# SYNTHESIS, CHARACTERIZATION, AND DFT STUDY OF A COPPER(II)-L-ISOLEUCINATE COMPLEX WITH POTENTIAL BIOLOGICAL ACTIVITY

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The importance of materials to humanity is well recognized, as evidenced throughout human history up to the present day[1]. The development and study of new materials are crucial to meet the demands of contemporary society. Among these, Cu(II) is essential for the human body, corresponding to a metal ion of great importance for the functioning of several enzymes and proteins, binding to DNA molecules, and exhibiting antibacterial, antifungal, and antitumor properties. Complexes formed from transition metal ions present are a promising solution, formed by bonding with ligands like L-isoleucine. They exhibit greater stability, and some ligands allow metal ions, such as Cu(II), to reach the target cell[2]. In this work, our objectives were to synthesize, characterize, and study properties of a Cu(II) complex with L-isoleucine using DFT calculations. Then, the complex was prepared using the slow solvent evaporation method, followed by crystal characterization via XRD, which included the definition of lattice parameters through Rietveld refinement. Finally, a theoretical study of the complex was conducted based on DFT. A solution was prepared in the ratio of 1 mMol of copper chloride to 2 mMol of L-isoleucine. The XRD analyses were performed in the 10° to 50° (2θ) range, with an angular step of 0.02° and a time of 2 s. Rietveld refinement was performed using the GSAS-II software, and the crystal structure was analyzed with the Mercury software. To date, the software Cremcraft has been used to explore the structure of the complex and to generate the corresponding Cartesian coordinate matrix for the computational calculations. Geometry optimization and vibrational frequencies calculations were performed using the PBE1PBE functional and the def2TZVP basis set. The solvation effect was included using the IEFPCM implicit solvation method[3]. All calculations were performed using Gaussian 16, yielding structural and spectroscopic data in good agreement with experimental results. The indices $R_{wp}$ = 7.3%, $R_p$ = 5.4%, and S = 1.13 demonstrate good agreement between the intensities observed in this study and those reported in the literature, confirming the good quality of the refinement and the successful synthesis of the target material. The Gibbs free energy ($\Delta G$) variations of -629.54 (in vacuum) and -194.41 kcal/mol (in water) confirm spontaneous complexation, and the electrophilicity (ω) of the complex of 5.19 eV (in vacuum) and 4.39 eV (in water) indicate a propensity for antitumor activity. Further physicochemical and biological analyses will be performed to investigate potential applications of this material.

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[1] JUNIOR, C. W. D.; RETHWISCH, D. G., John Wiley & Sons. 5. ed. 2012. EUA.
[2] WEEKS, CHARLES M.; COOPER, A.; NORTON, DORITA A., Structural Science, v. 25, 1969, p. 443.
[3] TOMASI J.; MENNUCCI B.; CANCÈS E., Journal of Molecular Structure: Theochem, v. 464, 1999, p. 211.