عنوان مقاله:

Quantum Chemistry Studies on Structures and Electronic Properties of the Tolazoline Drug on Nano Structure of Fullerene

محل انتشار:

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خلاصه مقاله:

Tolazoline is a non-selective competitive α-adrenergic receptor antagonist. It is a vasodilator that is used to treat spasms of peripheral blood vessels (as in acrocyanosis).Tolazoline is indicated in the treatment of persistent pulmonary hypertension in the newborn (persistent fetal circulation) when systemic arterial oxygenation cannot be maintained by supplemental oxygen and mechanical ventilation. The fullerene family especially C۶۰ derivatives have appealing photo-, electro-chemical and physical properties for biomedical applications including acting as pro- and anti-oxidants. In this research work at The first compounds [C۶۰- TOLAZOLINE -C۶۵-۲X] (X=F, Cl, Br) were optimized. Then the calculation of natural bond orbitals was performed with the NBO technique. All calculations using Hartree-Fock the ۶-۳۱G * basis set using Gaussian ۹۸ software and in gas phase has been done. The results showed that the energy levels of molecular orbital (HOMO & LUMO) in the R-۲F has the lowest value. C۶۵-X has the shortest length and the highest power in R-۲F. Comparison of the dipole moments of compounds shows this trend: R-۲H > R-۲Cl> R-۲Br> R-۲F. ratio Core / charge and the valence / charge for carbon atoms ۳۱, ۵۵, ۶۵ and ۶۳ in the RF has the highest value

کلمات کلیدی:

Tolazoline, Core / charge, Fullerene, valence / charge