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Synthesis, structural characterization, thermal behaviour and antimicrobial activity of copper, cadmium and zinc chelates of triazole-thiole ligand in comparison with theoretical molecular modelling

This research involved structural and molecular behaviour of the ligand HL, 4-amino-5-(2,2-dichloro-1-methylcyclopropyl)-4H-1,2,4-triazole-3-thiol towards the transition metal ions namely Cu(II), Zn(II) and Cd(II) had been studied using magnetic, electronic, elemental analyses, ¹H-NMR, FT-IR and thermal analyses (TGA and DTA). The interpretation of practical data obtained had been evaluated and confirmed by theoretical molecular modelling. The computations had been done by software of Gaussian 09 W package. The geometries of triazole-thiole ligand and its metal chelates were fully optimized using density functional theory B3LYP method. There are no symmetry constrains had been applied during geometry optimization. (DFT)/GENECP level by implementing Def2TZVP basis set was used for Cu, Cd and Zn-atoms; and basis set 6-311++G (d, p) was used for other atoms. The mixed basis set had been selected due to its flexibility. HOMO and LUMO energy values for chelates, chemical hardness and electronegativity had been calculated. NBO calculations had been done at the same level using (NBO 3.1) program involved in the software of Gaussian 09 W for measuring the intra-molecular delocalization in systems under investigation qualitatively. TD-DFT approximation at the same level of theory was used to calculate the electronic absorption spectra of the studied chelates. Their structures were confirmed via correlation between experimental and theoretical calculations. The antimicrobial results of the ligand and its metal chelates had been recorded against two bacteria positive (*Escherichia coli*) and negative (*Staphylococcus aureus*) and two fungus (*Aspergillus flavus* and *Candida albicans*).

Biography

Hayam Abd El Rahman Abd El Salam has completed her PhD from the Faculty of Science Ain Shams University. She is a Researcher in Green Chemistry Department, National Research Center, Dokki, Giza, Egypt. She has published more than seven papers in reputed journals and experience in extraction of natural organic compounds from many fatty wastes such as (swap stock, oils, free fatty waste) and used some extracted compound as complexing agents after modified the structure of this compounds.

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