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Synthesis, structural characterization, thermal behaviour and antibacterial activity of copper, cadmium and zinc chelates of traizole-thiole ligand in comparison with theoretical molecular orbital calculations

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This research involved structural and molecular behaviour of the triazole-thiole ligand towards the transition metal ions namely Cu(II), Cd(II) and Zn(II) had been studied using elemental analyses, magnetic, electronic, FT-IR, 1H-NMR, XRD and Thermal analyses (TGA and DTA). The interpretation of practical data obtained had been evaluated and confirmed by theoretical calculations. The computations had been done by software of Gaussian 09W package. The geometries of traizole-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 09W 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 ligand and its metal chelates biological activities had been tested against positive and negative bacteria such as *Proteus vulgaris, Escherichia coli, Staphylococcus aurous* and *Bacillus subtitles*. These biological activities are tested and give the order Zn-HL>Cd-HL>Cu-HL>>HL as a general trend in relation to transition metal cation present in chelate entity. This trend is also correlated to theoretical calculations of chelates electronegativity (X), polarizability and HOMO and LUMO values. Also this trend is correlated to theoretical calculations of energy gap values eV (Zn- HL=5.19, Cd-HL=4.32 and Cu-HL=2.08) and in reverse order to electronegativity (X) values. The results showed that the order of decreasing X (increasing CT within the molecules) is: Cu-HL>Cd-HL >Zn-HL>>HL. Some of them have the order of magnitude effects like standard amoxicillin.