SYNTHESIS AND CRYSTAL STRUCTURE OF COPPER(I) CHLORIDE π-COMPLEX WITH 2-ALLYLIMINO-3-(2-PYRIDIL)-1,3-THIAZOLIDIN-4-ONE

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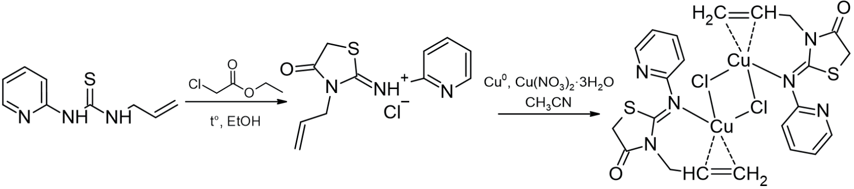
Copper(I) complexes are gaining significant interest due to their wide range of applications in catalysis, nonlinear optics, fluorescence, and biochemistry. Their biochemical activities range from antibacterial and anti-inflammatory effects to cytostatic and enzyme-inhibitory properties, with some showing promise as anticancer drugs. The crystal engineering of copper(I)-olefin complexes, particularly those involving allyl derivatives of heterocyclic compounds, has also been studied extensively. The presence of a C=C olefin bond in substituents attached to heterocyclic rings can facilitate selective coordination of transition metal ions through metal-olefin π-bonding. Allyl and pyridine derivatives turn out to be very effective ligands in coordinating with copper(I), enabling the construction of various inorganic fragments. Our current study examines the coordination behavior of allyl derivatives of binuclear heterocycles regarding Cu(I). In this work, we present the synthesis and structural characterization of a novel copper(I) halide π-coordination compound, [Cu_2(2-*Apithiaz*)$_2Cl_2$] (**1**) with 2-allylimino-3-(2-pyridyl)-1,3-thiazolidin-4-one (2-*Apithiaz*) as a ligand.

π-Complex **1** was prepared through an alternative-current electrochemical technique starting from acetonitrile solution of {2-*Apithiaz*(H^+)}Cl and copper(II) nitrate on copper electrodes (Scheme 1).



Scheme 1. Ligand and π-complex synthesis

The structure of the complex was studied by single-crystal X-ray diffraction. The π,σ-complex crystallizes in the centrosymmetric space group $P\bar{1}$ with one 2-*Apithiaz* molecule and one Cu(I) atom per asymmetric unit. Despite multiple donor centers in the ligand, it coordinates with the metal exclusively in a bidentate-chelating manner. The Cu(I) atom has a distorted trigonal-pyramidal environment, with the allyl C=C bond and two μ_2-bridging halogen atoms at the basal plane. At the same time, the imino nitrogen occupies the apical position of the copper polyhedron. Distances from Cu to the atoms of its coordination environment: d(Cu–Cl) = 2.2757(7) Å, d(Cu–Cl^i) = 2.3618(8) Å, d(Cu–N) = 2.35702 Å, d(Cu–m) = 1.967(2) Å, where i refers to symmetry code 2–x, –y, 1–z, and m is the center of a double bound. In addition, the C=C bond is slightly elongated compared to the usual one and equals 1.355(2) Å.

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