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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.

1. Introduction

In this report the studies have been done on *Cu* complexes of industrial dyes formazan. The ligands in the C_{16} position have been changed with the different groups. And then it has been researched about produced changes in Hartree Fock energy and stabilities of complexes, The energy of HOMO and LUMO orbital ,dipole moment, distance bond, bond angles, in the same bonds in the complexes and finally the amount coefficient factor of p orbital in $\sigma \& \pi$ bonds of complexes are studied. All calculations have been done in gas phase. The calculations for C, H, N, O atoms have been performed by the standard $6-31G*$ basis set, and for *Cu* standard LANL2DZ basis sets have been considered. The natural bond orbital analyses have been performed in the GAUSSIAN 98 [1-9].

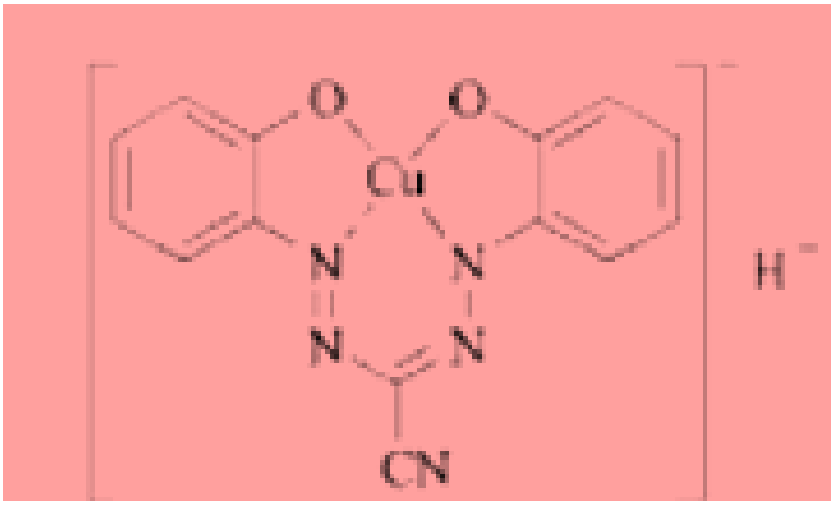

Fig 1. *Cu* complexes of industrial dyes formazan

2. Computational details

All Computations are performed by means of GAUSSIAN 03 packing [9]. Geometries for all compounds are computed by means of the density functional theory (DFT) with Becke's three-parameter functional (B3) plus Lee, Yang, and Parr (LYP) correlation functional. For all atoms, the standard 6-31G basis set is utilized. The structures of *Cu* complexes were designed primarily using of Gauss View 5.0.8 and nanotube modeler 1.3.0.3 soft wares. The interaction effects of Fluoxetine on Fullerene were investigated

through attachment to three different base positions. All these calculations are done under the assumption of standard state of gas phase, pressure of 1 atmosphere, and temperature of 25 degrees centigrade. The calculations are performed, using a Pentium 4 PC with a Windows 7 OS and a Core i5 processor.

3. Results

In this study, fluoxetine drug and its 3 fullerene derivatives investigated. The related structures are named in the following way:

The results showed that the calculated

Table1. Optimized bond length of C16-X and E(RHF) of formazan

complex	(C-X)%P	E(RHF)	C16-X
formazan	21.206	-2595.3119	1.08258
F-formazan	14.39515	-2693.9081	1.35000
Cl -formazan	-0.112339	-3054.205	1.76000
Br-formazan	-21.88678	-5164.4343	1.91000

Table 2. HOMO & LUMO orbitals Energies ,bond distance &bond angels (angstroms and degrees).The hybridizing coefficient of selected dond calculated by NBO method at the levels of HF/6-31G(d)

COMPOUND	E(RHF)	HOMO	LUMO	Dipole Moment
FORMAZAN	-2595.31197810	-0.301	-0.019	2.4647
FORMAZAN-F	-2693.90810395	-0.286	-0.122	5.4994
FORMAZAN-Cl	-3054.20503295	-0.307	-0.025	0.8949
FORMAZAN-Br	-5164.43431704	-0.279	-0.099	2.0709
FORMAZAN-CO	-2707.41481862	-0.295	-0.047	6.3778
FORMAZAN-COOH	-2782.90997345	-0.309	-0.026	0.7844
FORMAZAN-CN	-2686.82796062	-0.257	-0.121	6.0137
FORMAZAN-NO	-2723.94335645	-0.307	-0.029	1.5091
FORMAZAN-NO2	-2798.76020685	-0.316	-0.034	2.9259
FORMAZAN-CH3	-2634.15314393	-0.262	-0.098	6.8581

Table3.bond distance &bond angels (angstroms and degree)

COMPOUND	C18-C16-C11	C16-X	C16-C18	C16-C11
FORMAZAN	118.87339	1.08258	1.37021	1.40154
FORMAZAN-F	118.87342	1.35000	1.37021	1.40154
FORMAZAN-C1	118.87339	1.76000	1.37021	1.40154
FORMAZAN-Br	118.87341	1.91000	1.37021	1.40154
FORMAZAN-CO	118.87335	1.54000	1.37021	1.40154
FORMAZAN-COOH	118.87339	1.54000	1.37021	1.40154
FORMAZAN-CN	118.87343	1.54000	1.37021	1.40154
FORMAZAN-CH3	118.87343	1.54000	1.37021	1.40154
FORMAZAN-NO	118.87338	1.47000	1.37021	1.40154
FORMAZAN-NO2	118.87344	1.47000	1.37021	1.40154

Table 4.The hybridizing coefficient of selected dond calculated by NBO method at the levels of HF/6-31G(d)

COMPOUND	C16-X
FORMAZAN	$\sigma = 0.6113(sp^{2.27})_{c_{16}} - 0.7914(s)_{H_{23}}$
FORMAZAN-F	$\sigma = 0.8528(sp^{3.21}d^{0.02})_{c_{16}} - 0.5223(sp^{2.23}d^{0.01})_{F}$
FORMAZAN-Cl	$\sigma = 0.7298(sp^{3.14}d^{0.01})_{c_{16}} - 0.6836(sp^{4.46}d^{0.04})_{Cl}$
FORMAZAN-Br	$\sigma = 0.7030(sp^{3.28}d^{0.01})_{c_{16}} - 0.7112(sp^{5.79}d^{0.05})_{Br}$
FORMAZAN-CO	$\sigma = 0.7501(sp^{2.69})_{c_{16}} + 0.6613(sp^{0.48})_{C_{30}}$
FORMAZAN-COOH	$\sigma = 0.6885(sp^{2.53})_{c_{16}} - 0.7252(sp^{1.59})_{C_{30}}$
FORMAZAN-CN	$\sigma = 0.6971(sp^{2.56})_{c_{16}} - 0.7169(sp^{0.97})_{C_{30}}$
FORMAZAN-CH3	$\sigma = 0.6831(sp^{2.14})_{c_{16}} - 0.7304(sp^{2.97}d^{0.01})_{C_{30}}$
FORMAZAN-NO	$\sigma = 0.6617(sp^{2.67}d^{0.01})_{c_{16}} + 0.7498(sp^{2.51}d^{0.01})_{N_{30}}$
FORMAZAN-NO2	$\sigma = 0.7902(sp^{3.02}d^{0.01})_{c_{16}} - 0.6128(sp^{1.83})_{N_{30}}$

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