



A theoretical study about Substituted effect in current ring and aromaticity with NICS index in nano carrier Xylometazoline drug

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Abstract

Xylometazoline is a drug which is used as a topical nasal decongestant. It is applied directly into the nose, either as a spray or as drops. Xylometazoline is an imidazole derivative which is designed to mimic the molecular shape of adrenaline. It binds to alpha-adrenergic receptors in the nasal mucosa. Due to its sympathomimetic effects, it should not be used by people with high blood pressure, or other heart problems. In this report, At the first compounds [C60- Xylometazoline -C65-X] (X=F, Cl, Br) were optimized, then NMR calculations have been done. The results indicate In all noticed carbons atoms Chemical shielding tensor (σ) is lowest and chemical shift tensor(δ) is highest in R-F. On the other hand with increasing electroneativity in substituted atom, NICS Index shows this trend: R-F>R-Cl>R-Br. nucleic independent chemical shift (NICS) is considered for Aromaticity. If aromaticity is increased, so , stability is increased and reactivity is increased. All calculations is performed in 6-31g* basis set in HF method and in gas phase.

Keywords: Xylometazoline, 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 [1-5]. 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. Xylometazoline is an antidepressant of the selective serotonin reuptake inhibitor (SSRI) class. Xylometazoline 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]. Xylometazoline 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, Xylometazoline is used to treat trichotillomania if cognitive behavior therapy has been unsuccessful [10]. Xylometazoline's mechanism of action is predominantly that of a serotonin reuptake inhibitor [11-12]. Xylometazoline delays the reuptake of serotonin, resulting in serotonin persisting longer when it is released. Xylometazoline may also produce some of its effects via its weak 5-HT_{2C} receptor antagonist effects [13]. In addition, Xylometazoline has been found to act as an agonist of the σ_1 -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 [14-15]. Xylometazoline also functions as a channel blocker of anoctamin 1, a calcium-activated chloride channel.

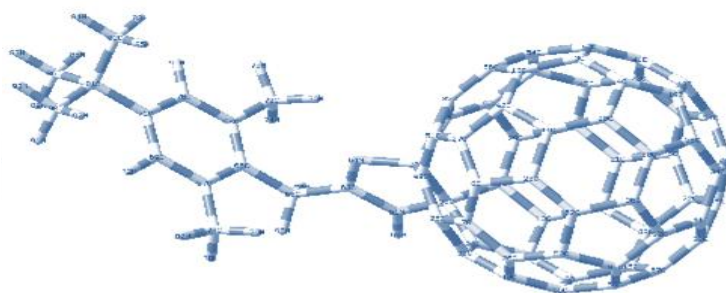


Fig 1. [C_{60} - Xylometazoline - C_{65} -X] (X=F, Cl, Br).

2. Computational details

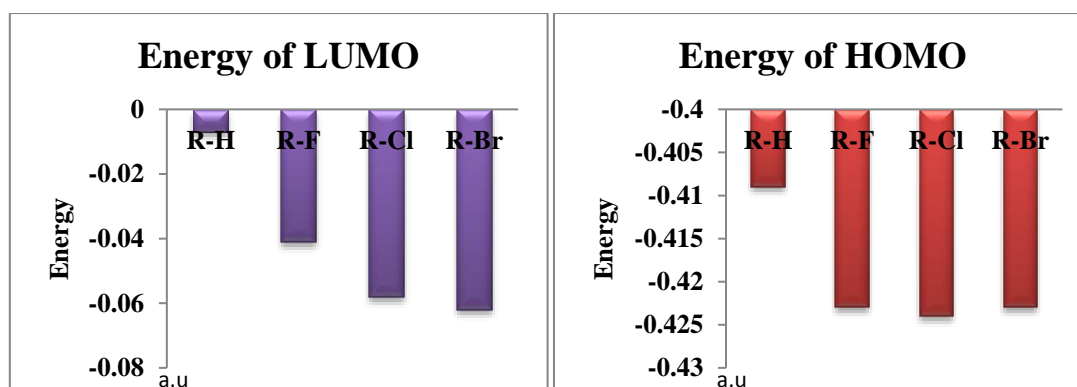
All Computations are performed by means of GAUSSIAN 03 packing [9]. Geometries for all compounds are computed by means of the density functional theory (DFT) with Becke's three-parameter functional (B3) plus Lee, Yang, and Parr (LYP) correlation functional. For all atoms, the standard 6-31G basis set is utilized. The structures of Xylometazoline 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 Xylometazoline 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[10-12].

3. Results

In this study, Xylometazoline drug and its 3 fullerene derivatives investigated. The related structures are named in the following way: The results showed that the calculated energy gap is typically much higher of the Xylometazoline than Xylometazoline attached to Fullerene in each three connection is different and the other hand the amount of that in each three Xylometazoline binds to Fullerene to connection forms is different and mostly the same compared with the accuracy of thousands.

Table (1): Energy Levels of HOMO and LUMO and energy chains in the composition of ONLY-Xylometazoline-C7-X2

	(ONLY) Energy		
	Energy of HOMO	Energy of LUMO	Gap of Energy
R-H	-0.409	-0.007	0.402
R-F	-0.423	-0.041	0.382
R-Cl	-0.424	-0.058	0.366
R-Br	-0.423	-0.062	0.361



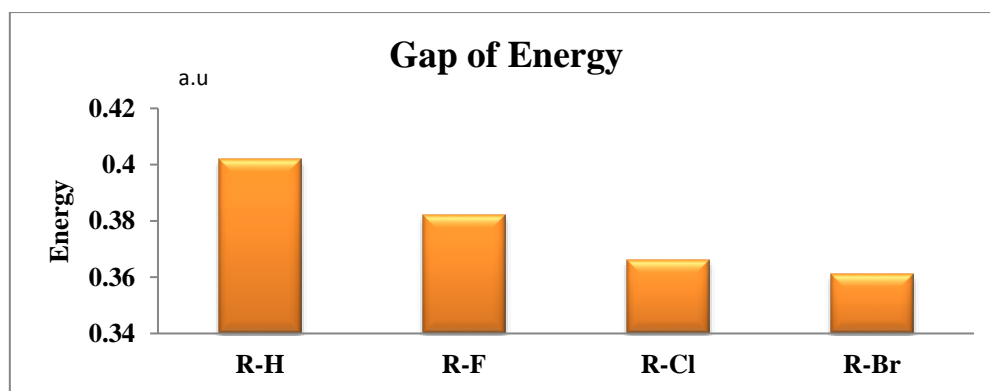


Fig2. Comparison diagrams of energy levels of HOMO and LUMO and energy chips in the ONLY-Xylometazoline-C7-X2 composition

Table (2): Energy Levels of HOMO and LUMO and Energy Changes in the C60-Xylometazoline-C65-X2 Compound

	(C ₆₀) Energy		
	Energy of HOMO	Energy of LUMO	Gap of Energy
R-H	-0.378	-0.107	0.271
R-F	-0.382	-0.111	0.271
R-Cl	-0.381	-0.110	0.271
R-Br	-0.379	-0.109	0.270

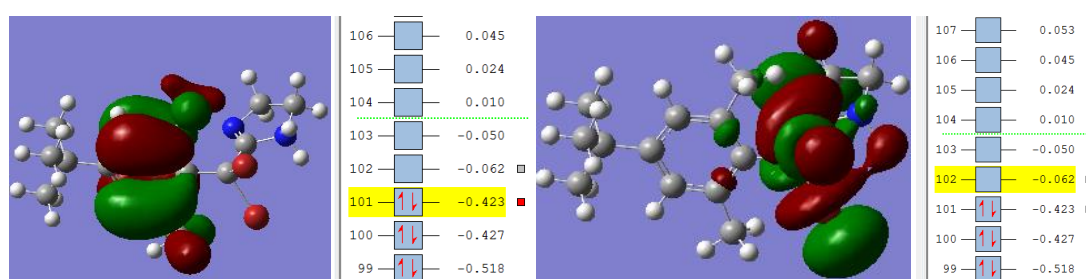


Fig 2. HOMO Ʌ LUMO of ONLY-Xylometazoline-C7-Br

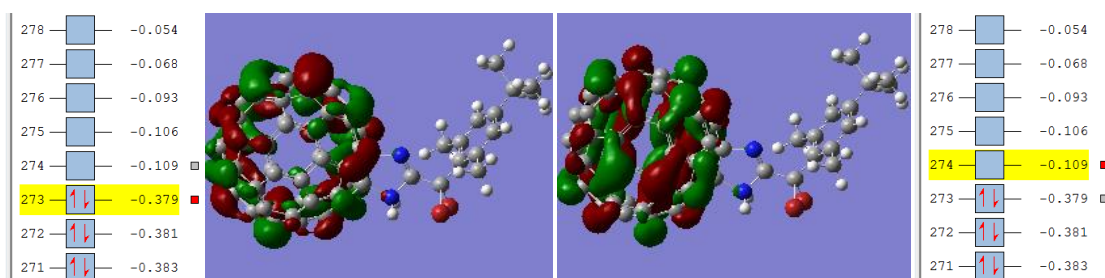


Fig3. HOMO Ʌ LUMO of ONLY-Xylometazoline-C7-Br of C₆₀-Xylometazoline-C₆₅-Br

5. Conclusion:

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