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Evaluation of Molecular Orbital Coefficients of Some Copper (II) Complexes of Naphthalene Analogues of 2'-Hydroxychalcones through their ESR Spectroscopic Investigations

E.R. AGHARIA

Department of Chemistry, SVKM's Mithibai College, Vile-Parle (West), Mumbai-400056, **INDIA**

Email: mhea22@rediffmail.com

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ABSTRACT

Some copper(II) complexes of naphthalene analogues of 2'-hydroxychalcones have been synthesized and characterized. The copper (II) complexes have the general formula CuL_2, where, L is the deprotonated ligand, the naphthylchalcone. In the present investigation, the molecular orbital coefficients α, α', β and γ were estimated from the experimental spin Hamiltonian parameters obtained from the ESR spectra of the Cu (II) complexes. The importance of these MO coefficients are discussed at length as in co-ordination chemistry, ESR or EPR or EMR plays a complementary role in elucidating the structure of coordination complexes, particularly Cu(II) complexes. These MO coefficients are calculated by using different formulae involving different EPR parameters. ESR and optical absorption spectra have been used many times to determine the covalent bonding parameters for the Cu^{2+} ion in various ligand field environments. The ESR parameters $g_{\parallel}$, $g_{\perp}$, $A_{\parallel}$ and $A_{\perp}$ and the separation of the d-orbitals ($^2B_{lg} \rightarrow {}^2B_{2g}$ corresponding to $|x^2-y^2>$ to $|xy>$ transition and $^2B_{lg} \rightarrow {}^2E_g$ corresponding to $|x^2-y^2>$to $|xz, yz>$) are used to evaluate the metal- ligand bonding parameters α^2, α'^2, β^2 and γ^2, which are in-plane σ- covalency, out-of-plane σ-covalency, in-plane π-bonding and out-of-plane π-bonding parameters respectively. The ESR study of the copper complexes provides supportive evidence to the optical results. The extent of departure of these coefficients from unity measures the extent of delocalization of the metal electrons due to metal-ligand bonding. Thus in general, if the MO coefficients are smaller than unity, then they indicate the covalent nature of bonding between metal and ligand orbitals. In the present study, the molecular orbital coefficients vary in the order $\alpha'^2 < \gamma^2 < \beta^2 < \alpha^2$ and they all are smaller than unity, indicating considerable amount of covalent nature of metal-ligand bond and also asserts them to be stable.

Keywords: ESR, EPR, chalcones, coordination complexes, bonding, molecular orbital coefficients, covalent.