MS15 Mineralogical and inorganic crystallography

## MS15-1-16 Synthesis and structural evaluation of a new copper(II) complex with a dithiocarbazate ligand #MS15-1-16

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## Abstract

The dithiocarbazates are Schiff bases that present huge versatility, their chemical properties can be modified with the introduction of different substituent groups in their structure, allowing the formation of metal complexes with different coordination polyhedra.<sup>1</sup> In addition, dithiocarbazates and their complexes are reported in the literature showing biological properties such as antifungal, antibacterial and antitumoral.<sup>2,3</sup> The current work reports the synthesis and structural evaluation of a new dithiocarbazate ligand (2-acetylpiridine-S-p-clorobenzyl-dithiocarbazate) and its Cu(II) complex. Both complex and ligand have been characterized by spectral measurements such as IR, and UV-Vis and the ligand was characterized also by <sup>1</sup>H NMR and <sup>13</sup>C NMR. The crystal structure and molecular interactions were evaluated by single-crystal X-ray diffraction and the analysis of the Hirshfeld surface. The Cu(II) complex was observed with a square planar geometry, coordinated by *NS*-donor atoms of the dithiocarbazate and a chloride ion. The ligand is coordinated to the centre atom with an anionic form and thiol tautomer. Intermolecular interactions were found between S1····H14 and Cl1····H2; those interactions contribute to the formation of the supramolecular arrangement in the crystal packing. Both compounds will be submitted for biological evaluation to investigate their promising biological properties.

## References

[1] Cavalcante, C. D. Q. O. et al. (2019) New J. Chem, 48, 15501-15514.
[2] Yekke-Ghasemi, Z. et al (2020). New J. Chem, 44, 8878-8889.
[3] Lima, F. C. et al (2018). Inorg. Chim. Acta 483, 464-472.

Molecular structure of the copper(II) complex.

