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Investigation of Chemical Properties in Fullerene Derivatives of Atenolol Drug: A DFT Study

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Abstract

In this study, the drug atenolol on C_{60} fullerene were the drug and its derivatives were optimized fullerene. NBO and NMR for complex computations required in the HF/6-31G (d) and B3LYP/6-31G (d) quantum chemistry method was used. Mechanical quantum calculations in theory level of B3LYP/6-31G were performed on structure of atenolol and nano fullerene atenolol with different positions of linking. The properties such as energetic levels and stability, HOMO and LUMO levels, chemical hardness, chemical potential and electrophilicity values were studied.

Keywords: Atenolol, Fullerenes, NBO, NMR.

1. Introduction

Today considerable advances in have been accomplished in applications of nano-particles specifically in medical sciences. Fullerene is one of the other artificial forms of carbon element. Long life cycle of medicines in the human body is a success factor in delivery of medicine to the specific place. Lots of nano-particles are being developed in this field. Considering medical point of view, achieving such goals is vital. The aim of present study was to evaluate the effect of atenolol chemical properties of antihypertensive clonidine drug in water by DFT methods. Studies NMR (σ iso) were performed for all conditions and

changes in chemical shift (δ) of the desired compound was considered. NBO studies and determine the coefficients of a hybrid of bonds (π, σ) to determine the p orbitals in bonding (π, σ) was. Others were examined in this study, the amount of energy transfer between donor and acceptor of electrons in the atoms of the compound and the chemical potential (μ) and chemical hardness (η) of the compound were studied. This drug is classified as a drug therapy as an adjuvant in the treatment of hypertension and congestive heart failure (CHF) is used.

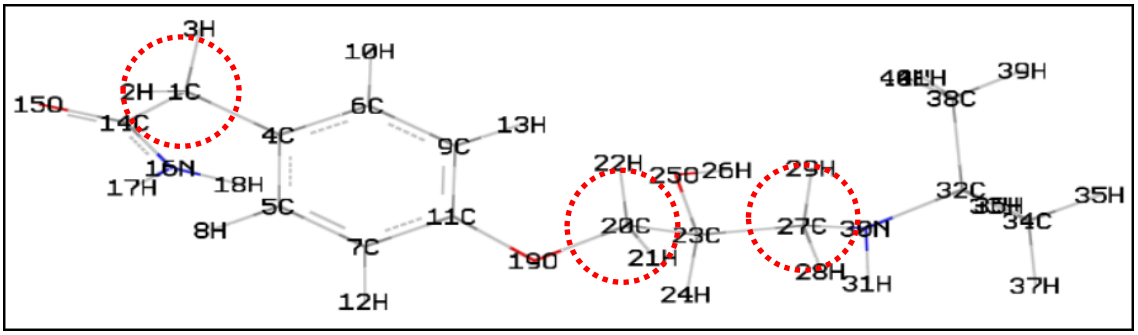


Fig 1. View of atenolol alone and location of connectable (1C, 20C and 27C) to Fullerene and shown briefly AT.

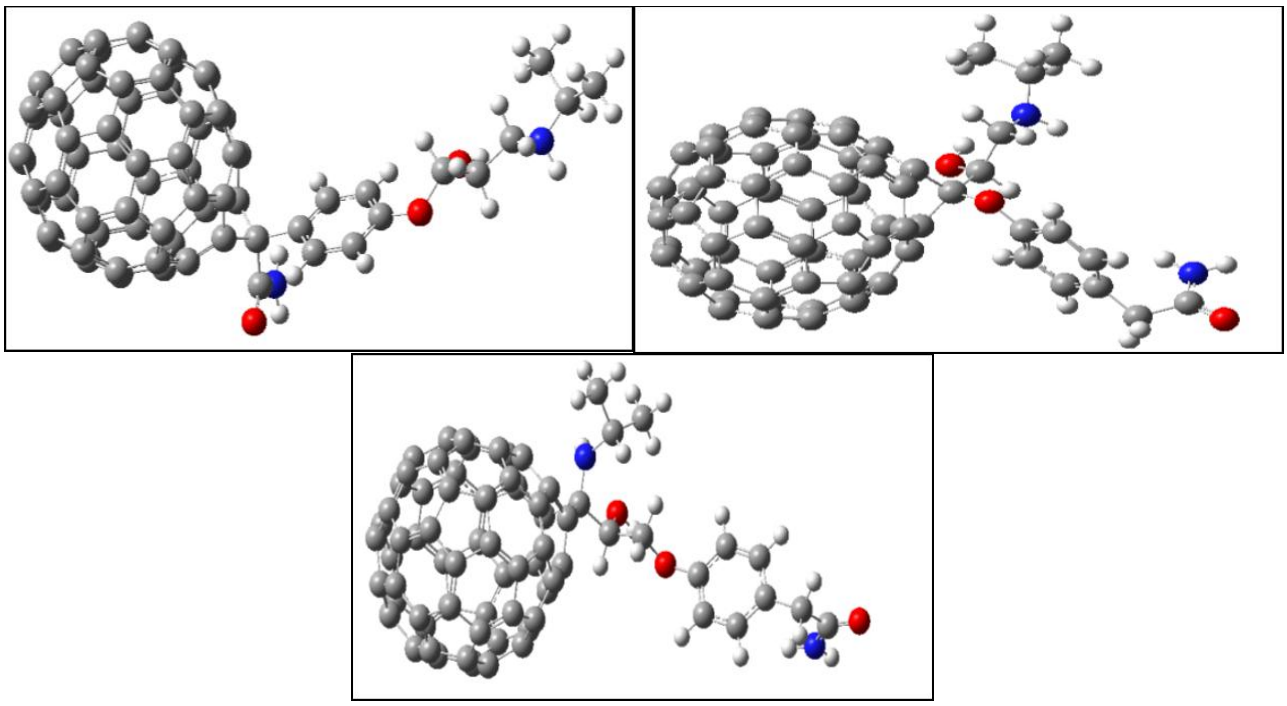


Fig 2. View of nano-drug atenolol has been obtained from carbon connection of atenolol in different position.

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 Beckes 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 atenolol 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 atenolol 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. Materials and methods:

All structure relating to structure of Atenolol and Nano Fullerene- Atenolol were designed primarily with use of Gauss view 5.0.8. In order to do final optimization, Gaussian 98 program of package HF method were used. However, for this purpose, 6-31G basis set was used. Computation was done in gas phase. Total computations were done with use of Pentium III with processor Intel core i5 with memory of 4 gigabytes and inside the operating of windows SEVEN. All computations were performed under gas phase, 1 atmosphere and 298 Kelvin temperature.

4. Results and discussion

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

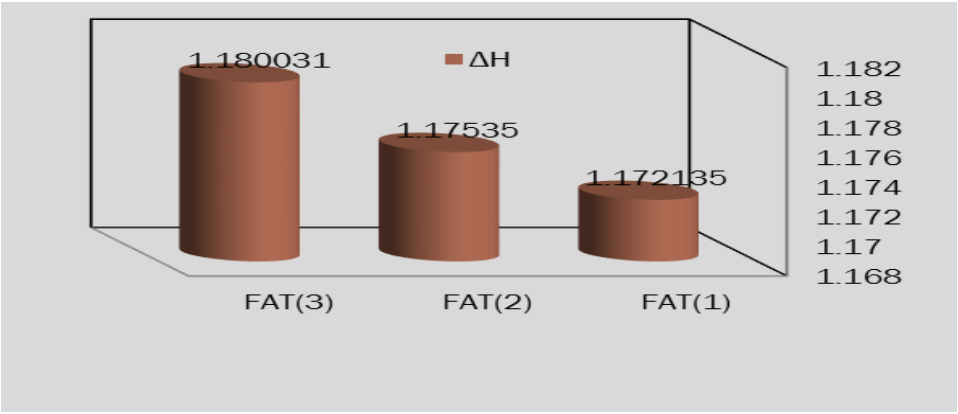
NO	Symbol	Matter
1	AT	Atenolol
2	FAT(1)	Nano-drug from binding of Atenolol C1 to Fullerene
3	FAT(2)	Nano-drug from binding of Atenolol C20 to Fullerene
4	FAT(3)	Nano-drug from binding of Atenolol C27 to Fullerene

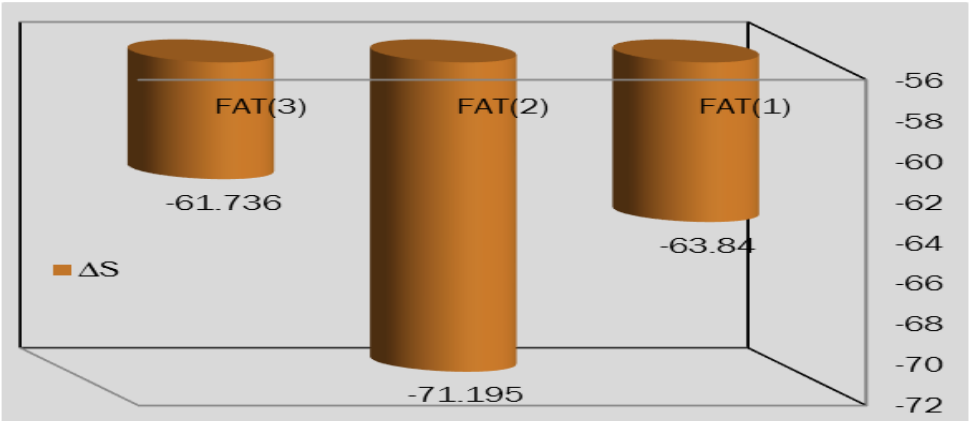
The results showed that the calculated energy gap is typically much higher of the Atenolol than atenolol attached to fullerene in each three connection is different and the other hand the amount of that in each three atenolol binds to fullerene to connection forms is different and mostly the same compared with the accuracy of thousands.

In this work Atenolol was linked to the fullerene, atenolol drug and its 4 fullerene derivatives investigated. Then compare Enthalpy (ΔH), Entropy (ΔS), Gibbs free energy (ΔG) parameters between atenolol alone and nano-fullerene- atenolol.

Table 1. Obtained energies, entropies of in fullerene Derivatives of Atenolol drug, calculated at the levels of B3LYP/6-31G (d) (Kcal/mole).

Energy parameters	ΔH	ΔS	ΔG
FAT(2)	1.172135	-63.84	1.202468
FAT(1)	1.17535	-71.195	1.209177
FAT(3)	1. 180031	-61.736	1.209364





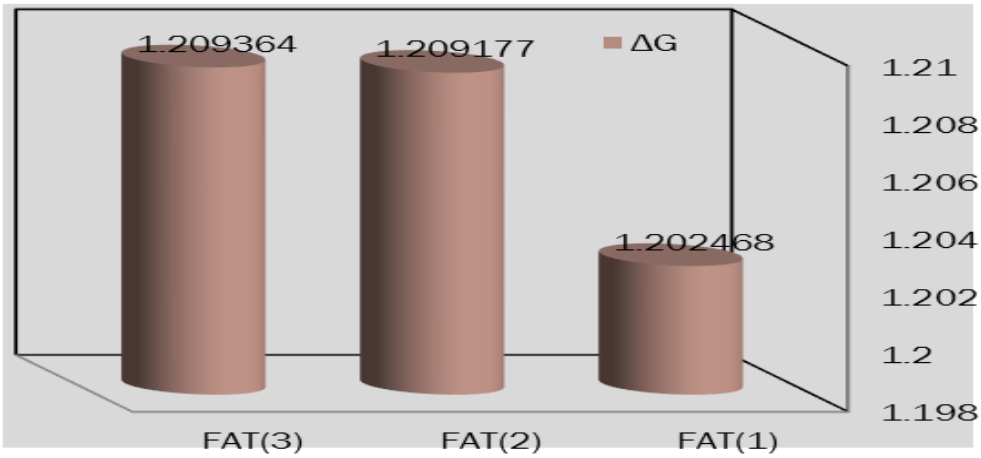


Fig 3. Obtained energies, entropies of in fullerene derivatives of atenolol drug, calculated at the levels of B3LYP/6-31G (d) (Kcal/mole).

4. Conclusion

Computational quantum mechanics at the theory level of B3LYP/6-31G on the structure of fullerene and fullerene derivatives of atenolol drug was done separately and only when the structure of atenolol 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 atenolol structure to fullerene structure will influence the Enthalpy (ΔH), Entropy (ΔS), Gibbs free energy (ΔG) changes are able to be investigated in the electrical and chemical parameters of fullerene derivatives structure.

- The calculation of the values in the table (ΔH> 0) (ΔS> 0) (ΔG> 0).

- Represents the energy, Enthalpy (ΔH), and the results show the reaction is endothermic FAT (3)> FAT (2)> FAT (1)

- Entropy (ΔS) represent irregularity and the results show a decrease in the amount of irregularities. FAT (3)> FAT (1)> FAT (2)

- Gibbs free energy (ΔG) is the amount of energy available to a process and when it is positive.

- When (ΔG> 0) is show non-spontaneous reaction, (ΔG= ΔH- ΔS) FAT (3)> FAT (2)> FAT(1).

The calculation of the values show this reaction is non-spontaneous.

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