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Investigating the resonance energy and charge transfer in the clonidine and C_{60}-clonidine-fullerene carriers with quantum chemistry calculations

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Abstract

Clonidine has two aromatic rings in which halogens are attached to one ring in this study, both in drug state and in fullerene nanostructure, and by changing the type of halogen at the * HF / 6-31G level and in The gas phase was first optimized and then the NBO calculations were performed. The results obtained in N61, N63 and N5, N3 indicate the highest rhizanese energy and load transfer that, with variations in the type of halogen from fluorine to bromine, in all resonance energies in the nanoparticle The drug shows more values, while in all situations, the amount of drug load in the drug is similar to the nano-carrier in the same conditions. Shows more

Keywords: Clonidine. Fullerene, resonance energy, load

1. Introduction

Clonidine boosts systemic blood pressure and also promotes cardiac pacing by stimulating receptors in the CNS and as an antihypertensive agent. Clonidine is used in various forms of increased pressure to stop aggression and high pressure. And also used in eye diseases to prevent gradual blindness [1]. The structure of the C60 molecule is completely stable. The structure of this molecule is so stable that the C60 molecule acquires its original shape after colliding with a steel plate at 7000 m / s. In fact, there are a large number of carbon atom clusters in this structure, the number of carbon atoms in that pair, these molecules are

collectively called fullerenes. Inside or out of the fullerenes, you can make some enzymes or drugs and hormones needed by the body [2-3]. In this way, nanomaterials can be used. Refer to Fig. 1.

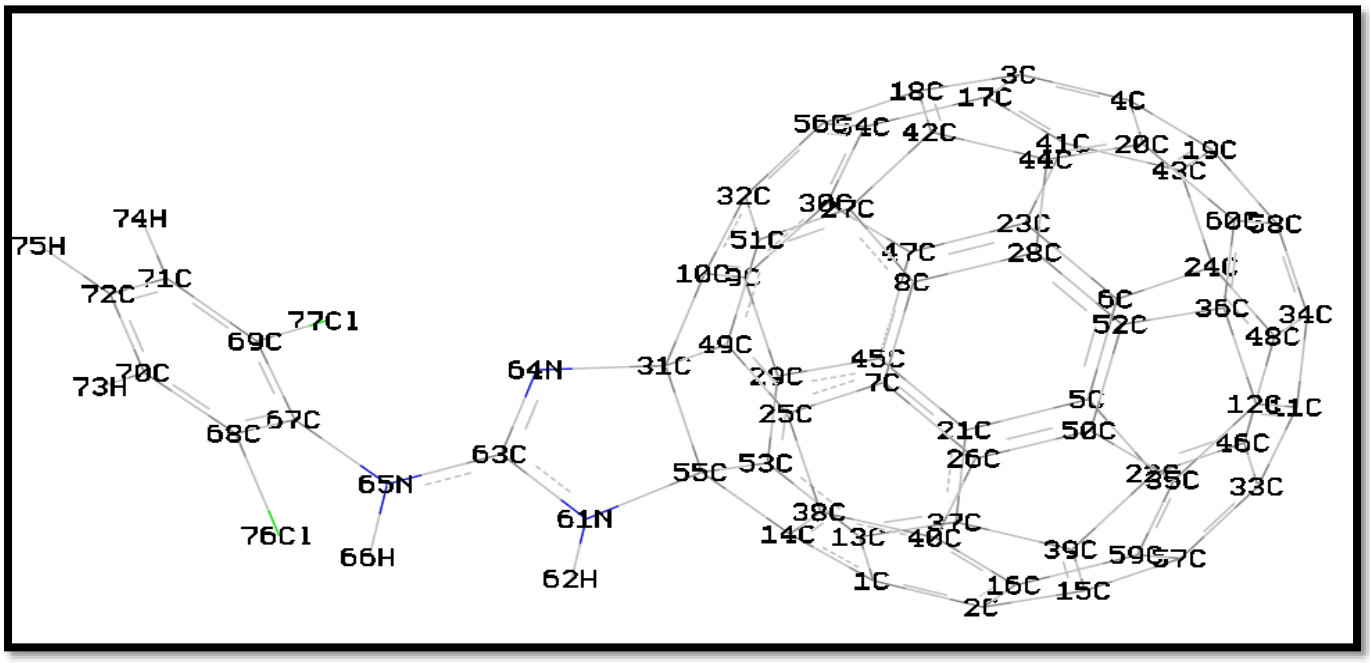

Figure 1 - X = F, Cl, Br) N61-X-C60-clonidine Compound

2. Method of work

In this study, using quantum chemistry calculations, the C60-clonidine and clonidine compounds were first optimized in the gas phase. Subsequently, quantum chemistry studies related to E2, Charge values on clonidine and clonidine on fullerene nanostructures by changing the halogenated halves of N61 N63, N5, N3 and using NBO software using Gaussian 98 software [4-9]. All calculations are performed on the HF level in the G * 31-6 base series.

3. Calculations and Results

Changes in halogen content in N61 and N3 and resonance energy changes of N61-C62-N63 and N64-C62-N63 and N3-C4-N5 and N6-C4-N5 bonds on clonidine and clonidine on fullerene nanostructures. Calculations show that the resonant energy in the nanoparticle is more than the drug. See Table 1 and Fig. 2 and Fig. 3.

Table 1 - Comparison of Resonance Energy Changes by Changing Hallucinations in N61 and N3 Positions on C60-Clonidine & Clonidine

	Atom	*E2* Lp N61 ⟹ BD* C62-N63 Lp N3 ⟹ BD* C4-N5	*E2* Lp N64 ⟹ BD* C62-N63 Lp N6 ⟹ BD* C4-N5
C60-Clonidine	F	58.99 Kcal/mol	76.26 Kcal/mol
	Cl	62.86 Kcal/mol	80.65 Kcal/mol
	Br	65.56 Kcal/mol	80.88 Kcal/mol
Clonidine	F	20.58 Kcal/mol	74.35 Kcal/mol
	Cl	61.12 Kcal/mol	76.29 Kcal/mol
	Br	62.68 Kcal/mol	75.77 Kcal/mol

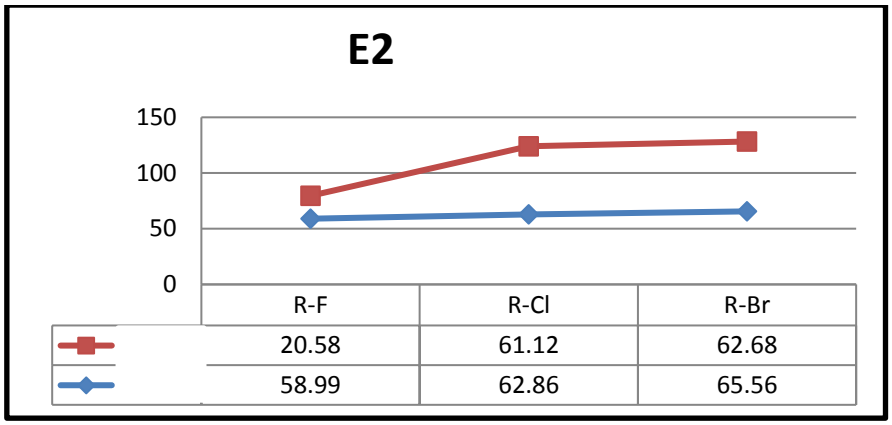

Figure 2: Changes of resonance energy by changing the halogen content of N61, N3 and E2 in N61-C62-N63 and N3-C4-N5 streams on the drug and nanoparticles

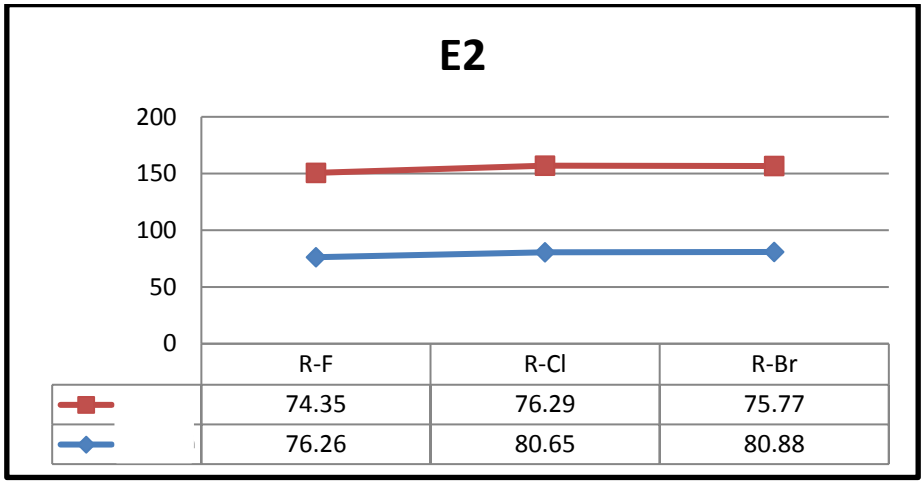

Figure 3: Changes in resonance energy with changes in halogenated atoms in N61, N3 position and E2 in N64-C62-N63 and N6-C4-N5 streams on drugs and nanoparticles

By investigating the change in the halogen content of N61 and N3 on clonidine and clonidine on the fullerene nanostructure, the transfer of charge from the drug to the nanoscale is carried out. Regarding the high electronegativity of F, the change trend for the two complexes is as follows Is: F <R-Cl <R-Br-R. Refer to Fig. 4

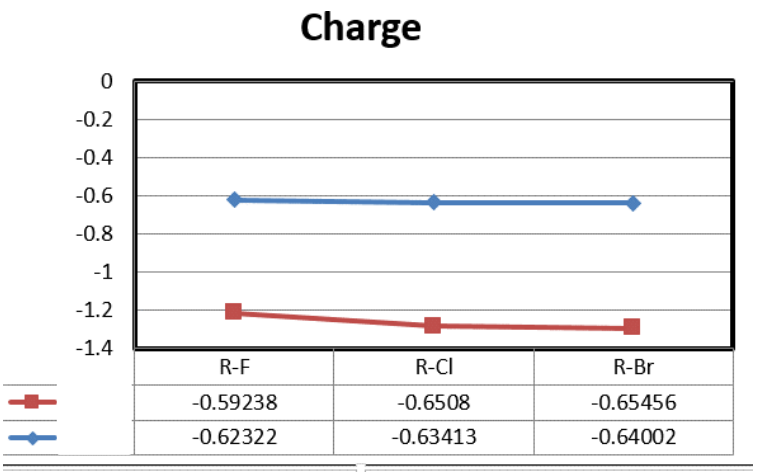

Figure 4. Changes in halogen content in N61 and N3 positions on clonidine and clonidine on fullerene nanostructures.

4 .Discussion and Conclusion

Investigations show that by changing the halogen content of N61 and N3, clonidine and clonidine on the fullerene nanostructure shows that the resonance energy in the nanoparticle is more than the drug. Resonance energy is directly related to reactivity. After the nanoscale in N61- C62-N63 and N64-C62-N63 have the highest reactivity. Refer to Table 1 and Fig. 2 and Fig. 3. In this regard, the connection of halogens in the N61 position is due to the high reactivity of this region. . Refer to Fig. 1. By investigating the trend of changing the halogenated components in the N61 and N3 position, the clonidine and clonidine drug on the fullerene nanostructure shows that the transfer of charge from the drug to the nanoparticle is carried out. By changing the halogen content, according to the electronegativity above F, the change trend for both complexes is as follows: F <R-Cl <R-Br-R. In general, by examining all three arguments, we can say Considering that the load is transferred from positive to negative, then, with regard to the data, when the drug is lonely in position N3, it has the highest amount of charge compared to the assessment of the position of N61 when the drug is attached to the fullerene, so transferring the drug from the drug to The nanoparticle is done. Refer to Figure 4.

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