Synthesis of a new Hg(II) complex with *α*-tetralone thiosemicarbazone ligand and a study of the hydrogen-bonded supramolecular network

Renan L. de Farias[1*] (PG), Adriano B. de Oliveira[1] (PQ), Christian Näther[2] (PQ), Inke Jess[2] (PQ), Fillipe V. Rocha[3] (PQ), Adelino V. G. Netto[3] (PQ)

***renanlira1402@yahoo.com.br**

[1] *Departamento de Química, Universidade Federal de Sergipe, 49100-000 São Cristóvão – Brasil*
[2] *Institut für Anorganische Chemie, Christian-Albrechts Universität, D-24118 Kiel- Germany*
[3] *Instituto de Química, Universidade Estadual Paulista, 14800-060 Araraquara- Brasil*

Palavras Chave: *Coordination Chemistry, Single Crystal - DRX, Hg(II) complex, Thiosemicarbazones*

Introduction

Thiosemicarbazones (TSC's) are important and versatile ligands, due to the *N,S*-donors that matched with *π*-delocalized system along main chain, C=N-NH-C(S)-N, resulting at a variety of coordination modes[1]. Metal complexes of TSC's have been intensively studied, because their biological activity against several pathogenic agents[2]. Our interest and on-going research concerning the structural chemistry of TSC and their metal complex covers a wide range of properties, from hydrogen-bonded supramolecular networks of molecules to their pharmacological properties[2,3]. We would like to report herein the crystal structure of a new Hg(II) complex, $Hg(TTSC)_2Cl_2$. The study of its supramolecular network is important due to the possible chemical structure-biological relationship.

Results and Discussion

The *α*-Tetralone thiosemicarbazone (10 mmols) and $HgCl_2$ (5 mmols), were stirred and refluxed in ethanol (80 mL) for 6h. After cooling and filtering, the $Hg(TTSC)_2Cl_2$ were obtained. Suitable crystals for single crystal X-ray diffraction of the compound grow in DMSO after slow evaporation of the solvent. The title compound crystallizes in monoclinic space group $P\ 2_1/c$ (nº 14), Z = 8, with a = 8.1612(2) Å, b = 18.1003(4) Å, c = 40.1136(11) Å, β= 95.691(2)^0. The asymmetric unit consists of two disordered DMSO solvates (they were refined over two sets of sites with occupancy ratios of 0.80:0.20 for S atoms and *─CH$_3$─* groups) and two Hg(II) complexes with different orientations showing the TTSC coordinated as terminal ligands. Finally, two chloride ligands complete the slightly distorted tetrahedral coordination spheres (dihedral angles of 89.3º and 85.3º) **Figure 1**. In the crystal, the molecules are connected *via* intermolecular N─H•••Cl and N─H•••O H-interactions, stacked along *a*-axis forming channels. Those are filled with DMSO molecules. Two intramolecular N─H•••Cl and an N─H•••N hydrogen bonding are also observed.

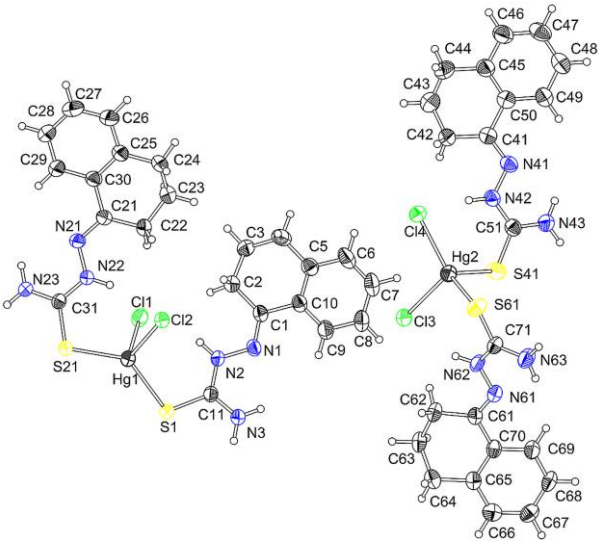

Figure 1. ORTEP of the Hg complexes showing with the displacement ellipsoids drawn at the 40% probability level. The two DMSO solvates were removed for clarity.

We suggest that this compound can be a promising biologically active molecule due the presence of two TSC-ligands with proven pharmacological properties, as well as, two weak chloride ligands that can be easily dislocated.

Conclusions

This work shows the synthesis of a new Hg(II) complex structurally characterized by single crystal X-ray diffraction. The monodentate coordination was observed for TSC-ligands and the presence of the two chloride ligands complete the tetrahedral geometry in the neighborhood of metal center. We suggested that the compound can be suitable for biological trials.

Acknowledgements

We gratefully acknowledge Professor Dr Wolfgang Bensch (Uni-Kiel).

[1] Lobana, T. S. *et al., Cood. Chem. Rer.* **2009**, 253, 977.
[2] Rocha, F. V. *et al. Polyhedron.* **2013**, 65, 2014.
[3] Oliveira, A. B. *et al. Acta Cryst E.* **2014**, E70, 101.