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The usage comparison of occupancy parameters, gap band energy, ΔN_{max} at Xylometazoline medicine ratio its medical conveyer nano

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ABSTRACT

For analyzing of compositions molecular orbitals in this article in order to combination only- xylometazolin-C_7 X_2 (XY) and C_{60}– xylometozolin-C_{65}-X_2 (FXY), first got energies of highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) by using NBO analyze in Gaussian 03 software. Then, occupancy parameter, gap of energy, and ΔNmax were calculated by support of these energies. All calculations were implemented in gaseous phase by using of (DFT) method and basis series 6-31G**.

Keywords: *Xylometazoline; Fullerene; Conveyer nano; ΔN_{max}; Density Functional Theory (DFT).*

INTRODUCTION

Xylometazoline is a sort of medicine used to treat the hyperemia in people's noses [1]. This medicine is applied directly as driblet or spray into the nose [1, 2]. Xylometazoline cure the issues through contracting the nasal veins. Such feature occurs due to decrease in blood pressure in capillary veins and accordingly less water permeates through them so the water leakage is lowered [3,4]. Xylometazoline is one of the Imidazole derivatives and the objective of creating such medicine is stated as imitation of adrenaline molecular form. This medicine attaches to alpha adergenic receptors exist in nasal parts [5, 6]. Since it imitates the sympatric aspects, xylometazoline should not be used by people who suffer from high blood pressure or other cardiovascular disease [6] (Figure 1). Nowadays, nanotechnology is widely utilized as a research tool in medical areas and medicine transport [7]. Fullerene (C_{60}) derivatives have demonstrated photochemical, electrochemical and physical properties which could be used in biomedical applications. So Fullerene in the present study have been utilized as nano-carriers for xylometazoline [8, 9] (Figure2).

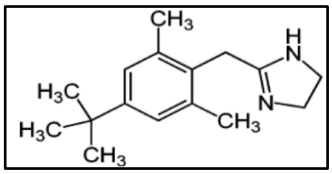


Fig. 1. Structure of xylometazoline (XY)

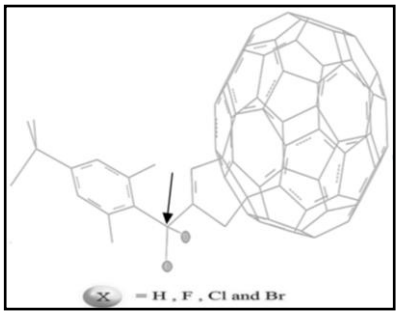
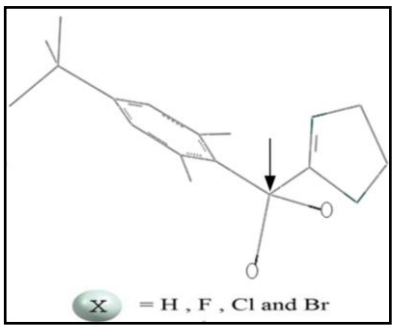


Fig. 2. Structure of C_{60}- Xylometazoline-C_{65}-X_2 (FXY) without Hydrogens

In this investigation, xylometazoline is placed on Fullerene tested using a variety of halogens so that optimized structure of each complex could be identified in accordance with halogens' placements [10] (Figures 2, 3). NBO and NMR Calculations are made using Gaussian.03 and Gauss View as software platforms. Estimations are than carried out using Density Functions Theory (DFT) under basic series of 6-31(G^{**}) [11].



Figures 3. Structure of only- xylometazoline- C_7-X_2 (XY) without Hydrogens

EXPERIMENTAL

Computational methods

Optimization of the present combination is required in this research in order to carry out the calculations. So input files were calculated using Gauss View software for only- xylometazoline- C_7-X_2 (XY) and the medicine attached to Fullerene nano-carrier C_{60}- xylometazoline- C_{65}-X_2 (FXY). (Figures 2 and 3). Indicate that halogen compounds are placed on carbon no.7 of single combination while halogen compounds in combinations are attached to Fullerene on the equivalent carbon, that is, carbon no.65. Totally, there are 4 compounds as hydrogen, fluorine and chlorine as well as bromine combined with carbon no.65. Such compounds are optimized and recalculated under 6-31(G^{**}) series using (DFT) and Gaussian 0.3 as the platform software [10, 11].

RESULTS AND DISCUSSION

Considering the study objectives as applied comparison of orbital occupancy, gap band energy and maximum electron charge transferred (ΔN_{max}) of xylometazoline with its nano-carrier medicine, energy values of highest and lowest occupied levels (HOMO and LUMO respectively) for the C_{60}- xylometazoline-C_{65}-X_2(FXY), only-xylometazoline- C_7-X_2 (XY) were calculated using NBO analysis in Gaussian software (Figure 4).

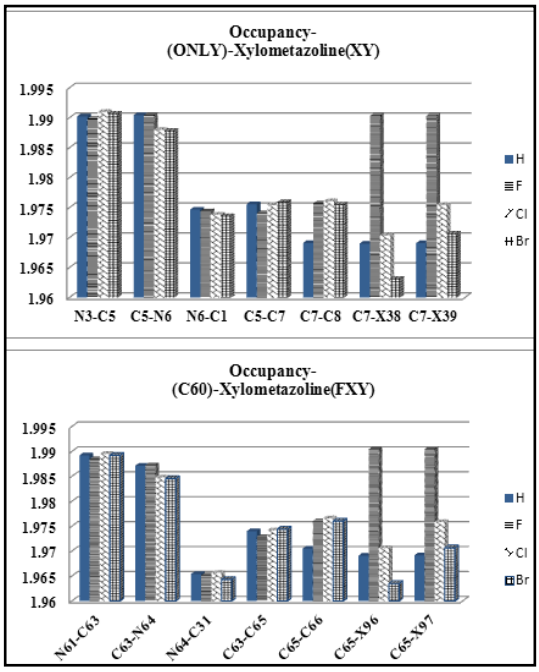


Fig. 4. Comparison orbital occupancy of same bonds in C_{60}-xylometazoline- C_{65}-X_2(FXY) and only – xylometazoline- C_7-X_2(XY) in (a.u)

Parameters such as orbital's occupancy, gap band energy and maximum electron charge transfered (ΔNmax) were then calculated. (Tables 1, 2)

Table 1. Energy of HOMO, LUMO and band GAP in only-xylometazoline- C_7-X_2 (XY) and C_{60}- xylometazoline- C_{65}-X_2 (FXY) in (a.u)

Compound	(XY) Energy		
	E(HOMO)	E(LUMO)	Gap band 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
	(FXY) 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

Table 2. Comparison of maximum electron charge transferred in XY and FXY in (a.u)

Compound	ΔNmax	
	(XY)	(FXY)
R-H	0.517	0.895
R-F	0.607	0.910
R-Cl	0.658	0.906
R-Br	0.672	0.904

Maximum electron charge (ΔNmax) is increased due to attachment of C_{60} to the medicine so it could be said that Fullerene nano-carriers are more reactive compared to medicine only (Figure 5). Besides, considering Table 1 It could be concluded that energy gap decreases if halogen's electronegative properties of xylometazoline and the same attached to nano-carriers no.65 decrease. In other words, energy gap decreases in accordance with following trend;

R-H> R-F > R-Cl> R-Br.

As specified before, lower energy gap makes the molecule to demonstrate higher electronic properties because the electron can easily shift from (HOMO) level to (LUMO). (Figure 6)

Having compared Tables 1, one can conclude that energy gap decrease to 0.7 its value in single mode due to attachment to Fullerene nano-carriers so electronic properties increases because of its attachment to C_{60}.

Orbital occupancy of some compounds in single medicinal compositions and the one attached to Fullerene revealed to increase the dependency of orbital occupancy to halogen type as we move from Imidazole ring to halogen compounds (Table 3).

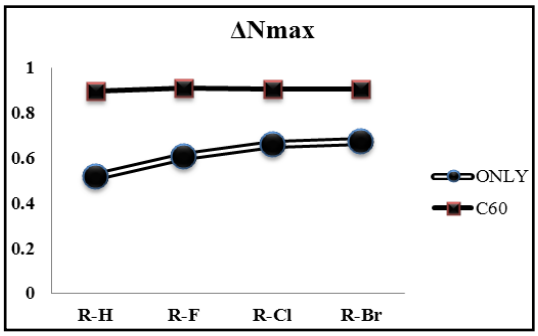


Fig. 5. Maximum electron charge transferred in XY and FXY in (a.u)

Table 3. Comparison of Corporation of p orbitals in bonds of C_{60}- xylometazoline- C_{65}-X_2(FXY) and only- xylometazoline-C_7-X_2(XY) in (a.u)

XY	Corporation of p orbitals in bonds			
Bond	H	F	Cl	Br
N_3-C_5	-0.3683	-0.1219	-0.1265	-0.1174
C_5-N_6	0.1889	0.1384	0.1806	0.1852
N_6-C_1	0.5292	0.5674	0.5491	0.5398
C_5-C_7	-0.7848	-0.4752	-0.3987	-0.3842
C_7-C_8	-0.0308	-0.4309	-0.4253	-0.4116
C_7-X_{38}	1.2662	0.9231	-1.0080	-1.9858
C_7-X_{39}	1.2664	0.9196	-1.0432	-1.9923
FXY	**Corporation of p orbitals in bonds**			
Bond	**H**	**F**	**Cl**	**Br**
N_{61}-C_{63}	-0.2624	-0.0602	-0.0653	-0.0660
C_{63}-N_{64}	0.1906	0.1354	0.1780	0.1856
N_{64}-C_{31}	0.5898	0.6617	0.6381	0.6189
C_{63}-C_{65}	-0.7512	-0.4434	-0.3692	-0.3586
C_{65}-C_{66}	-0.0276	-0.4178	-0.4161	-0.4029
C_{65}-X_{96}	1.2667	0.9144	-1.0025	-1.9562
C_{65}-X_{97}	1.2707	0.9187	-1.0236	-1.9576

In addition, it's been observed that the existing trends are the same for single compounds and the one attached to C_{60}.

Since orbital occupancy (e.g. orbital-p) is influenced by electronegative aspects, it is more evident in lateral compounds while it is not serious in compounds with larger distance, even zero!

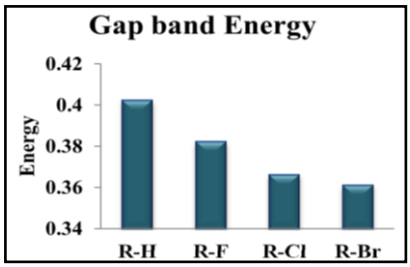


Fig. 6. Gap band energy values in XY and FXY in (a.u)

CONCLUSIONS

Considering analysis made here, it is obvious that increase in maximum value of electron charge would lead to rise in energy gap and orbital occupancy as well as medicinal properties of xylometazoline in Imidazole ring, so reactivity of the medicine effectual properties and xylometazoline nano-carriers is enhanced.

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