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Computational Investigation on the Effect of Changes in Halogenated on Afrin with Fullerene

Arya Jalili*

Department of Chemistry, K. N. Toosi University of Technology (KNTU), P. O. Box 15875-4416, Tehran, Iran.
*Corresponding Author e-mail Address: **Aryajalili@yahoo.com**

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Abstract

In this research at the first Afrin drug or and its fullerene derivative were optimized. Afrin is a nasal congestion drug that acts by contraction of the blood vessels of the arteries and veins. Afrin acts directly on the nasal vessels. Eclipse of the blood vessels in your nose and the sinuses causes the water to be collected and the nasal congestion is reduced. And this medicine is used for colds. The fullerene is made up of a large number of carbon atoms, which is round and spherical. In this research, the early studies [2X- [C60-Afrin-C65 (X = F, Cl, Br) were optimized. All computations were performed using the Hartree-Fake method in the 6-31G * series, using GaussianVoucin 2003 software and in the gas phase. Calculations have shown that by changing the halogenated equations based on the size and changing the electronegative size, the lengths of the connections and The angles change. The results indicate that the C65-X has the shortest bond length and bond strength. As well as the angles, C65-C66-C67 was investigated which has this process. R-F <R-Cl <R-Br. The data in tables and graphs and shapes were compared and discussed.

Keywords: Afrin, Fullerenes, Chemical potential, Nano drug carriers.

1. Introduction

Nanostructures can be categorized into following forms according to their structures: diamonds with sp^3 hybridization, Graphite with sp^2 hybridization, Hexagonal diamonds with sp^3 hybridization, fullerenes with SP^2 hybridization, Nanoparticles, Graphene, single-layer and multi-layer nanotubes, Crystal Nanostructures. All these forms of nanostructures produce unique Pharmaceutical and electronic properties. Graphenes have a two-dimensional structure of a single layer of carbon chicken wire [1-3]. A fullerene is any molecule composed of carbon in the form of a hollow sphere, ellipsoid, tube, and many other shapes. Spherical fullerenes are also called Bucky balls, and they resemble the balls used in football (soccer). Cylindrical ones are called carbon nanotubes or Bucky tubes. Fullerenes are similar in structure to graphite, which is composed of stacked Graphene sheets of linked hexagonal rings; but they may also contain pentagonal (or sometimes heptagonal) rings. The first fullerene molecule to be discovered, and the family's namesake, buckminsterfullerene (C_{60}), was prepared in 1985 by Richard Smalley, Robert Curl, James Heath, Sean O'Brien, and Harold Kroto at Rice University. The discovery of fullerenes greatly expanded the number of known carbon allotropes, which until recently were limited to graphite, diamond, and amorphous carbon such as soot and charcoal. Buckyballs and buckytubes have been the subject of intense research, both for their unique chemistry and for their technological applications, especially in materials science, electronics, and nanotechnology [4]. It was approved by the U.S. Food and Drug Administration for the treatment of major depressive disorder in December 1987 [5]. Afrin is used for the treatment of major depressive disorder (including pediatric depression), obsessive-compulsive disorder (in both adults and children), bulimia nervosa, panic disorder and premenstrual dysphoric disorder. In addition, Afrin is used to treat trichotillomania if cognitive behavior therapy has been unsuccessful. Afrin's mechanism of action is predominantly that of a serotonin reuptake inhibitor [6]. Afrin delays the reuptake of serotonin, resulting in serotonin persisting longer when it is released. Afrin may also produce some of its effects via its weak 5-HT2C receptor antagonist effects. In addition, Afrin has been found to act as an agonist of the σ1-receptor, with a potency greater than that of citalopram but less than that of fluvoxamine. However, the significance of this property is not fully clear. Afrin also functions as a channel blocker of anoctamin 1, a calcium-activated chloride channel. The base of fullerenes is the pages in the graphite, except that in the atomic structure of the fullerenes, instead of the regular hexagons in the graphite plates, there is a series of hexagonal and regular pentagons that are arranged together in one another. Taken and Fulleran Butter. The placement of these pentagons and hexagons together is essential for the formation of a spherical structure. In fact, without the presence of pentagons in the graphene structure, we can not obtain the graphene of spherical structur. Determine the fullerenes according to the number of atoms in their building. To name the fullerenes, a letter C is used that represents the carbon atom in their structure. After the letter C, the number of carbon atoms in the

fullerene spherical network unit is mentioned. For example, the C_{60} molecule contains 60 carbon atoms. The number of atoms in the generated fullerenes is from 28 to hundreds of carbon atoms

Afrin is an aldaveridia drug rather than an anti-congestion drug. Constipation drugs are available locally and edibly. Contraindications include oral and hypodermic epinephrine. Afrin is the most common topical anesthetic and has the chemical formula C13H24N2O [7-11].

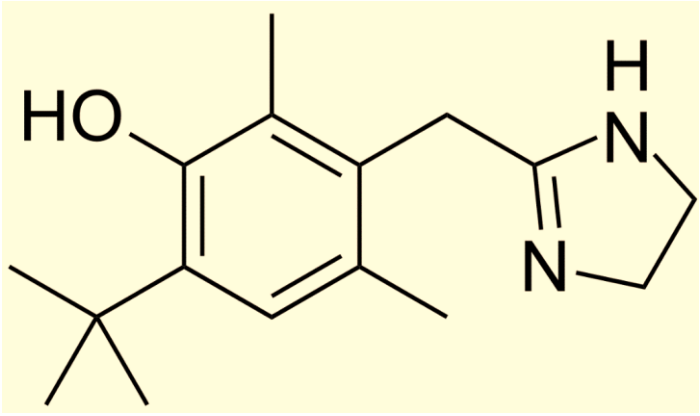

Fig 1. View of Afrin

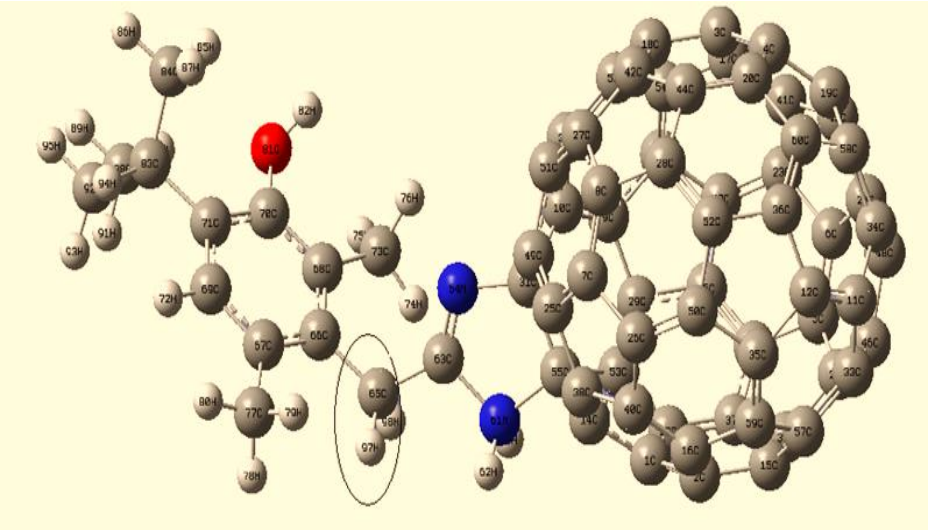

Fig 2. View of Nano-drug Afrin has been obtained from carbon connection of Afrin to Fullerene .

2. Computational details

All Computations are performed by means of GAUSSIAN 03 packing [12-15]. 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 Afrin 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 Afrin 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, Afrin drug and its fullerene derivatives investigated. Using Gaussian software (X = F, Cl, Br ([C60-Afrin-2X] + on a computer compilation in this paper, the calculations of 2003 and Gossoyou were carried out. Compounds with different substitutions first, using the Hartree-Fake method Changes in the lengths of the links and angles were optimized by adding halogenated groups, and then, 6-31 G* Was evaluated and evaluated

Table 1. The length of the transplantation of the compounds -2 X C60-Afrin, (X = F, Cl, Br) in the C65-X graft

Complex	Bond length
C_{65}-F_{97}	1.395
C_{65}-Cl_{97}	1.883
C_{65}-Br_{97}	2.018

Table 2. N61-C63 bond lengths in combination [C60-Afrin-2X] + by changing the type of halogen in the carbon position 63 at HF level

Complex	N_{61}-C_{63}
R-2F	1.487
R-2Cl	1.4901
R-2Br	1.4935

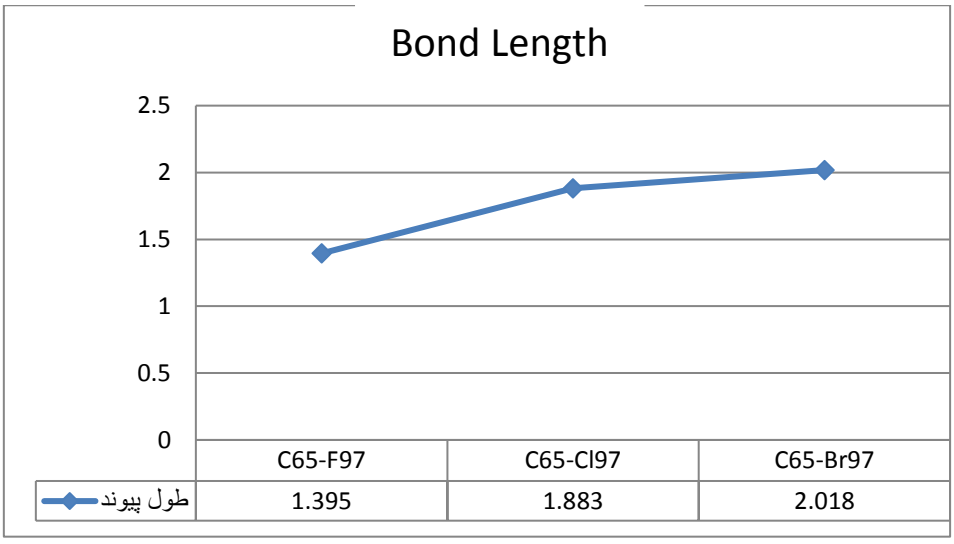

Fig 3. Results of the Bond Length of the three Fullerene derivative in B3LYP/6-31 level

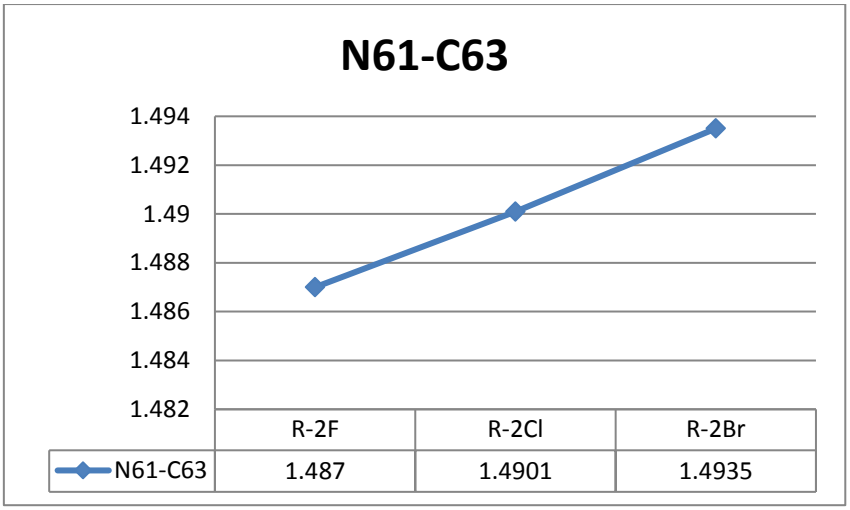

Fig 4. Comparison of the length of the N61-C63 bond [C60-Afrin-2X] +, (X = F, Cl, Br) at the HF surface

Table 3. Comparison of C65-C66-C67 graft angle in compounds [C60-Afrin-2X] +, (X = F, Cl, Br) at HF level

Complex	C65-C66-C67
R-2F	121.81845
R-2Cl	123.74638
R-2Br	124.70344

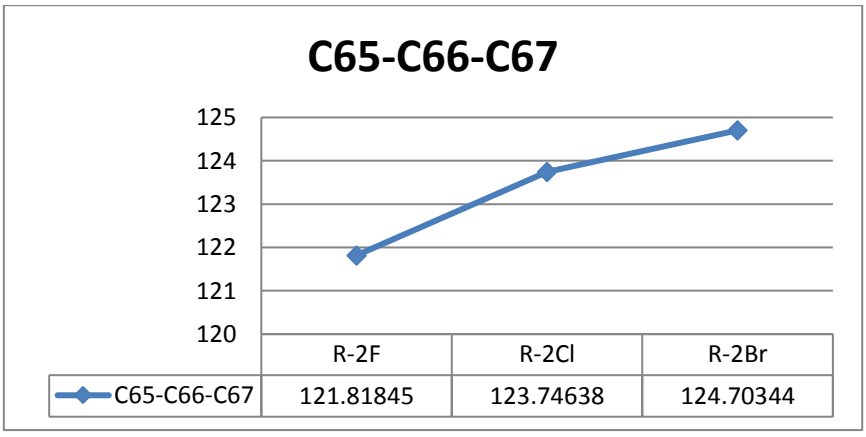

Fig. 4 shows the angular displacements in the compounds [C60-Afrin-2X] +, (X = F, Cl, Br) at the HF surface

5. Conclusion:

Computational Quantum Mechanics at the theory level of B3LYP/6-31G on the structure of Fullerene and Fullerene Derivatives of Afrin drug was done separately and only when the structure of Afrin 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 Afrin 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. The presence of halogens causes changes in the length of the bonds and as a result of the strength of the bonds. The modifications of these changes depend on the type of halogen and its location. By changing the refractories on the composition, it was observed that, as much as possible, more and the amount of added substituents added to the composition The gravity of the electron gravity nucleus gravity becomes larger and the electronegativity of the atom increases and the relative desire of the atom to absorb the pair of adjacent electrons of the neighboring atoms in a stable molecule increases, that is, the relative relative tendency of that atom to pull the electrons of a covalent bond toward the nucleus It is self-propagating and the length of the strain is strain It gives you Fluorine is the electronegative atom in the halogens group, which has the shortest bond length and the highest binding strength (Tables 1,2) and (Figures 2,3). Comparison of angles showed that in the combination of fluorinated C65-C66-C67 the lowest amount of compounds [C60-Afrin-2X] + (X = F Cl Br)

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