ iPrOH and [1]⁺ PF₆⁻ MeOH, which is characteristic in HS states, while the complexes [2]⁺ Cl⁻ iPrOH, [1]⁺ PF₆⁻ iPrOH [2]⁺ and [2]⁺ ClO₄⁻, shows a minor distortion according to LS states. On the other hand, [1]⁺ ClO₄⁻ is a SCO complex with a typical geometry for both spin states at 120 K (LS) and 298 K (HS). Finally, we studied the intermolecular interactions using Crystal Explorer Software[2] between the iron complexes, the counterion and/or the solvate molecule, for instance, in the [2]⁺ PF₆⁻ MeOH complex, the most remarkable feature observed are Br...Br intermolecular interactions (figure 2). ACKNOWLEDGMENTS: FONDECYT N° 1130640, FONDEQUIP EQM120095 and Beca CONICYT folio 21130944

[1] Tissot, R Bertoni, E2. Collet, L. Toupet, M-L Boillot, (2011) *J. Mater. Chem.*, 21, 18347-18353., [2] M. A. Spackman, D. Jayatilaka, (2009) *CrystEngcomm* 11, 19.

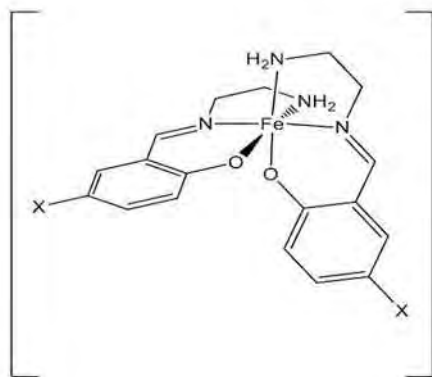


Figure 1: Schematic structure for [1]⁺; X = Cl and [2]⁺; X = Br

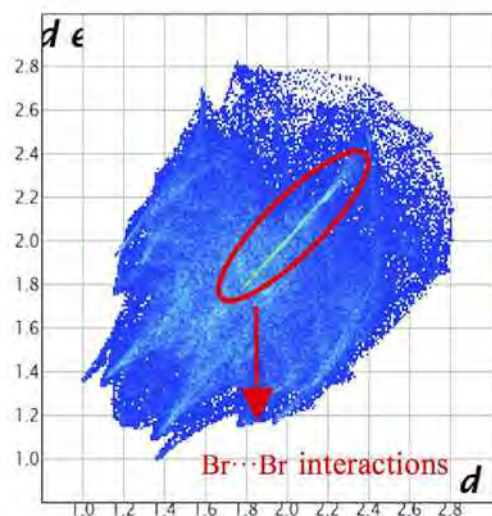


Figure 2: Hirschfeld surface for [2]⁺ PF₆ MeOH

Keywords: iron complexes, Schiff base ligands, spin-crossover complexes