



Investigating the resonance energy and charge transfer in the clonidine and C₆₀-clonidine-fullerene carriers with quantum chemistry calculations

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Abstract

Clonidine has two aromatic rings in which halogens are attached to one ring in this study, both in drug state and in fullerene nanostructure, and by changing the type of halogen at the * HF / 6-31G level and in The gas phase was first optimized and then the NBO calculations were performed. The results obtained in N61, N63 and N5, N3 indicate the highest rhizanese energy and load transfer that, with variations in the type of halogen from fluorine to bromine, in all resonance energies in the nanoparticle The drug shows more values, while in all situations, the amount of drug load in the drug is similar to the nano-carrier in the same conditions. Shows more

Keywords: Clonidine. Fullerene, resonance energy, load

1. Introduction

Clonidine boosts systemic blood pressure and also promotes cardiac pacing by stimulating receptors in the CNS and as an antihypertensive agent. Clonidine is used in various forms of increased pressure to stop aggression and high pressure. And also used in eye diseases to prevent gradual blindness [1]. The structure of the C₆₀ molecule is completely stable. The structure of this molecule is so stable that the C₆₀ molecule acquires its original shape after colliding with a steel plate at 7000 m / s. In fact, there are a large number of carbon atom clusters in this structure, the number of carbon atoms in that pair, these molecules are