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Theoretical study of chemical properties of Fulleromethyldopa and derivatives

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Abstract

In recent years, many studies have been done on structure of fullerene derivatives as medicine nano-carrier compounds. In this work mechanical quantum calculations in theory level of B3lyp/6-31g* and HF/6-31G in the gas phase were performed on structural of methyl dopa (MD) and fulleromethyle dopa (FMD) with different halogen substitutions. In the other hand some different properties such as HOMO and LUMO levels, Chemical hardness, Energy gap, Conductivity, ΔNmax and Dipole moment value were studied. Also the activity of chemical sites such as acid and base site and the hydrogens of benzene ring were investigated. The result showed that the value of energy gap and chemical hardness decreased by linking structure of methyl dopa to fullerene (C_{60}) and the value of Chemical potential, ΔNmax and Dipole moment were increased in fullerene methyl dopa (FMD). However, after binding of methyldopa to fullerene, acidic sites, it is more acidic than before link. And the activities of the alkali site are reduced. These structures showed that change in substitution (X=F, Cl, Br and H) changed values of these parameters. These changes show dependency of the results on power of electro negativity and atomic radius of substitution X. Finally, the data were compared and discussed.

Keywords: DFT, Electrophilicity, Chemical hardness; Chemical potential,

1. Introduction

In the recent years, many studies have been done on the structure of fullerene and their derivatives. Fullerene derivatives have been studied due to the outstanding properties such as electron accepting and it is caused to use as a carrier for gen delivery systems [1-5].1 and