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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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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