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Investigation of Chemical Properties in Fullerene Derivatives of Fluoxetine Drug : A DFT Study

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Abstract

In this research at the first fluoxetine drug and its fullerene derivative were optimized. NBO calculations and NMR for the complexes were carried out at the B3LYP/6-31G*quantum chemistry level. Different parameters such as energy levels, the amount of Chemical Shift in different atoms, the amount of HOMO/LUMO, chemical potential (μ), chemical hardness (η), Thermodynamic Properties was determined and the coefficients of hybrid bonds (π, σ) and the orbital portion of the bonds p (π, σ) was performed. In another part, the core and the valence electrons of atoms were compared. This drug as a major therapeutic category is antidepressant drug. In this study of fullerenes, we used nano drug carriers. The data in tables and graphs and shapes were compared and discussed.

Keywords: Fluoxetine, Fullerenes, Chemical potential, Nano drug carriers.

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