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Ab Initio Studies: effect of various substituted on structural parameters and charge transfer energy of the Nafazolin drug and its nano carrier on fullerene

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Abstract

A fullerene is any molecule composed entirely of carbon, in the form of a hollow **s**phere. Naphazoline is a sympathomimetic agent with marked alpha adrenergic activity. It is a vasoconstrictor with a rapid action in reducing swelling when applied to mucous membrane. It acts on alpha-receptors in the arterioles of the conjunctiva to produce constriction, resulting in decreased congestion. It is an active ingredient in several over-the-counter formulations including Clear Eyes and Naphcon eye drops.In this research work at The first compounds $[C60\text{-}Nafazolin\text{-}Cn\text{-}2X]^+$ and $[Nafazolin\text{-}Cn\text{-}2X]^+$ (X=F,Cl,Br) were optimized. Then the calculation of natural bond orbitals was performed with the NBO technique. All calculations using Hartree- fock the 6-31G * basis set using Gaussian 98 software and in gas phase has been done. The results showed that the energy levels of molecular orbital (HOMO & LUMO) in the RF has the lowest value. C65-X has a length of the shortest bond and the bond has most power. Comparison of the dipole moments of compounds shows this trend: RF> R-Cl> R-Br but to be noticed that with same trend in nano carrier dipole moment is reducing. The values of Charge transfer energy for $\sigma \Longrightarrow \sigma^*$ (C_7 - X_{26} $\Longrightarrow$ C_5 - N_6) show this order R-Br> R-Cl > R-F

Keywords: Nafazolin , nano carrier, fullerene , charge transfer energy..

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 [1-5]. 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. Nafazolin is an antidepressant of the selective serotonin reuptake inhibitor (SSRI) class. Nafazolin was first documented in 1974 by scientists from Eli Lilly and Company [6]. It was approved by the U.S. Food and Drug Administration for the treatment of major depressive disorder in December 1987 [7-8]. Nafazolin 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 [9]. In addition, Nafazolin is used to treat trichotillomania if cognitive behavior therapy has been un successful [10]. Nafazolin's mechanism of action is predominantly that of a serotonin reuptake inhibitor [11]. Nafazolin delays the reuptake of serotonin, resulting in serotonin persisting longer when it is released. Nafazolin may also produce some of its effects via its weak 5-HT2C receptor antagonist effects [12]. In addition, Nafazolin 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 Nafazolin also functions as a channel blocker of anoctamin 1, a calcium-activated chloride channel.

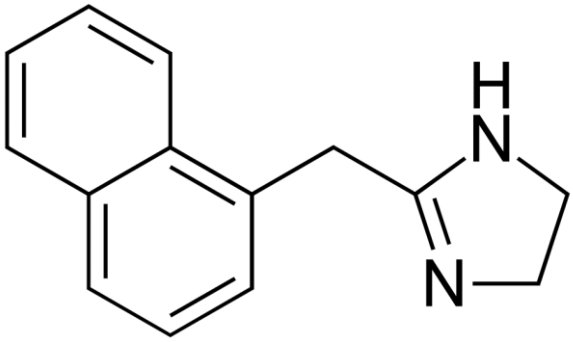

Fig 1. View of Nafazolin alone

2. Computational details

All Computations are performed by means of GAUSSIAN 03 packing [13]. 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 Nafazolin 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 Nafazolin 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

Table 1. The values of the length of the links with the substitution of F, Cl, Br halogens at HF level

compound	C_{65}-X_{85}	C_{65}-C_{63}	C_{63}-N_{64}	N_{64}-C_{31}
C_{60}- $C_{14}H_{12}N_2H^+$_2F	1.41066 Å	1.70118 Å	1.39236 Å	1.59805 Å
C_{60}- $C_{14}H_{12}N_2H^+$_2Cl	1.89544 Å	1.64585 Å	1.49236 Å	1.49383 Å
C_{60}- $C_{14}H_{12}N_2H^+$_2Br	2.02151	1.52584 Å	1.58236 Å	1.37315 Å

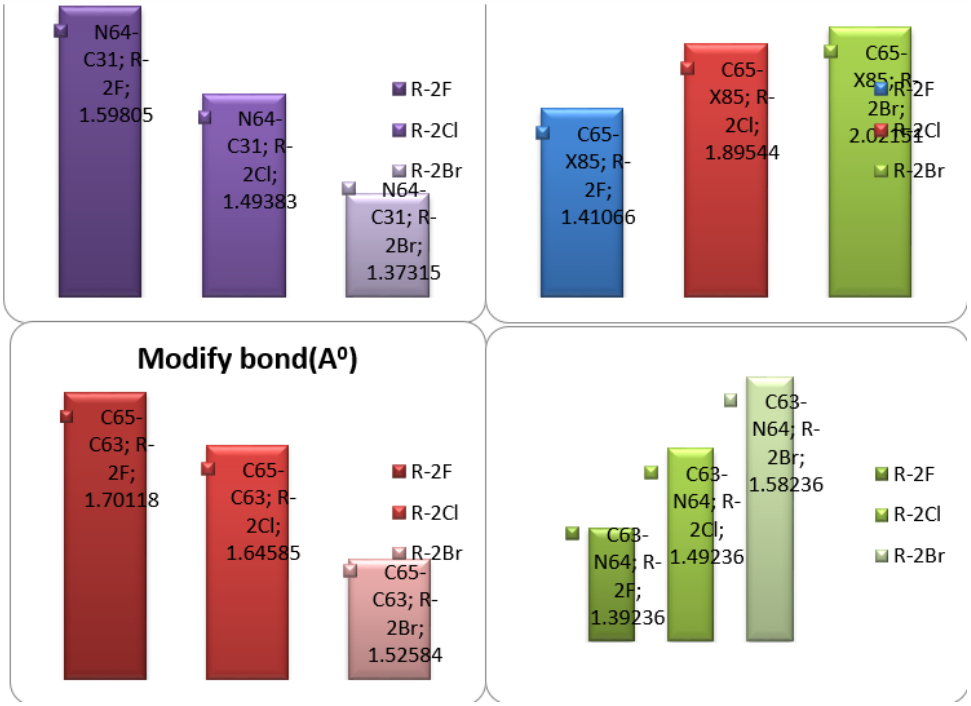

Chart 1. Changes in the length of the C65-X89, C65-C63, C31-N64, C63-N64 graft by changing the halogens

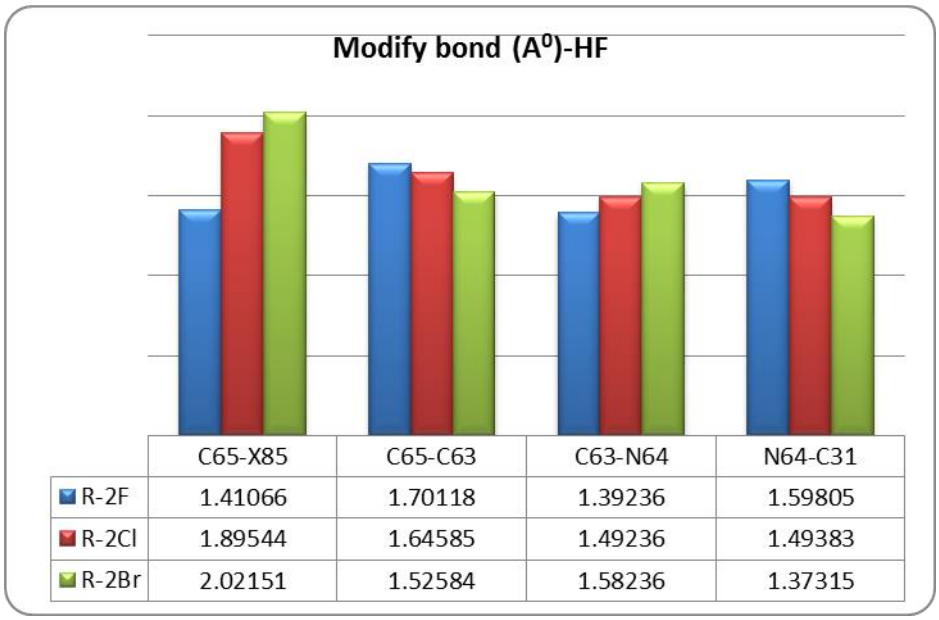

Chart 2. Comparison of changes in the length of the C65-X89, C65-C63, C31-N64, C63-N64 graft by changing the halogens

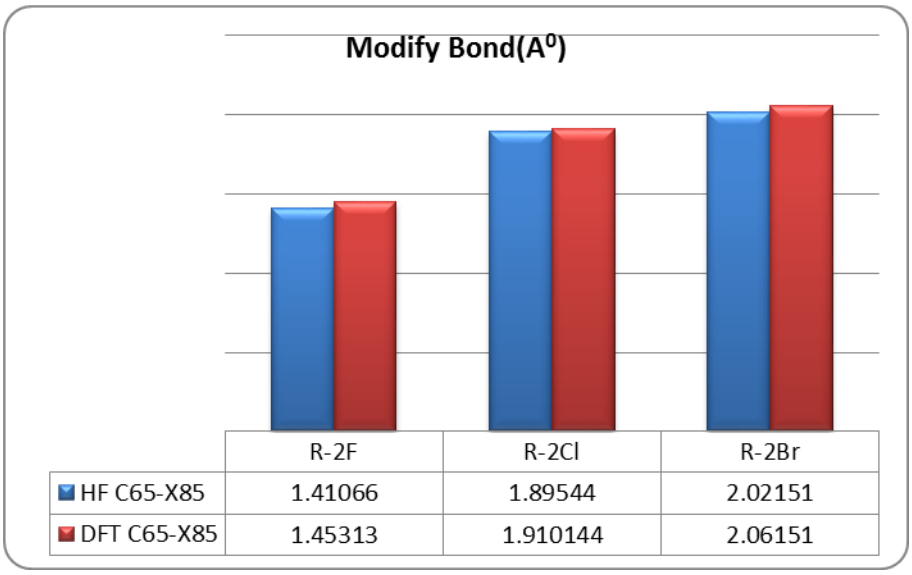

Chart 3. Comparison of changes in the other length of the C65-X89, C65-C63, C31-N64, C63-N64 graf bonds by changing the halogens

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

5. Conclusion:

Computational Quantum Mechanics at the theory level of B3LYP/6-31G on the structure of Fullerene and Fullerene Derivatives of Nafazolin drug was done separately and only when the structure of Nafazolin 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 Nafazolin 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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