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Electronic and vibrational properties of complexes of (4E)-4-(4-metoxibenzilidenoamino)-1,2-dihidro-2,3-dimetil-1-fenilpirazol-5-ona with Cu(II) and Zn(II) with Antiprotozoal Activity.

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The Schiff bases, known as imines and their transition metal complexes have a variety of biological applications in the fields of Pharmacology, Chemistry and Physics. Despite the toxicity of some transition metals, the use of essential metal properly coordinated to specific ligands decreases the possibility of toxicity. The synthesis of Schiff bases, with a fundamental mechanism of addition-elimination, followed by elimination of water to form a double bond carbon-nitrogen. In this study we have chosen the 4-aminoantipyrine portion with pharmacological action and *p*-methoxybenzaldehyde. The complex formed by the imine and transition metals such as Cu (II) and Zn (II) has shown antiprotozoal activity, nominally trypanocidal and leishmanicidal against epimastigotes and promastigotes strains [1]. Moreover, the study of vibrational properties of organic compounds and their complexes with Cu (II) and Zn (II) made by FT-IR and FT-RAMAM, aims to evaluate the vibrational modes, which occur in different regions of spectrum, with emphasis on the region between 1590-1650 cm-1 attributed to the involvement of C = N bond in the orientation of the metal ion. The vibrational modes between 450-470 cm^{-1} which can be attributed to (Zn-O) bond. The vibrational modes between 380-405 cm^{-1} associated with the ν(Cu-O) [2]. In this we have made a study of structural and electronic properties of the ligand $C_{19}H_{19}N_3O_2$ coordinated with Cu (II) and Zn (II) in different conformations by comparing their binding energies using *ab initio all-electron* method. The method was PAw [3], a method known as *ab-initio all-electron*, related to Theory of the Density Functional (DFT) by CP-PAw computational code. In addition, was held with the study of spin polarization to investigate the contribution of the unpaired electron of Cu (II). We carried out comparative studies of energy and structural connection between the metal ions Cu (II) and Zn (II) in its oxidized and reduced states. Noting the differences in the characteristics of the frontier orbitals for the different metals. The Figure 1 shows the schematic representation for the ligand (4*E*) -4 - (4-metoxibenzilidenoamino)-1,2-dihydro-2 ,3-dimethyl-1-fenilpirazol-5-one. Thus, it was investigated the possible forms of coordination of the ligand, $C_{19}H_{19}N_3O_2$, the Cu (II) and Zn (II) observed structural differences found by evaluating the orbital border and electronic distribution, to correlate with the reported biological action found for these complexes.

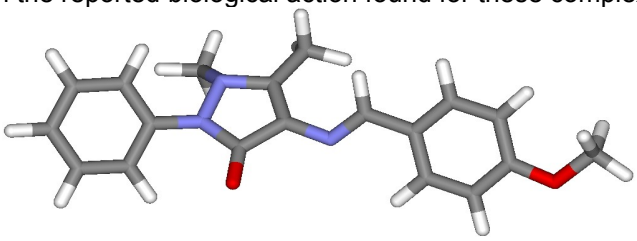

Figure 1: Schematical representation of (4E)-4-(4-metoxibenzilidenoamino)-1,2-dihidro-2,3-dimetil-1-fenilpirazol-5-ona.

References

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