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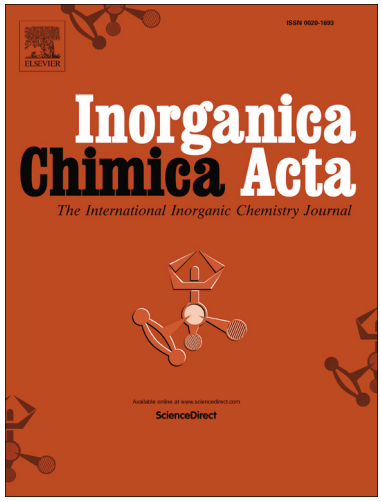

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Synthesis, structural characterization and DFT analysis of an unusual tryptophan copper(II) complex bound *via* carboxylate monodentate coordination: tetraaquabis(L-tryptophan) copper(II) picrate

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ABSTRACT

Herein, we report the synthesis, spectroscopy, crystal structure and theoretical studies of a new Cu(II) complex with formula $[Cu(L\text{-}trp)_2(H_2O)_4](pic)_2 \cdot 4H_2O$ (**1**), which exhibits an unusual tryptophan coordination to copper(II) *via* carboxylate monodentate binding. The complex has been prepared using the mixed ligand approach. Single crystal X-ray diffraction structural analysis of **1** revealed that, in the complex, the Cu(II) site shows a distorted octahedral geometry, and the tryptophan (trp) ligand is coordinated through the carboxylate group in a monodentate fashion. The picric acid (pic) co-ligand, which is present in the anionic form, resides outside the coordination sphere forming a charge-separated complex. Density Functional Theory (DFT; including time-dependent DFT) has been employed to calculate the equilibrium geometry of the complex as isolated species in dimethylsulfoxide (DMSO) solution, and also its electronic spectrum, which was used to understand details of the experimentally obtained ultraviolet-visible (UV-Vis) spectrum. The structural analysis was complemented by additional spectroscopic studies [infrared (IR) and electron paramagnetic resonance (EPR) spectroscopies], and the thermal stability of the complex evaluated by thermogravimetric analysis (TGA).

Keywords: Crystal structure, tryptophan, picric acid, TGA, UV-Visible, IR, EPR, DFT.