Journal of Molecular Structure

Volume 1294, Issue 1, 2023, Pages -

Synthesis, characterization, DFT/M06 studies, NBO, QTAIM and RDG analyses of new copper (II) complexes with bis-phosphonamide obtained under microwave irradiation

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Abstract: We have devised a novel one-step approach for synthesizing bis-phosphonamides utilizing primary amines and phenylphosphonic dichloride (PPDC) under ultrasound irradiation. The bis-phosphonamides obtained were used as organophosphorus ligands for the synthesis of new copper (II) complexes with metal ions. The synthesis of these complexes was accomplished via a novel eco-friendly method employing microwave irradiation. The desired complex obtained, as a green powder in 65% yield, which were fully characterized by spectroscopic methods (FT-IR, UV–vis, XDR). To gain and further insights into structure and properties of studied complexes, several calculations such as Natural Atomic Orbitals (NAO), Natural Bond orbitals(NBO), Quantum Theory of Atoms in Molecules (QTAIM) analysis were performed at M06/6-311++g(d, p) level. Using the Reduced electron Density Gradient (RDG) approach, the non-covalent interactions were explored and visualized in two and three-dimensional spaces.

Keywords : Phenylphosphonicdichloride, Bis-phosphonamide, Organometallic complexes, Green chemistry, Ultrasound Microwave