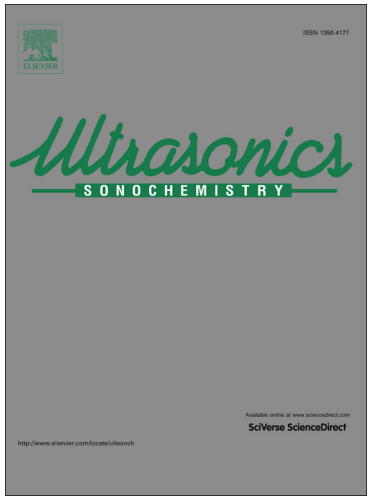

Sonochemical Synthesis, *In vitro* Evaluation and DFT Study of Novel Phenothiazine base Schiff bases and their Nano Copper Complexes as the Precursors for New Shaped CuO-NPs

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Sonochemical Synthesis, *In vitro* Evaluation and DFT Study of Novel Phenothiazine base Schiff bases and their Nano Copper Complexes as the Precursors for New Shaped CuO-NPs

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Key words: Phenothiazine, Schiff base, Nano copper complex, MEP, ESP, DPPH, CuO NPs.

Abstract

The current work reports the ultrasound-assisted synthesis of two nano binuclear copper complexes derived from novel tetradentate (N_2O_2) phenothiazine based Schiff bases. The synthesized compounds were characterized using the physicochemical methods, including ^{1}H NMR, ^{13}C NMR, FE-SEM, Mass, FT-IR, UV-Vis, elemental analysis, magnetic moment and molar conductance measurements. It is found that the geometrical structure of $Cu^{II}_2L^nCl_4$ is distorted tetrahedral around the copper atoms using the results of ^{1}H NMR, UV-Vis and magnetic moment studies. In addition, CuO nano particles were produced in the nano range (14.3-12.1 nm) by the thermal decomposition of the copper complexes CuO NPs were characterized using FT-IR, FE-SEM, XRD, UV-Vis and photoluminescence methods and indicated a close accordance with the standard pattern. Also, the antioxidant studies revealed that the copper complexes exhibit comparable scavenging effects (against O_2 and OH) with the standard antioxidants, such as vitamin C, while, they show more antioxidant activity than ligands. Similarly, the complexes show more antibacterial activity against four gram positive and gram negative bacteria in comparison to their Schiff base ligands. furthermore, The optimized structure, Molecular orbital (M.O.), Mulliken population analysis (MPA), contour of Electrostatic Potential (ESP) and Molecular Electrostatic Potential (MEP) map of the titled compounds were calculated base on DFT calculations that were carried out at the B3LYP levels of theory with a double basis set LANL2DZ for copper, and 6-311+G(d,p) basis set for the other atoms.

Introduction