XXI Brazilian Meeting on Inorganic Chemistry
X Brazilian Meeting on Rare Earths
III Workshop on Theoretical Bioinorganic Chemistry
Belo Horizonte, September 12 - 15th 2024

Crystal structure and Hirshfeld surface analyses of copper(I) complexes with thiosemicarbazides

Pedro H. O. Santiago and **Javier Ellena**

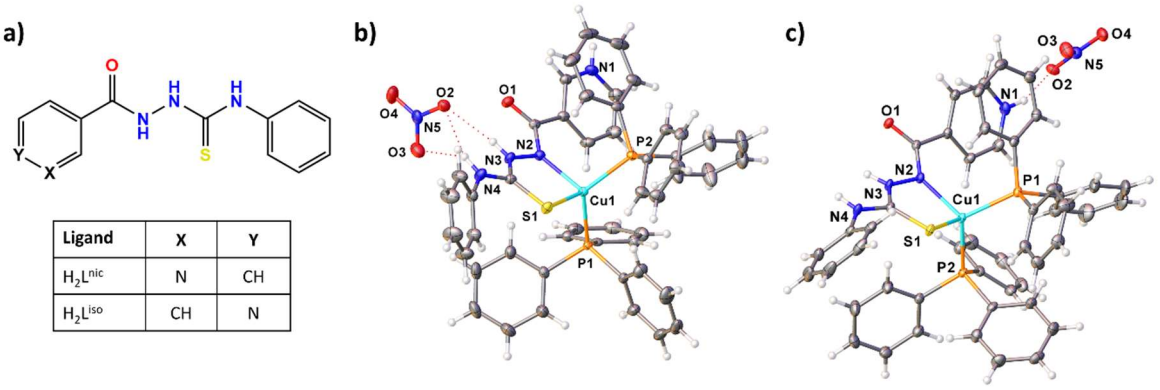
[1]*São Carlos Institute of Physics, University of São Paulo, São Carlos-SP, Brazil*
E-mail: pedrophs.santiago@gmail.com

Thematic Area: Biological Inorganic Chemistry

Keywords: Copper(I) complex, Thiosemicarbazide, Crystallography

Thiosemicarbazides are organic compounds that have been mainly used as precursors for the synthesis of biologically active heterocycles [1]. The use of these compounds as chelating agents has attracted interest due to the possibility of obtaining metal complexes with pronounced biological, luminescent and catalytic properties [2–4]. Aiming to obtain metal complexes with pharmacological potential, herein we report the synthesis and structural analysis of two copper(I) complexes with the isomeric thiosemicarbazides H_2L^{nic} and H_2L^{iso} as ligands (Figure 1).

The single crystal X-ray diffraction results reveal the formation of the cationic and isostructural complexes $[Cu(H_2L^{nic})(PPh_3)_2]^+$ and $[Cu(H_2L^{iso})(PPh_3)_2]^+$, which have a nitrate as counterion. Both complexes are formed by a copper(I) cation coordinated to two triphenylphosphine ligands and one bidentate and *zwitterionic* thiosemicarbazide, being inserted into a distorted tetrahedral geometry. The difference in the position of the nitrogen atom in the structure of the ligand enabled the obtaining of different crystal structures, with the complex $[Cu(H_2L^{nic})(PPh_3)_2]NO_3$ crystallizing as an anhydrous complex, while $[Cu(H_2L^{iso})(PPh_3)_2]NO_3$ was obtained was a methanolic solvate. The Hirshfeld surface analysis was performed to evaluate the intermolecular interactions in the two structures, with different patterns of non-covalent interactions being observed for each structure.



Ligand	X	Y
H_2L^{nic}	N	CH
H_2L^{iso}	CH	N

Figure 1. (a) Representation of the thiosemicarbazides and ORTEP type illustration of the complexes (b) $[Cu(H_2L^{nic})(PPh_3)_2]NO_3$ and (c) $[Cu(H_2L^{nic})(PPh_3)_2]NO_3$, with ellipsoid drawn at 50% of probability.

Acknowledgments: FAPESP (Process number 2021/10066-5), IFSC-USP

References

[1] M.A. Metwally *et al.*, J. Sulfur Chem., **32**, 489–519 (2011).
[2] H.H. Nguyen *et al.*, J. Mol. Struct., **1249**, 131680 (2022).
[3] A.P. Borges *et al.*, Polyhedron, **155**, 170–179 (2018).
[4] S.S. Clinton *et al.*, Catal. Sci. Technol., **13**, 3358–3365 (2023).