International Journal of New Chemistry, 2016, 3 (4), 87-92
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Published online 2016 in http://www.ijnc.ir/.
Original Article

Online ISSN 2383-188X
Open Access

Computational Investigation of the Effect of Changes in Halogenated on Factors in Nano-Carriers of 1-cyclohexyl-1-phenyl-3-pyrrolidin-1-yl-propan-1-ol hydrochloride and C_{60}

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Received 6 September 2016; Accepted 28 October 2016; Published 1 November 2016

Abstract

In this study, the drug combination of 1-cyclohexyl-1-phenyl-3-pyrrolidin-1-yl-propan-1-ol hydrochloride or Procychelidine was applied on fullerene and its dual halogen derivatives were optimized in the position of carbon 62. In this study, using initial computation methods, the rate of participation of atomic orbitals and hybrid coefficients in adjacent adjacent atoms was calculated, and the Procyclidine 2X-C60 composition was studied by varying substitutions such as Br, Cl, F. The results indicate the change in the rate of orbital participation and the degree of sustainability affected by these changes in this link.

Keywords: 1-cyclohexyl-1-phenyl-3-pyrrolidin-1-yl-propan-1-ol hydrochloride, Fullerene, Participation of atomic orbital

1. Introduction

Fullerene, the first known carbon-spherical carbon molecule, is arranged in the shape of a ball in the form of a ball. The base of the fullerenes is the plates in the graphite, with the difference that in the atomic structure of the fullerenes, instead of regular hexagons in the graphite plates, there is a series of

hexagons and regular polygons, It is located in the middle of each other and forms the fullerene sphere. Because of the spherical and empty building, they are used as drug carriers. [1].Procyclodine, introduced in the 1950s, is an anticholinergic drug used to treat Parkinson's disease, especially in the early stages of the disorder, for treating vibration and muscle stiffness, and secretion of excess saliva. Parkinson's disease is a paralysis of the brain disorder that causes tremor, stiffness and muscle weakness. Prodaccilidine is used as a tablet, infusion or oral liquid. [2-5]. The combination is part of the anticholinergic). 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. Procychelidine is an antidepressant of the selective serotonin reuptake inhibitor (SSRI) class. Procychelidine 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]. Procychelidine 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 [8]. In addition, Procychelidine is used to treat trichotillomania if cognitive behavior therapy has been un successful [9]. Procychelidine's mechanism of action is predominantly that of a serotonin reuptake inhibitor [10-11]. Procychelidine delays the reuptake of serotonin, resulting in serotonin persisting longer when it is released. Procychelidine may also produce some of its effects via its weak 5-HT2C receptor antagonist effects [12]. In addition, Procychelidine 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 [14-15]. Procychelidine also functions as a channel blocker of anoctamin 1, a calcium-activated chloride channel [13].

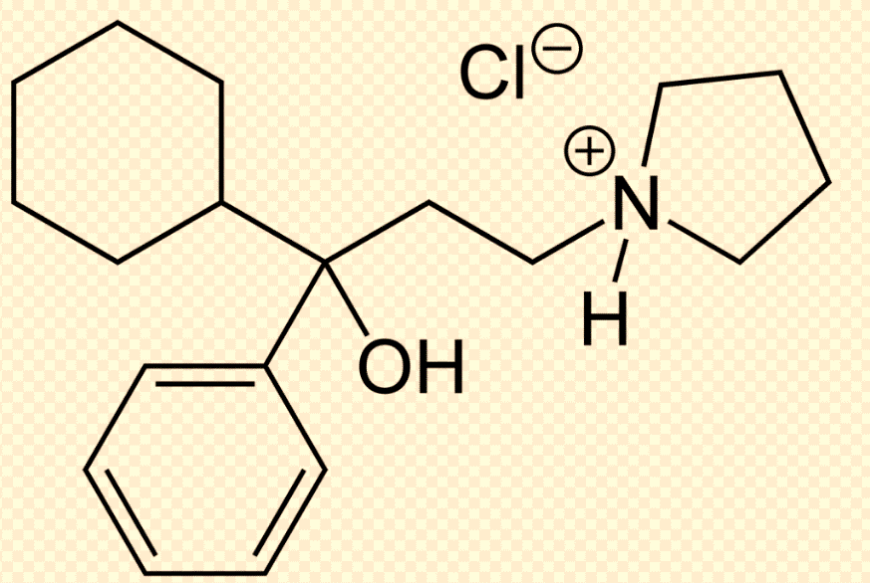

Fig 1. View of **1-cyclohexyl-1-phenyl-3-pyrrolidin-1-yl-propan-1-ol hydrochloride or Procychelidine**

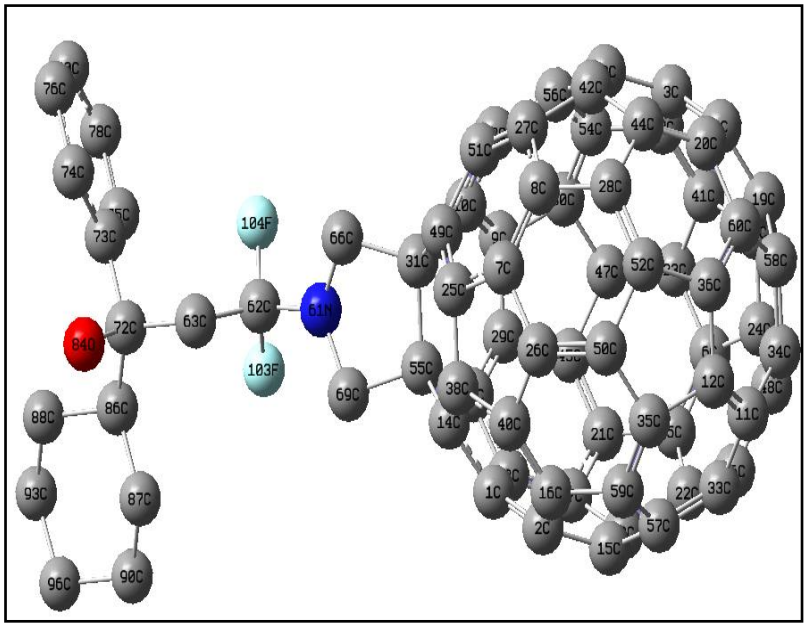

Fig 2. View of Structural image of the composition - Procyclidine 2F-C60

2. Computational details

All Computations are performed by means of GAUSSIAN 03 packing [14-15]. 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 Procychelidine 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 Procychelidine 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, Procychelidine drug and fullerene derivatives investigated. The results showed that the calculated energy gap is typically much higher of the Procychelidine than Procychelidine attached to Fullerene in each three connection is different and the other hand the amount of that in each three Procychelidine binds to Fullerene to connection forms is different and mostly the same compared with the accuracy.

Table 1. **Table 1: The amount of orbitals involved in the 2X-C60-procyclidine composition by changing the substitutions F, Cl, Br at**

NBO	2F	2Cl	2Br
C_{62}- X_{103}	2.19232	3.19414	4.34730
C_{62} – X_{104}	2.16785	3.21109	4.37317
C_{66} - N_{61}	1.94069	1.96178	2.00241
C_{69} - N_{61}	1.93834	1.95643	1.98790

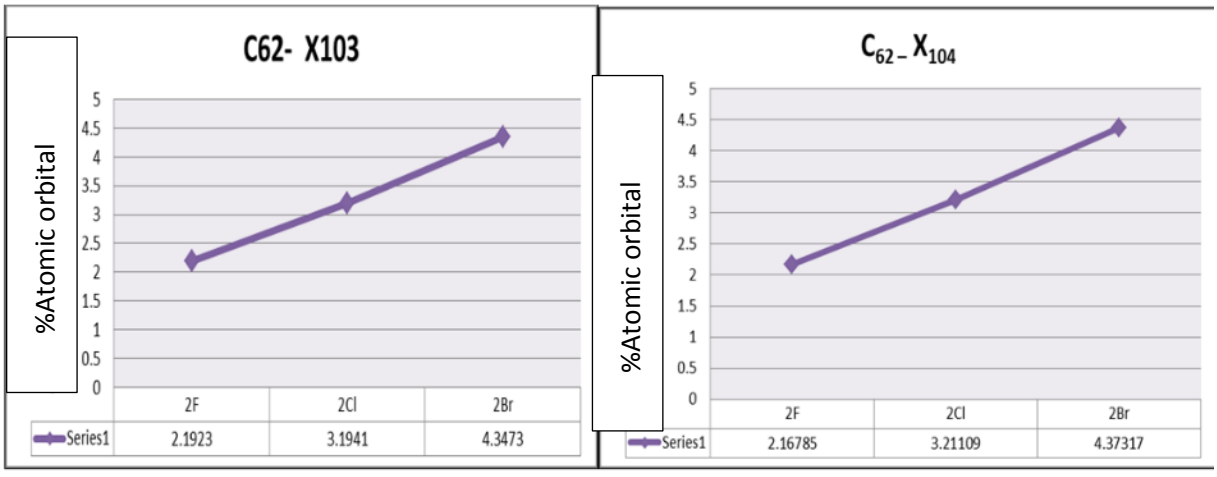

Fig 3. The amount of orbitals involved in the 2X-C_{60}-Procyclidine combination by changing the F, Cl, Br substitutions at position C_{62}

Table 2: Hybrid coefficients of bonding with F, Cl, Br calculated by NBO method in base series 6-31G

Bond	2F	2Cl	2Br
$C_{62}-X_{103}$	0.029	3.194	4.347
$C_{62}-X_{104}$	0.011	3.211	4.373

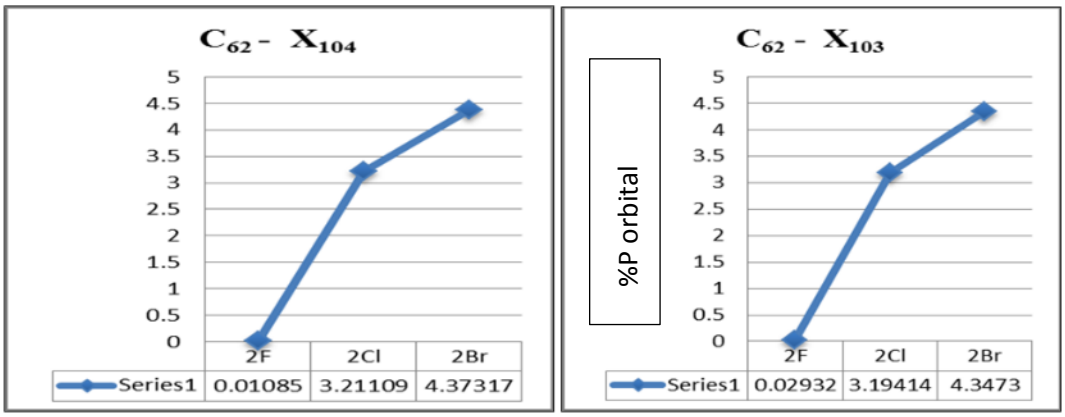

Fig 4. Hybrid Factors of C_{60}-Procyclidine Compounds with F, Cl, Br Compounds Calculated by NBO Method in Base Series 6-31 G*

5. Conclusion:

Computational Quantum Mechanics at the theory level of B3LYP/6-31G on the structure of Fullerene and Fullerene Derivatives of Procychelidine drug was done separately and only when the structure of Procychelidine 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 Procychelidine 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.In this project, NBO calculations for the C60-Procyclidine complex were performed with the HF method in the base series 6-31 G *. [3]. The percentage of orbital participation p with substitutions of Br is higher than other halogens - Given that the fluorine electronegative is chlorine and bromine, the amount of orbital p-participation in the C62-F linkage is reduced and, as a result, C62 gives a greater share of orbital p in the C62-C63 bond.

In general, it can be stated that the lower the electronegativity of the halogenated substituent (and the larger the size of the halogen), the greater the orbital p-bond ratio of C62-X, and therefore the contribution of the orbital p contribution to the atoms around the C62 is less.

As it was observed, the rate of orbital p involvement in the C62-X103 and C62-X104 bond in the Br component is more than F and Cl, which is more explicit with respect to the larger radius of chlorine and fluorine and having an orbital share of p. As a result, the bindings around the bromide have less orbital p participation. The following trend is the same for the participation rate of atomic orbitals and hybrid coefficients.

$$C_{62} - 2Br > C_{62} - 2Cl > C_{62} - 2F$$

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