International Journal of New Chemistry, 2016, 3 (1), 12-17.
Published online January 2015 in http://www.ijnc.ir/.
Original Article

Online ISSN 2383-188X
Open Access

A theoretical study of dipole moments, energy levels and structural parameters in the Oxymetazoline drug as a nano carrier based on fullerene with changing substitution

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Received 1 December 2015; Accepted 28 December 2015; Published 30 January 2016

Abstract

Oxymetazoline is a decongestant. It works by constricting (shrinking) blood vessels (veins and arteries) in your body. The nasal formulation acts directly on the blood vessels in your nasal tissues. Constriction of the blood vessels in your nose and sinuses leads to drainage of these areas and a decrease in congestion. Oxymetazoline is an adrenomimetic that nonselectively agonizes α_1 and α_2 adrenergic receptors. The fullerenes family especially C60 derivatives have appealing photo-, electro-chemical and physical properties for biomedical applications including acting as pro- and anti-oxidants. In this report at The first compounds [C60- Oxymetazoline -C_{65}-2X] (X=F,Cl,Br) were optimized. Then the calculation of natural bond orbitals was performed with the NBO method. All calculations using Hartree- Fock the 6-31G * basis set using Gaussian 98 software and in gas phase has been done. The results indicated that the energy levels of molecular orbital (HOMO & LUMO) in the [C60- Oxymetazoline -C_{65}-2F] have the lowest value. C65-X has a length of the shortest bond and the bond has most power. Comparison of the dipole moments and amount of (C_{63}-C_{65}-C_{66}) angle in these compounds show this trend: RF> R- Br > R- Cl. Both C_{63}-C_{65} and C_{65}-C_{66} bonds have this order: R- Cl> R- Br> RF

Keywords: Oxymetazoline , nano carrier, fullerene , Hartree- Fock

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

Fig 1.

3. Results

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

Table1. Optimized bond length of R-2 X (X =F, Cl, Br) of complexes in HF, B3LYP methods

	bond length					
	R-2F		R-2Cl		R-2Br	
	HF	B_3LYP	HF	B_3LYP	HF	B_3LYP
C_{65}-X_{97}	1.39516	1.42584	1.88302	1.99665	2.01332	2.04328
C_{65}-X_{98}	1.40699	1.45505	1,89256	1.91663	2.0185	2.11475
C_{65}-C_{66}	1.49724	1.48148	1.50939	1.48549	1.51139	1.48896
C_{63}-N_{61}	1.48706	1.51943	1.49011	1.52299	1.49356	1.52614

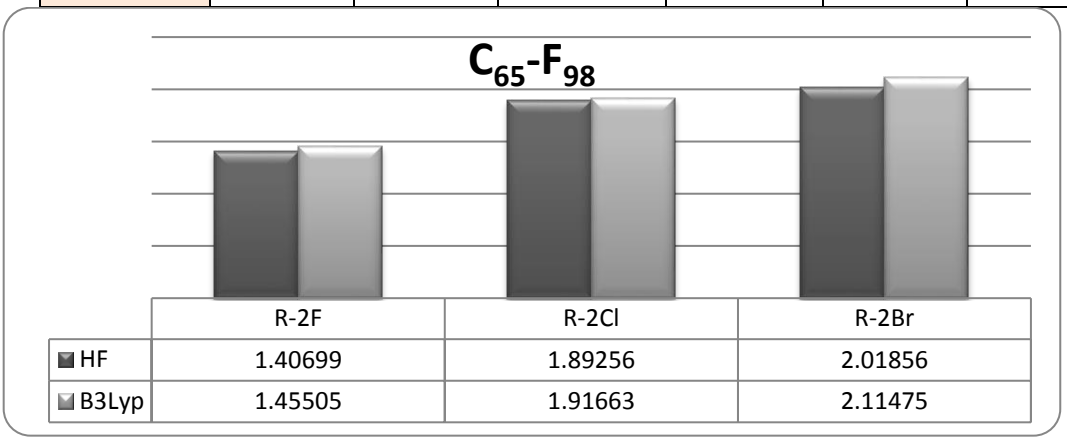

Table2. P Contribution in Fullerene + Medicines and in the in HF, B_3LYP methods HF/6-31G*

Bond	Atom		Orbital P Contribution
б	C_{31} - N_{64}	nano drug /HF	$0.6355\ (S^1P^{3.80})_{C31} + 0.7721\ (S^1P^{2.39})_{N64}$
		Drug/HF	$0.7551(S^1P^{3.8۹})_{N64} + 0.6556(S^1P^{3.۵۰})_{C31}$
б	C_{63} - C_{65}	nano drug /HF	$0.7286\ (S^1P^{1.67})_{C63} + 0.6849\ (S^1P^{2.64})_{C65}$
		Drug/HF	$0.7448\ (S^1P^{1.6۵})_{C63}\ 0.6673(S^1P^{2.۹۴})_{C65}$
б	C_{65}- C_{66}	nano drug /HF	$0.7231\ (S^1P^{1.71})_{C65} + 0.6907\ (S^1P^{2.62})_{C66}$
		Drug/HF	$0.7352\ (S^1P^{2.۰۷})_{C65} + 0.6779\ (S^1P^{2.۴۹})_{C66}$
б	C_{65}- F 97	nano drug /HF	$0.5096\ (S^1P^{4.62})_{C65} + 0.8604(\ S^1P^{2.65})F_{۹7}$
		Drug/HF	$0.6232\ (S^1P^{3.75})_{C65} + 0.7821\ (S^1P^{8.68}F_{97}$
б	C_{65} - F 98	nano drug /HF	$0.5086\ (S^1P^{4.66})_{C65} + 0.8610\ (S^1P^{2.78})\ F_{98}$
		Drug/HF	$0.6242\ (S^1P^{3.76})_{C65} + 0.7813\ (S^1P^{8.92})\ F_{98}$
Bond	**Atom**		**Orbital P Contribution**
б	$C_{۳1}$ - N_{61}	nano drug /HF	$0.7802(S^1P^{2.54})_{C31} + 0.6256\ (S^1P^{3.62})_{N64}$
		Drug/HF	$0.7551\ (S^1P^{3.89})_{N64} + 0.6556\ (S^1P^{3.50})_{C31}$
б	C_{63} - C_{65}	nano drug /HF	$0.7133\ (S^1P^{1.63})_{C63} + 0.7009\ (S^1P^{2.43})_{C65}$
		Drug/HF	$0.7135\ (S^1P^{1.57})_{C63} + 0.7007(S^1P^{2.43})_{C65}$
б	C_{65}- C_{66}	nano drug /HF	$0.7382\ (S^1P^{1.65})_{C65} + 0.6746\ (S^1P^{2.56})_{C66}$
		Drug/HF	$0.7392(S^1P^{1.66})_{C65} + 0.6735\ (S^1P^{2.6})_{C66}$
б	C_{65}-Cl 97	nano drug /HF	$0.\ 6853\ (S^1P^{4.96})_{C65} + 0.7282(\ S^1P^{7.10})_{Cl97}$
		Drug/HF	$0.6857(S^1P^{4.91})_{C65} + 0.7278(S^1P^{7.05})_{\text{Cl }97}$
б	C_{65} - Cl 98	nano drug /HF	$0.6799\ (S^1P^{5.03})_{C65} + 0.7333\ (S^1P^{7.08})_{Cl98}$
Bond	**Atom**		**Orbital P Contribution**
б	$C_{۳1}$ - N_{61}	nano drug /HF	$0.6372\ (S^1P^{\mathbf{3.73}})_{C31} + 0.7707(S^1P^{\mathbf{2.38}})_{N64}$
		Drug/HF	$0.7799\ (S^1P^{2.46})_{N64} + 0.6259(S^1P^{3.63})_{C31}$
б	C_{63} - C_{65}	nano drug /HF	$0.7130\ (S^1P^{1.59})_{C63} + 0.7012\ (S^1P^{2.39})_{C65}$
		Drug/HF	$0.7130\ (S^1P^{1.54})_{C63} + 0.7011\ (S^1P^{2.39})_{C65}$
б	C_{65}- C_{66}	nano drug /HF	$0.7389\ (S^1P^{1.64})_{C65} + 0.6738\ (S^1P^{2.53})_{C66}$
		Drug/HF	$0.7394\ (S^1P^{1.64})_{C65} + 0.6733(S^1P^{2.54})_{C66}$
б	C_{65}-Br 97	nano drug /HF	$0.7228\ (S^1P^{5.06})_{C65} + 0.6910\ (S^1P^{9.07})_{Br97}$
		Drug/HF	$0.7233(S^1P^{5.06})_{C65} + 0.6905(S^1P^{9.14})_{Br97}$
б	C_{65} - Br 98	nano drug /HF	$0.0.7179\ (S^1P^{5.11})_{C65} + 0.6961\ (S^1P^{8.99})_{Br98}$
		Drug/HF	$0.0.7190\ (S^1P^{5.11})_{C65} + 0.6951\ (S^1P)_{Br98}$

Atom	Charge	Core	Valence	Rydberg	Total
O81	-0.78564	1.99976	6.78031	0.00557	8.78564
N61	-0.70367	1.99941	5.69219	0.01206	7.70367
C73	-0.69921	1.99935	4.69126	0.00859	6.69921
C77	-0.69341	1.99935	4.68724	0.00682	6.69341
C92	-0.67905	1.99937	4.66953	0.01015	6.67905
C88	-0.66966	1.99934	4.66097	0.00934	6.66966
C84	-0.66446	1.99934	4.65607	0.00904	6.66446
N64	-0.34514	1.99921	5.33236	0.01357	7.34514
C69	-0.24412	1.99898	4.2326	0.01253	6.24412
C66	-0.13735	1.99873	4.12047	0.01814	6.13735
C83	-0.0601	1.99911	4.0507	0.01028	6.0601
Cl98	-0.0484	9.99981	7.04004	0.00855	17.0484
C65	-0.0236	1.99861	3.99668	0.02831	6.0236
C68	-0.0055	1.99892	3.99305	0.01353	6.0055
Cl97	-0.00332	9.9998	6.99424	0.00928	17.00332
C71	0.02163	1.99892	3.9592	0.02025	5.97837
C67	0.04308	1.99897	3.94346	0.01449	5.95692
H74	0.21559	0	0.78276	0.00165	0.78441
H87	0.22985	0	0.76907	0.00108	0.77015
H91	0.231	0	0.76795	0.00104	0.769
H94	0.23213	0	0.76676	0.0011	0.76787
H93	0.23304	0	0.76588	0.00108	0.76696
H89	0.23305	0	0.76596	0.00099	0.76695
H85	0.23426	0	0.76446	0.00128	0.76574
H86	0.23938	0	0.75963	0.00099	0.76062
H76	0.2429	0	0.75548	0.00162	0.7571
H95	0.24678	0	0.75233	0.00089	0.75322
H78	0.24951	0	0.74935	0.00114	0.75049
H80	0.25074	0	0.74828	0.00098	0.74926
H72	0.25296	0	0.74577	0.00128	0.74704
H79	0.25658	0	0.74238	0.00104	0.74342
H90	0.26067	0	0.73835	0.00098	0.73933
H75	0.2859	0	0.71275	0.00135	0.7141
C70	0.31522	1.99845	3.66958	0.01675	5.68478
C63	0.42394	1.99889	3.5463	0.03087	5.57606
H82	0.50603	0	0.49273	0.00124	0.49397
H96	0.50738	0	0.49042	0.0022	0.49262
H62	0.50806	0	0.48933	0.00261	0.49194

5. Conclusion:

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

We are appreciating and thanking Islamic Azad University of Yeager-e-Imam Khomeini (Rah) Share Rey.

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