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Synthesis and structural elucidation of one one-dimensional coordination polymer of Cu (II) by Single Crystal X-ray Diffraction

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Coordination polymers (CPs) are a class of compounds defined, according to IUPAC (International Union of Pure and Applied Chemistry), as the repetition and extension of coordination entities—formed by a central atom surrounded by atoms or groups of atoms called ligands—in one (1D), two (2D), or three (3D) dimensions [1]. Due to the stable structural arrangement of CPs, many materials have been developed within this class. Consequently, these polymers can exhibit properties relevant to different areas of application, such as catalysis [2], adsorption [3], and luminescence [4]. When using fluconazole as a ligand, the luminescent physical-chemical property is prominent. Fluconazole contains several available acceptor/donor groups, including difluoro phenyl, triazole, and hydroxyl, which form weak interactions such as pi-stacking interactions and hydrogen bonding to stabilize supramolecular structures [5]. In this context, a one-dimensional coordination polymer of Cu(II) was synthesized using fluconazole and 4-sulfobenzoic acid as ligands. To analyze the physicochemical properties of this compound, it is necessary to characterize it structurally. For this purpose, single-crystal X-ray diffraction (SCXRD) characterization was employed—a crucial technique that allows determination of atomic positions, bond lengths, and angles. Therefore, it was observed that the Cu(II) polymer crystallized in the $P\bar{1}$ space group. The structural analysis show that the compound is a 1D coordination polymer (figure 1).

(a) (b)

Figure 1: Structure's asymmetric unit (a) and expansion along the c axis (b). Hydrogen atoms and H2O molecules were hidden for better visualization of the structure. The Oxygen, Nitrogen, Carbon, Sulfor, Fluor and Copper atoms are represented respectively with the colors red, blue, gray, yellow, green and orange.

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