

MS13-2-12 Structural study of a new family of heteroleptic iron(III) [Fe(NSO)(N₂O)] coordination compounds #MS13-2-12

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Abstract

Spin-crossover properties of homoleptic Iron(III) complexes containing two tridentate Schiff base ligands [FeN₄O₂] have been amply reported in the last decade[1]. However, to the best of our knowledge, few examples of a heteroleptic iron(III) coordination compound with Spin-crossover (SCO) properties has been recently published[2]. According to this, and intending to develop new materials with SCO properties, we carried out the synthesis and characterisation of three new heteroleptic iron(III) [Fe(NSO)(N₂O)] **C1-3** coordination compounds. These complexes are the first complexes that contain tridentate organometallic Schiff base ligands derivate of ferrocenyl b-diketones.

The structural analysis, by single-crystal X-ray Diffraction, revealed that the structures of the compounds are isostructural and crystallize in the tetragonal space group I4/a, containing a molecule of the neutral Fe(III) complex in the asymmetric unit. In addition, this analysis showed that the metallic centre of iron is coordinated by the NSO atoms belonging to the organic ligand H₂thsa (thiosemicarbazone-salicylaldimine) L1 and the N₂O atoms corresponding to one of the different organometallic ligands **L2**. (**Fig 1**). Regarding to this, the octahedral distortion parameters for **C1-3** exhibit large values, consistent with the high-spin electronic state (HS) of the Fe(III) complexes at 170K and 290K.

We are currently carrying out structural studies through XRD at 100K and magnetic properties through magnetic susceptibility, with the purpose of deepening key aspects that govern the structural and magnetic properties, crucial for the rational design of SCO systems.

References

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[2] W. Phonsri, V. Martinez, C.G. Davies, G.N.L. Jameson, B. Moubaraki, K.S. Murray, *Chem. Commun.* (2016), 52, 1443–1446. W. Phonsri, L. C. Darveniza, S. R. Batten, K. S. Murray, *Inorganics* (2017), 5, 13747–13753.

Fig 1. Ball and stick diagram for C1-C3.

