Poster

Copper complexes of new unsymmetrically NNOO ligands: X- ray structure, NLO properties, catalytic oxidation and bromoperoxidase activities

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A series of mononuclear copper **CuL^{Bz}**, **CuL^{T}** complexes containing unsymmetrical tetradentate Schiff base ligands were synthesized and fully characterized by conventional spectroscopic techniques. Crystal structure data of **CuL^{T}**, solved by **X-ray diffraction**, shows a monoclinic system with ***Cc*** space group and **Z= 4** molecules per unit cell. The central copper ion adopts a nearly ideal square planar coordination geometry **(Fig. 1)**.

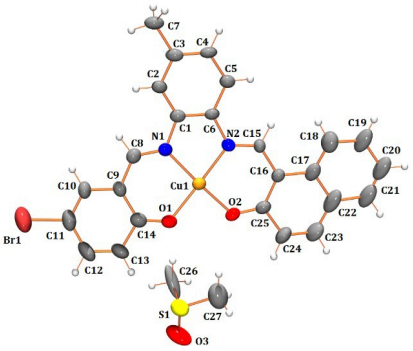

***Fig. 1. ORTEP** diagram of the X-ray crystal structure of **CuL^{T}. DMSO** complex with atom labelling scheme. Displacement ellipsoids are drawn at the **50%** probability level. **H** atoms are shown as circles of arbitrary radius.*

Cyclic voltammetry of the copper complexes revealed quasi reversible redox couples corresponding to **Cu^{I}/Cu^{II}** redox processes. The quantum calculations, performed by **DFT** and **TD-DFT** theory at the **M062X/6-311**G/ SDD** level, agree well with the experimental data. The results show that the copper compounds have larger static and dynamic hyperpolarizability values than the urea. For instance, the **β_0** value of **H_2L^T** is about 68 times larger than that of the urea. The results predict that the studied compounds have the ability to be excellent second and third-order **NLO** materials. The prepared complexes catalyzed effectively homogeneous oxidation reaction of cyclohexene in the presence of **H_2O_2** as oxidant. Higher conversion of **98%** is attained using **CuL^{Bz}** as catalyst. The bromoperoxidase activity is explored in the oxidative bromination of phenol red as a trap employing the studied complexes which can be considered as potential functional models of bromoperoxidase, **CuL^{Bz}** catalyst exhibits the better catalytic activity, the reaction rate constant **k** is equal to **2.203×10^5 (mol L^{-1})$^{-2}$s^{-1}**.

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