

MS36-P02

Powder X-ray diffraction structural characterization and applications of cis-[Co^{II}(κ²N,N'-1,10-phenanthroline-5,6-dione)₂Cl₂]

Olufunso Olumide Abosedel¹, José Fernandes², Simona Galli²

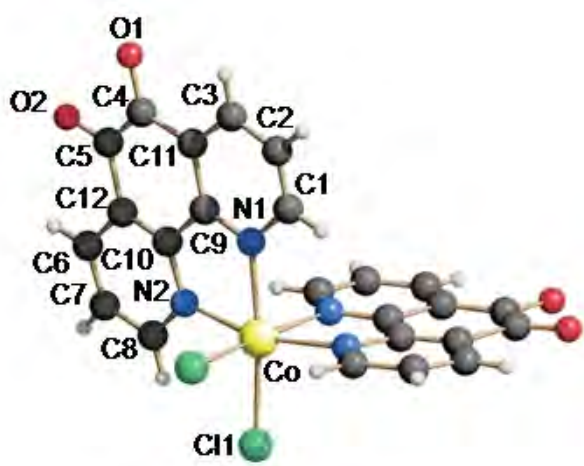
1. Department of Chemistry, Federal University Otuoke, Otuoke via Yenagoa, Nigeria
2. Dipartimento di Scienza e Alta Tecnologia, Università dell'Insubria, via Valleggio 11, 22100, Como, Italy

email: abosedeo@fuotuke.edu.ng

1,10-phenanthroline-5,6-dione (phendione) is a versatile ligand that has been used in the preparation of stable homo- and hetero-metallic complexes with a wide range of transition metal ions [1]. Phendione itself possesses electrochemical and strong biological activity including antifungal, DNA and cytotoxic activity [2-3]. It has been shown that its biological activity increases upon complexation with a wide range of metal ions, such as Ag⁺, Cu²⁺, Pt²⁺ [2-3].

This poster presents the synthesis and powder X-ray diffraction (PXRD) structural characterization of cis-[Co^{II}(κ²N,N'-1,10-phenanthroline-5,6-dione)₂Cl₂]. PXRD details, unit cell parameters, and space group for cis-[Co^{II}(κ²N,N'-1,10-phenanthroline-5,6-dione)₂Cl₂], C₂₄H₁₂Cl₂CoN₄O₄, are reported [a = 41.4951 (13) Å, b = 8.2768 (2) Å, c = 12.4994 (3) Å, unit cell volume V = 4292.9 (2) Å³, Z = 8, and space group Fdd2].

Spectroscopic characterization and the antibacterial activity of this complex against *Bacillus subtilis*, *Staphylococcus epidermidis*, *Staphylococcus aureus*, and *Klebsiella pneumonia* will also be presented and discussed.



References:

- [1] Viganor. L. et al. (2016) *J. Antimicrob. Chemother.* 71, 128-134.
- [2] Roy S. et al. (2008) *ChemMedChem* 3, 1427-1434.
- [3] McCann M. (2012) *Toxicol. Res.* 1, 47-54.

Keywords: powder X-ray diffraction, 1,10-phenanthroline-5,6-dione, crystal structure

MS36-P03

The dimeric nature of the Re(I) complexes of the thiosemicarbazone derived of 4-(dimethylamino)benzaldehyde

Saray Argibay Otero¹, Ezequiel Vázquez-López¹, Rosa Carballo¹

1. Departamento de Química Inorgánica, Instituto de Investigación Sanitaria Galicia Sur-Universidade de Vigo, Vigo, Spain

email: saargibay@uvigo.es

Dimeric thiosemicarbazone complexes [Re₂(CO)₆(L)₂] (see Figure 1) are often isolated from solutions of the corresponding mononuclear rhenium(I) complexes, [ReX(CO)₃(HL)], containing the protonated species of those bidentated ligands [1]. The deprotonation of the HL ligand and the labilization of the halogen in adduct produces the dimerization of the rhenium complexes by linking the sulfur atom of a neighboring molecule at the position previously occupied by the halogen atom. The Re-S bond to the sulfur atom belonging to the chelating system of the neighboring rhenium atom is larger (around 0.1 Å) than its own chelate.

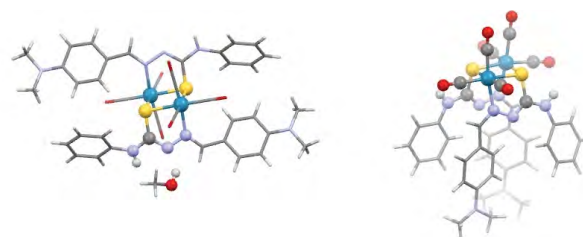
When basic media is used to remove the halide group, the dinuclear complex is usually formed in stoichiometric amounts. The stability of thiosemicarbazone specie depends also of ligand nature, so that the thiosemicarbazones derived from aldehyde give the dimer more easily than those derived from ketones.

Recently, we had tried the synthesis of rhenium(I) complexes of the thiosemicarbazone derived of 4-(dimethylamino)benzaldehyde and we have observed the systematic formation of the dinuclear complex as crystal from solutions of the monomer in several solvents and at different temperatures.

In addition, we have isolated two different compounds depending of the ligands disposition respect to the Re₂S₂ diamond: the centrosymmetric arrangement (Figure 1 left) and the dissymmetric arrangement (Figure 1 right). Both dimers were able to isolated as separated single crystals and also as a co-crystal.

In the present work, we study the structural differences between both kind of structures and we describe the possible factors determining the formation of one or other symmetric disposition.

Acknowledgements: Financial support from Ministry of Economy, Industry and Competitiveness (Spain) and European Regional Development Fund (EU) (CTQ2015-71211-REDT and CTQ2015-7091-R) is gratefully acknowledged.



References:

- [1] A. Nuñez-Montenegro, R. Carballo, U. Abram, E.M. Vázquez-López. *Polyhedron* 65 (2013) 221-228.

Keywords: Dimer, thiosemicarbazone, crystal