Structural Investigation of a Novel Copper(II) Complex with Pyridoxal Thiosemicarbazone

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Abstract: The Schiff-bases with pyridoxal moieties, forms found in vitamin B6, and their metal complexes have been attracting special attention for many years.[1-2] Furthermore, Cu(II) complexes with this class of compounds appear to be very promising candidates for pharmacological application, as some of them have shown antifungal, antibacterial and antitumor activities.[3] The synthesis and crystal structure of Cu(II) complex with pyridoxal thiosemicarbazone (pyridoxal-N^4-thisemicarbazone – H_2L^1) $[Cu(H_2L^1)Br]Br{\cdot}H_2O$ is reported in this work. The X-ray data collection was accomplished on a Bruker CCD SMART APEX II single crystal diffractometer with Mo Kα radiation (0.71073 Å). The data were processed with SAINT and SADABS was used to scale the data and perform the multi-scan absorption correction. The refinement of the structure (R1 = 5.60% and Goof = 1.052) was performed using SHELXL-2016 and suggest the centrosymmetric monoclinic space group $P2_1/n$. The ORTEP drawing depicted in Figure 1, show the complex in thiolate tautomeric form. The ligand H_2L^1 it is in cationic and zwitterionic form in the complex, is coordinated by *ONS*-donor atoms, with an additional bromide ion. The ligand based on thiosemicarbazone and pyridoxal moieties adopts an *E* configuration with respect to the C(8)=N(2) and N(3)=C(9) bonds, respectively. The metal center present a distorted square-planar geometry. The crystal packing revealed by single crystal X-ray diffraction analysis showed the compound stabilized by relevant intra and intermolecular hydrogen bonding. A network in three dimensional is formed connected the cation complex, the bromide ion and the water solvent molecule. Interestingly, are the intra and intermolecular hydrogen bonding connected the Br(2) with two cation complex molecules Br(2)···O(2) distance of 3.199(6) Å and Br(2)···N(1)^a (a: 2-x, 1-y, 2-z) distance of 3.216(6) Å. These interactions are important for the crystallization of the compound and in the formation of a supramolecular structure.

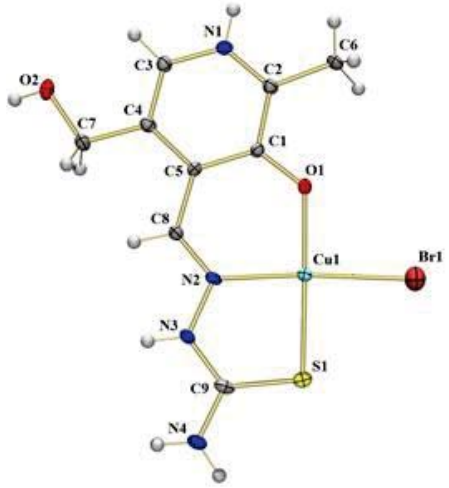

Figure 1. Molecular structure of $[Cu(H_2L^1)Br]Br{\cdot}H_2O$ with crystallographic labelling (30% probability displacement ellipsoids).

1) Vidovic, D.; Radulovic, A.; Jevtovic, V. *Polyhedron* **2011**, *30*, 16.
2) Zangrando, E.; et.al., *Inorganica Chimica Acta* **2015**, 427, 278.
3) Liu, Y.-H.; et.al., *Dalton Transactions* **2016**, *45*, 8036.

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