Structural study by X-ray diffraction of iron (III) complexes

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The compounds with Spin-crossover (SCO) phenomenon have a reversible exchange between a low spin (LS) state that is stable at low temperatures and a high spin (HS) state that is stable at high temperatures. In general, the reversible process in solid systems is controlled by intermolecular cooperatives interactions [1]. The correlation between the structures with the physical properties is crucial for the interaction's identification and the understanding of the complex processes that control the phenomenon SCO. Most of the materials SCO studied are complexes with 3d4 – 3d7 metals with coordination sphere N2O4 [1-2]. Structural studies were performed comparing the structures of a series of complexes informed in this work and previously described by our research group [2] to establish relationships with magnetic properties [3].

This work aims to carry out a structural study of complexes with coordination sphere N4O2, for which purpose iron (III) complexes have synthesized from FeBr2 and FeCl3 salts with hexadentate and tridentate ligands forming octahedral systems. These complexes have been characterized by FT-IR, UV-vis spectroscopy and single-crystal X-ray diffraction.

Using the crystallographic data is possible to determine, in octahedral complexes, the distortion of the coordination sphere during the spin transition determining the distortion parameters. For instance, in the complex [C1] Br, the distances between Fe atom to atoms in the coordination sphere were similar in the range of 170 K to 298 K, wherefore the octahedral parameters not undergo a significant change ($\sum^{o}$/ 79.5 a 170 K y 80.1 a 298 K y Θ^{o}/ 226.1 a 170 K y 229.1 a 298 K). These parameters indicate that in that temperature range, this complex is in High Spin State.

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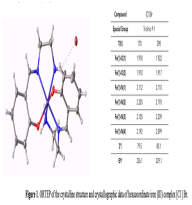

Figure 1