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# Quantum chemistry studies on structures and electronic properties of the Tolazoline drug on nano structure of fullerene

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## Abstract

Tolazoline is a non-selective competitive α-adrenergic receptor antagonist. It is a vasodilator that is used to treat spasms of peripheral blood vessels (as in acrocyanosis).Tolazoline is indicated in the treatment of persistent pulmonary hypertension in the newborn (persistent fetal circulation) when systemic arterial oxygenation cannot be maintained by supplemental oxygen and mechanical ventilation. The fullerene family especially C60 derivatives have appealing photo-, electro-chemical and physical properties for biomedical applications including acting as pro- and anti-oxidants. In this research work at The first compounds [$C_{60}$-TOLAZOLINE -$C_{65}$-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 R-2F has the lowest value. $C_{65}$-X has the shortest length and the highest power in R-2F. Comparison of the dipole moments of compounds shows this trend: R-2H > R-2Cl> R-2Br> R-2F. ratio Core / charge and the valence / charge for carbon atoms 31, 55, 65 and 63 in the RF has the highest value

**Keywords:** Tolazoline, Core / charge, fullerene , valence / charge

## 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 [1-2]. 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. Tolazoline is an antidepressant of the selective serotonin reuptake inhibitor (SSRI) class. Tolazoline was first documented in 1974 by scientists from Eli Lilly and Company [3]. It was approved by the U.S. Food and Drug Administration for the treatment of major depressive disorder in December 1987 [4]. Tolazoline 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 [5]. In addition, Tolazoline is used to treat trichotillomania if cognitive behavior therapy has been un successful [6]. Tolazoline's mechanism of action is predominantly that of a serotonin reuptake inhibitor [7]. Tolazoline delays the reuptake of serotonin, resulting in serotonin persisting longer when it is released. Tolazoline may also produce some of its effects via its weak 5-HT2C receptor antagonist effects [8]. In addition, Tolazoline 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 [9]. Tolazoline also functions as a channel blocker of anoctamin 1, a calcium-activated chloride channel.

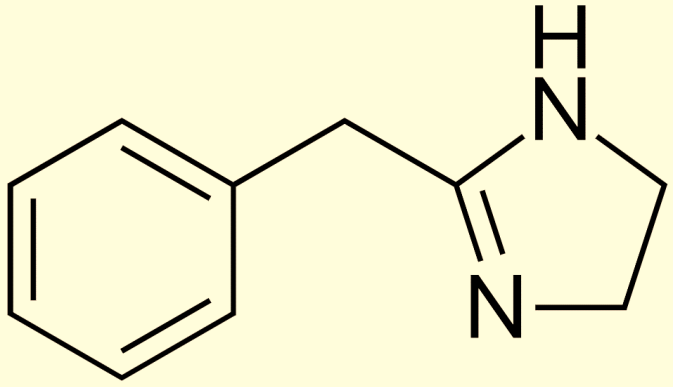


Fig 1. The structure optimized by HF / 6-31G * for Tolazoline

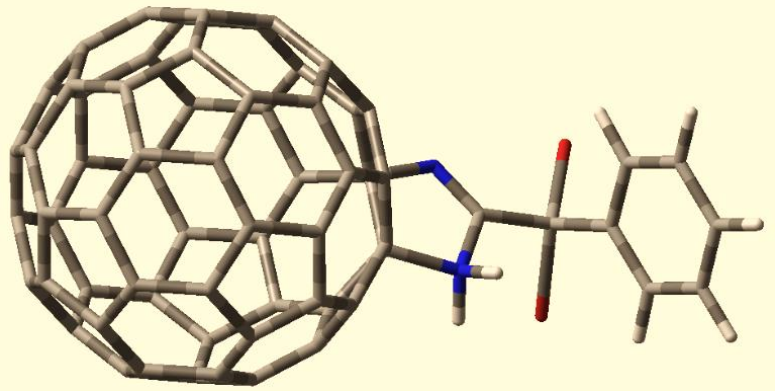

Fig 2. The structure optimized by HF / 6-31G * for the derivative C68H7Br2N2 (+1)

## 2. Computational details

All Computations are performed by means of GAUSSIAN 03 packing [10]. 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 Tolazoline 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 Tolazoline on Fullerene were investigated [11].

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, Tolazoline drug and its 3 fullerene derivatives investigated. The related structures are named in the following way:

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

| | Bond length | | |
|---|---|---|---|
| | F | Cl | Br |
| C65-X 78 | 1.36746 | 1.83257 | 1.95422 |
| C65-X 79 | 1.39722 | 1.87324 | 1.99575 |
| C65-C63 | 1.50626 | 1.49877 | 1.49311 |
| C65-C66 | 1.50101 | 1.51456 | 1.51555 |
| C63-N61 | 1.48254 | 1.49008 | 1.49001 |
| C63-N64 | 1.23991 | 1.24129 | 1.24193 |
| C66-C68 | 1.38928 | 1.38838 | 1.38848 |

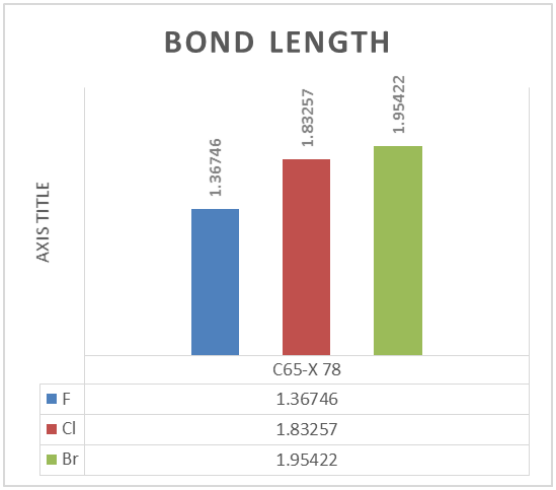


Fig3. Changes in the length of the C65-X78 bond by changing the halogens. (X = F, C, Br)

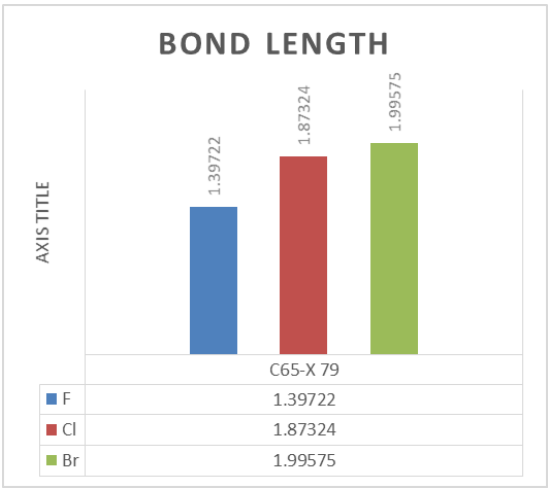


Fig3. Changes in the length of the C65-X79 bond by changing the halogens. (X = F, C, Br)

## 4. Conclusion:

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

## Acknowledgment

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