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Theoretical Study of effect ligands on Molecular & Orbital Properties of Cu complexes of industrial dyes formazan

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Abstract

In this research at the first complexes were optimized. NBO calculations and NMR for the complexes were carried out at the B3LYP/6-31G*quantum chemistry level. Different parameters such as energy levels, the amount of Chemical Shift in different atoms, the amount of HOMO/LUMO, chemical potential (μ), chemical hardness (η), Formazan dyes have become important reactive dyes for cotton. Formazan dyes are also used in analytical chemistry because of the high color intensity of many of their metal complexes. The chemistry of formazans was first exploited in 1962 by MacDonald to produce color photographs [1].The complexes assume a planar tetragonal structure so that two monodentate ligands can occupy free coordination sites at the apices of an octahedron. The copper complex of 1,5-bis(2-hydroxyphenyl)-3-cyanoformazan probably exists as tricyclic structure (Fig 1) because of the increased acidity of the phenolic hydroxyl group. Metal complexes of tri- and tetra dentate formazans are much more stable. At last the data in tables and graphs and shapes were compared and discussed.

Keywords: Formazan dyes, monodentate ligands, Metal complexes.