The study of electron-orbital properties of bipolar energy of complex (2,6-diaminopyridinium bis (4-hydroxy-pyridine-2,6,6-dicarboxylate) dihydrate chromate III))) with alteration of ligands by computational methods

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Abstract

In this report, using the ab initio method of stability and electron-orbital properties of the complex (2,66-diaminopyridinium bis (4-hydroxy-pyridine-2, 6-dicarboxylate) dihydrate chromate III) with a change of ligand at position 17 It has been studied with ligands such as F, Cl, Br,,, and. The results indicate changes in energy levels, bipolar moments, and sustainability rates due to these changes in these bonds.

Keywords: (2,6-diaminopyridinium bis (4-hydroxy-pyridine-2,6,6-dicarboxylate) dihydrate chromate III))).

1. Introduction

The reaction of Chromium III, 6 acepyridine 2,6 diamino and 4 hydroxypyridine-2,6-dicarboxylic acid in a 1: 2: 2 molar ratio of aqueous solution leads to the formation of a compound (or the pyda of the same pyridine 2 and 6 diamine and the same 4-hydroxy Pyridine is a 2,6-dicarboxylic acid. Each atom with four O atoms and two N atoms is hexadecimal, which acts as a triangular ligand in the complexity of the geometric actahedral geometry. The atoms of the two atoms of 4-hydroxypyridine 2 , Dicarboxylic 6 is cordoned, groups that act as three-toothed ligands, a pyridine nitrogen atom and two atoms of carboxylate oxygen. Atoms and from The geometry of the surrounding quadrilateral can be explained as an octahedral gap. The four groups of carboxylates from the dianions around the atoms are Flat tetra form are arranged [1-5]
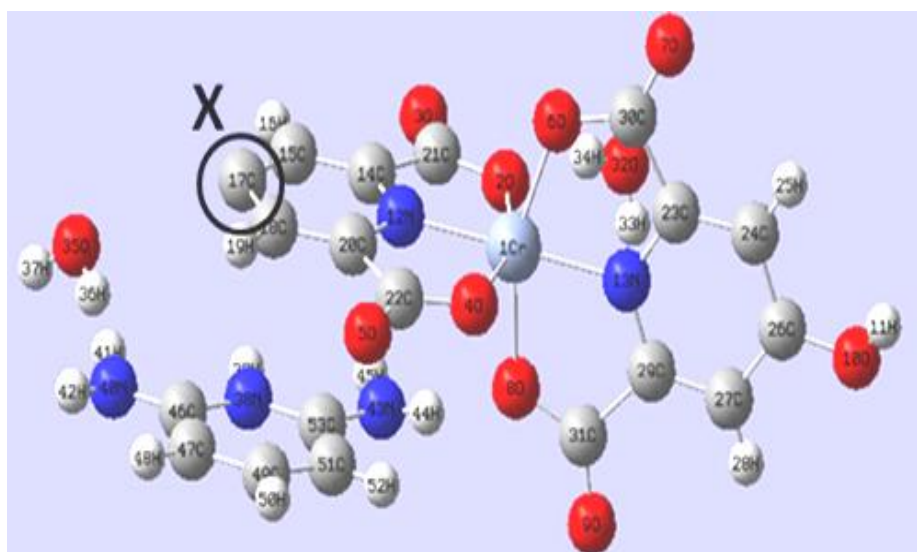

Fig 1. Figure 1 – Combination $[Cr(C_7H_3NO_5)_2]$

2. Computational details

   All Computations are performed by means of GAUSSIAN 03 packing [6-8]. 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 compounds 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

In this report, the complex structure was first optimized at two levels of HF, DFT. Then, studying the electron-orbital properties of the chromium complex and different species of this complex with different ligands using the Gaussian 98 software by the NBO method, which is based on the base series in Two levels of HF and DFT are calculated from ab initio starting methods and ultimately concluded [9-10].

3. Results

Electron-Orbital Properties

The electron-orbital and molecular orbital-electron properties (HOMO & LUMO), limited in the base series, were carried out in two different HF and DFT methods for complex ligands attached to the complex. These studies show that by changing the ligand at position 17 on the complex (2,66-diaminopyridinium bis (4-hydroxy-pyridine-2, 6-dicarboxylate) dihydrate chromate III)), the HOMO & LUMO energy sequence is as follows..

Table 1. Limit values of molecular orbital (HOMO, LUMO) chromium complex with different ligands in two methods: HF, B3LYP

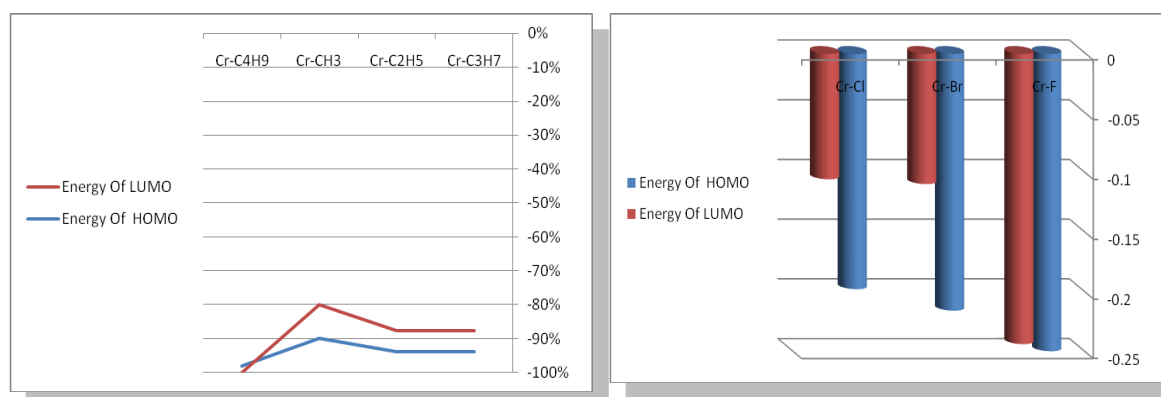|	*Energy Of HOMO*	*Energy Of LUMO*
B3LYP-NBO-Cr-F	-0.249	-0.243
B3LYP-NBO-Cr-Cl	-0.197	-0.105
B3LYP-NBO-Cr-Br	-0.215	-0.109
HF-Cr-CH3	-0.251	0.028
HF-Cr-C2H5	-0.364	0.024
HF-Cr-C3H7	-0.365	0.024
HF-Cr-C4H9	-0.239	-0.005

Fig 1. HOMO, LUMO energy for the chromium complex with CH3, C2H5, C3H7, C4H9, F, Cl, Br, ligand in B3lyp, HF

Energy and dipole moment

The stability and duopoly duration of Cr complex has been studied by changing the ligands attached to them, and the results show the sustainability level affected by these changes.

Complex Cr + Br> Complex Cr + Cl> Complex Cr + F

Complex Cr $^+$> Complex Cr $^+$> Complex Cr $^+$> Complex Cr$^+$

Table 2. Energy values and the dipole moment obtained by complex with different ligands in two methods: HF, DFT

|	*Energy(a.u)*	*Hartree Energy(kcal/mol)*	*Dipole moment(Debye)*
B3LYP-NBO--Cr-Cl	-3380.201574	-2121091.699	18.819
B3LYP-NBO--Cr-Br	-5491.726113	-3446082.849	19.5355
B3LYP-NBO--Cr-F	-3000.379101	-1882751.388	44.1118
HF-Cr-Cl	-3367.613098	-2113192.373	21.3454
HF-Cr-Br	-5477.841435	-3437370.151	33.7405
HF-Cr-F	-3007.412686	-1887164.994	26.1615
HF-Cr-CH3	-2947.562735	-1849608.88	24.483
HF-Cr-C2H5	-2986.786173	-1874221.764	22.6707
HF-Cr-C3H7	-3025.683589	-1898630.068	22.6438
HF-Cr-C4H9	-3064.488549	-1898630.068	15.3742
HF-Cr-COOH	-3096.353871	-1942975.988	19.8566
HF-Cr-CO	-3020.565291	-1895418.313	31.8739
HF-Cr-CN	-3000.499067	-1882826.667	18.8065
HF-Cr-NO2	-3112.230163	-1952938.432	18.2325
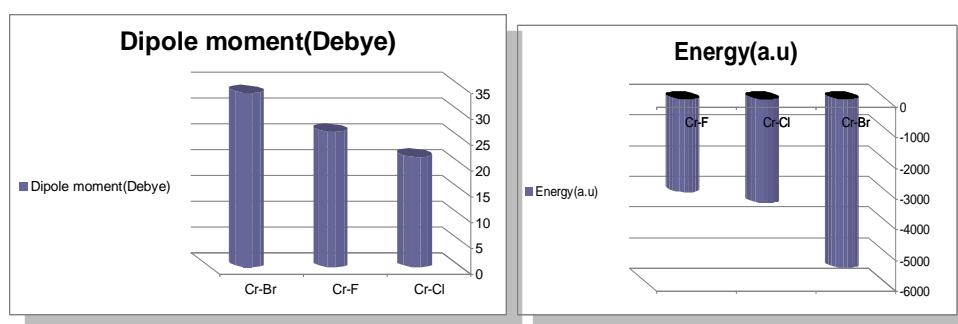
Chart 2 - Computational energy values of the HF method for chromium complexes by changing the ligands F, Cl, Br at position 17
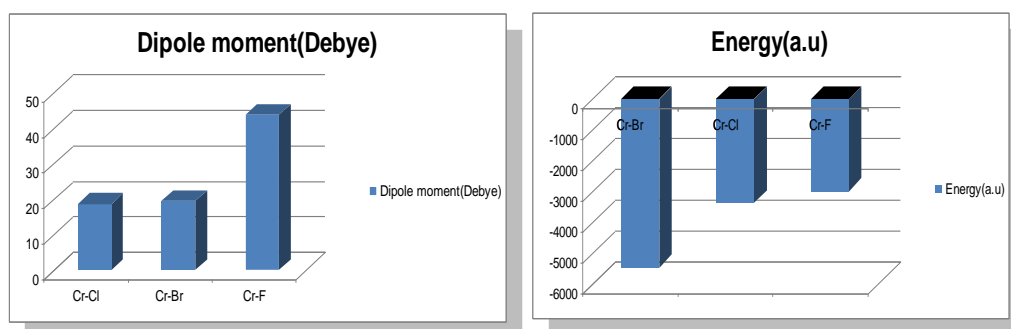
Graph 3 - Computational energy values of the DFT method for chromium complexes by changing the ligands F, Cl, Br at position 17

Dipole moment(Debye
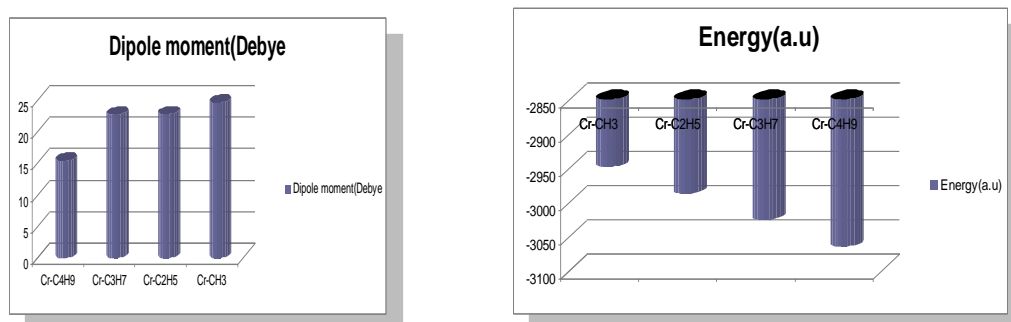
Energy(a.u)

Graph 4 - Computational energy values of the DFT method for chromium complexes by changing the ligands F, Cl, Br in position
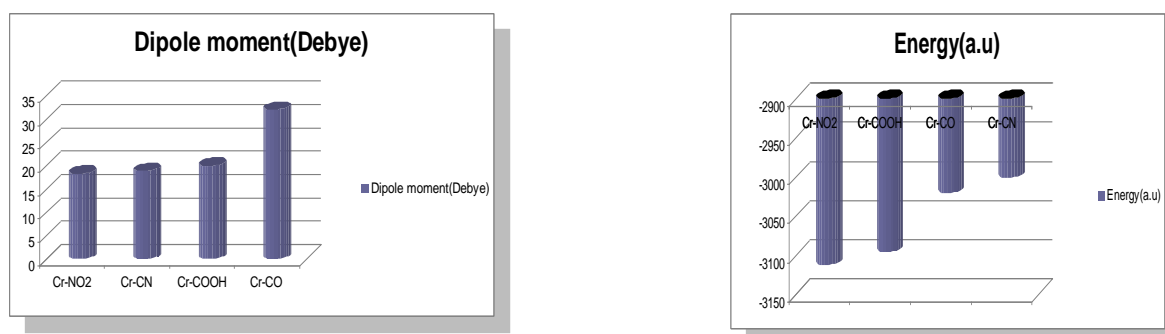
Dipole moment(Debye)

Energy(a.u)

Chart 5 - Energy values and bipolar moments of the HF method for chromium complexes by changing the NO2 ligand. CO, CN, COOH at position 17

4 Conclusion

Molecular orbital HOMO, LUMO show a similar trend in the HF, DFT method for each complex separately. From about 1 to 3 carbons, they have a good process, but with the increasing number of carbon, the trend disappears, which is due to the weight of the alkyl and its molecular mass. As the ligand has less electronegative halogen, the resulting complex is more stable, and the alteration of the alkylated ligands also shows that the more acidic the molecule is, the more complex the resulting energy is more stable. .In HF, DFT, the process is one, which suggests the overall accuracy of these two methods in computing and sustaining these complexes.

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