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Computational study of structures and electronic properties of the Catapres on nano structure of fullerene with calculations method

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Abstract

Abstract

In this report, using computational methods of quantum mechanical the study of structural, electronic and orbitals properties of Catapres on nanostructured fullerenes using software Gaussian 98 is done. At the first compounds were optimized, then NBO calculations have been done. The results indicate changes of energy levels HOMO & LUMO, dipole moments, bond distance of N_{61}-C_{62}, N_{61}-C_{62} and N_{61}-C_{62} and the ratio Core / charge of halogens. Interesting that in all cases studied listed the lowest values for each case to combine computing with fluorine substitute is concerned. All calculations is done in 6-31g* basis set in HF method and in gas phase

Keywords: Catapres , Orbital Molecular level , fullerene , Gas phase.

1. Introduction

Catapres (catapresis, catapresants) was synthesized by Stahl in 1962 at the Department of Chemistry, C.H.Boehringer sohn Ingelheim. Catapres is a white powder with a molecular weight of 266.57. Its melting point ^{0}C is 313. Catapres is known as nasal congestion, low blood pressure, acute adjunctive addiction control, and also a growth stimulus. The two loops in the drug building are not relative to each other due to the spatial inhibition of the two chlorine atoms, and the angle between the two loops, according to The quantum chemistry calculations are 34 degrees and the X-ray study is 75 degrees. Researchers have recently discovered that nanotubes have the power to infiltrate fibroplastic nuclei, so that the drug can be coupled to the drug to reach the head of the cell. Because this batch of substances at low doses It does not pose a risk to

the body, so it has a lot of use in medical sciences. Fullerenes consist of a large number of carbon molecules. In a general hollow form, they are circular, elliptical, or tubular in nano-metric dimensions. The hybrid carriers of carbon atoms are sp2. (Figure 1) [1-5]

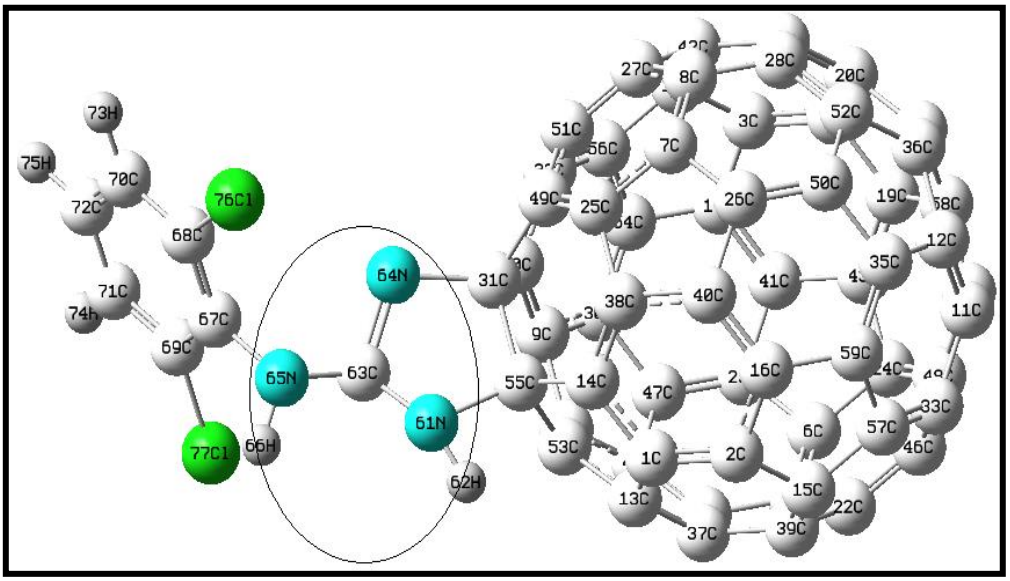


Fig 1. View of Catapres linked to Fullerene, N61-X-C60-Catapres (X = F, Cl, Br – Compound

In this study, using quantum chemistry calculations, the structure of compounds N61-X-C60-Catapres (X = F, Cl, Br) was first optimized in the gas phase. Then, quantum chemistry studies related to the orbital and structural electrons properties of Catapres on the fullerene nanostructures by changing the position of the N61 halogen solutes by using The Gossin 98 software was implemented using the NBO method. All calculations are performed on the HF level in the G * 31-6 base series. [6-8].

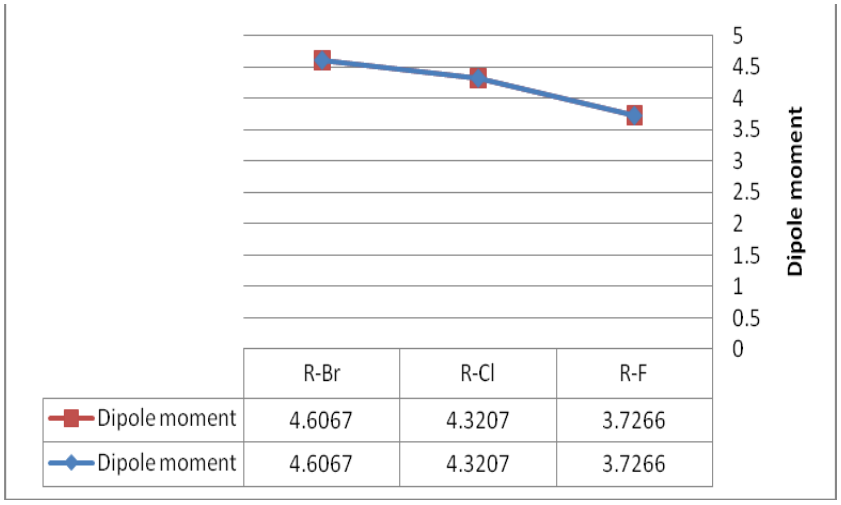
2. Computational details

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 Catapres on Fullerene were designed primarily using of Gauss View 5.0.8 and nanotube modeler 1.3.0.3 soft wares. The interaction effects of Catapres 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 [10] .

3. Results

The investigation of the electron-orbital properties of compounds N61-X-C60-Catapres (X = F, Cl, Br) has been carried out. These studies show that the energy of HOMO & LUMO in combination with halogen fluoride is lower than that of other compounds. . figure 2)



	R-Br	R-Cl	R-F
Dipole moment	4.6067	4.3207	3.7266
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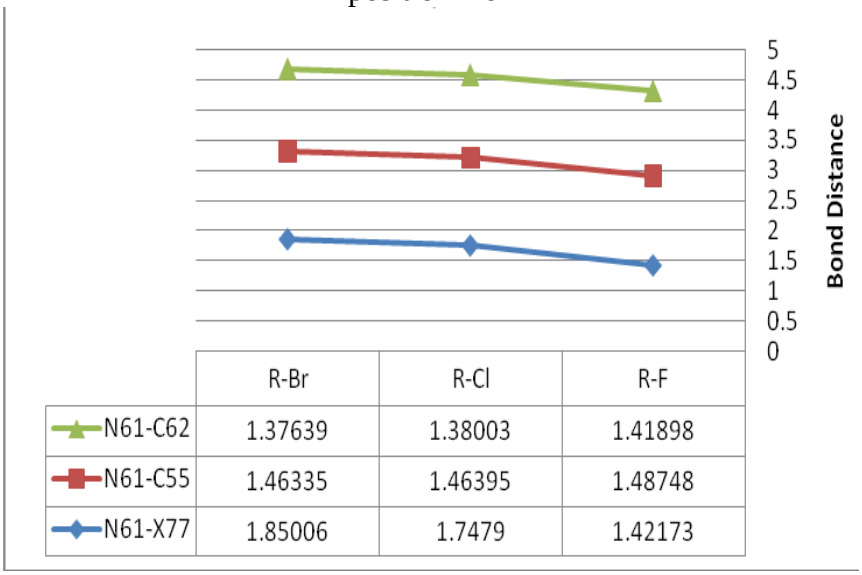
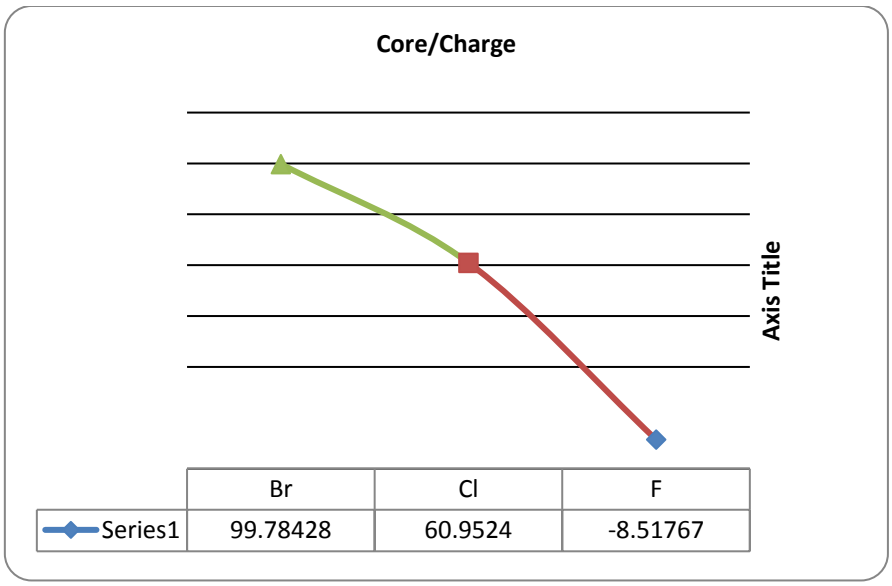
Fig. 4. Changes in the bipolar momentum of 3C9H9Cl2N-C60 complex by changing the type of halogen at position N61



	R-Br	R-Cl	R-F
N61-C62	1.37639	1.38003	1.41898
N61-C55	1.46335	1.46395	1.48748
N61-X77	1.85006	1.7479	1.42173

Fig. 4: Changes in the lengths of N61-C62, N61-C62 and N61-C62 complexes of 3C9H9Cl2N-C60 complexes by changing the type of halogen at position N61



	Br	Cl	F
Series1	99.78428	60.9524	-8.51767

Fig. 5. Core / charge ratio for halogen atoms in 3C9H9Cl2N-C60 complex by changing the type of halogen at position N61 at HF/ 6-31 G* [11-14].

4. Conclusion

Studies show that the energy of HOMO & LUMO levels in combination with halogen fluorine is less than that of N61 in the N61-X-C60-Catapres composition. Fig. 2, which is due to the electronegativity of the fluorine atom. The bipolar momentum variation was evaluated and compared since the bipolar momentum is a measure of the polarization in the molecule. A polar molecule is a molecule that has a serial and negative state, that is, one side is positive and the other is negative. For each polar bond, a polarized vector can be considered which is directed towards the electronegative atom and its length is due to the electronegativity difference Two atoms depend. The greater the electronegativity difference between the two atoms, the longer the bipolar momentum and the polar bond. In the compounds studied in this study, there are two chlorine atoms at positions 76 and 77. Fig. 1, due to their large electronegativity, seems to be It turns out that the magnitude of the dipole moment is affected, and it is observed that the bipolar momentum of the opposite trend is observed. R-Br> R-Cl> RF. Figure 3: Changes in the lengths of the N61-C62, N61-C62 and N61-C62 complexes of 3C9H9Cl2N-C60 complexes by changing the type of halogen at position N61 show that in all of the investigated links in this study, the increasing trend is as follows: R-Br> R (4) The Core / charge ratio for halogen atoms in the 3C9H9Cl2N-C60 complex is opposite, respectively. Br> Cl> F Fig. (5)

5. Conclusion:

Computational Quantum Mechanics at the theory level of B3LYP/6-31G on the structure of Fullerene and Fullerene Derivatives of Catapres drug was done separately and only when the structure of Catapres was attached to Fullerene and the results of this computation can be classified as follows:

The investigation of all the parameters show that the attachment of Catapres structure to Fullerene structure will influence the energy levels and dipole moment changes and these changes are able to be investigated in the electrical and chemical parameters of Fullerene Derivatives structure.

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