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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

medicine nano-carrier compounds. according to the discovery of the nano-scale synthesis, the chemistry of this fascinating molecules have been investigated.2 The fullerene family specially C_{60}, has appealing photo, physical and electro chemical properties can be used in various medical fields in modern material nano science concerns carbon-based materials, among which fullerenes take one of the first places. Fullerene the most abundant reprehensive of the fullerene family was produced for the first time on a preparative scale in 1990, by resistive heating of graphite. Fullerene molecules are composed of carbon, in form of sphere, ellipsoid, and tube [6-10]. Among them sphere form of fullerene are referred to as Bucky balls [11-16]. The C60 surface contains 20 hexagons and 12 pentagons all the ring are fused. All the double bonds are conjugated. Fullerene and their derivatives have potential antivirial activity, which has strong implications on the treatment of HIV-infection. According to this character is based on biological properties including their unique molecular architecture and antioxidant activity 3. One of the derivatives of fullerene is fullerene-polyhydropolyamino-caproic-acid being used for the treatment of HIV-infection.4 Methyldopa is useful in the treatment of mild to moderately severe hypertension. It. lowers blood pressure chiefly by reducing peripheral vascular resistance, with a variable reduction in heart rate and cardiac output. [17-22]. Methyldopa is useful in the treatment of mild to moderately severe hypertension. It lowers blood pressure chiefly by reducing peripheral vascular resistance, with a variable reduction in heart rate and cardiac output. In this report 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 fullerомethyle dopa (FMD) with different halogen substitutions.

The electrophilicity index, which measures the stabilization in energy when the system acquires an additional electronic charge, ΔN, from the environment is given by equation 8 and is presented in terms of the electronic chemical potential, μ (the negative of electronegativity, χ) and the chemical hardness, η. Both quantities may be approximated in terms of the energies of frontier molecular orbitals (εHOMO and εLUMO) as μ= (εH + εL)/2 and η=εL - εH (Eqs. 9 and 10). Electrophilicity can also be approximated in terms of the ionization potential (I) and electron affinity (A) (Eqs. 8-10) [23-30]. High values of μ and low values of η, characterize a good electrophone species. The maximum amount of electronic charge, ΔN_{max}, that the electrophone system may accept is given by equation 11 as [26]. Thus, while the quantity of ω describes the propensity of the system to acquire additional electronic charge from the environment, the quantity of ΔNmax describes the charge capacity of the molecule [30-32].

$$HLG=E_{LUMO} - E_{HOMO} \quad (1)$$

$$\eta = (E_{LUMO} - E_{HOMO})/2 \quad (2)$$

$$\mu = (E_{LUMO} + E_{HOMO})/2 \quad (3)$$

$$\omega = \mu^2/2\eta \quad (4)$$

$$\Delta N_{max}=- \mu/ \eta \quad (5)$$

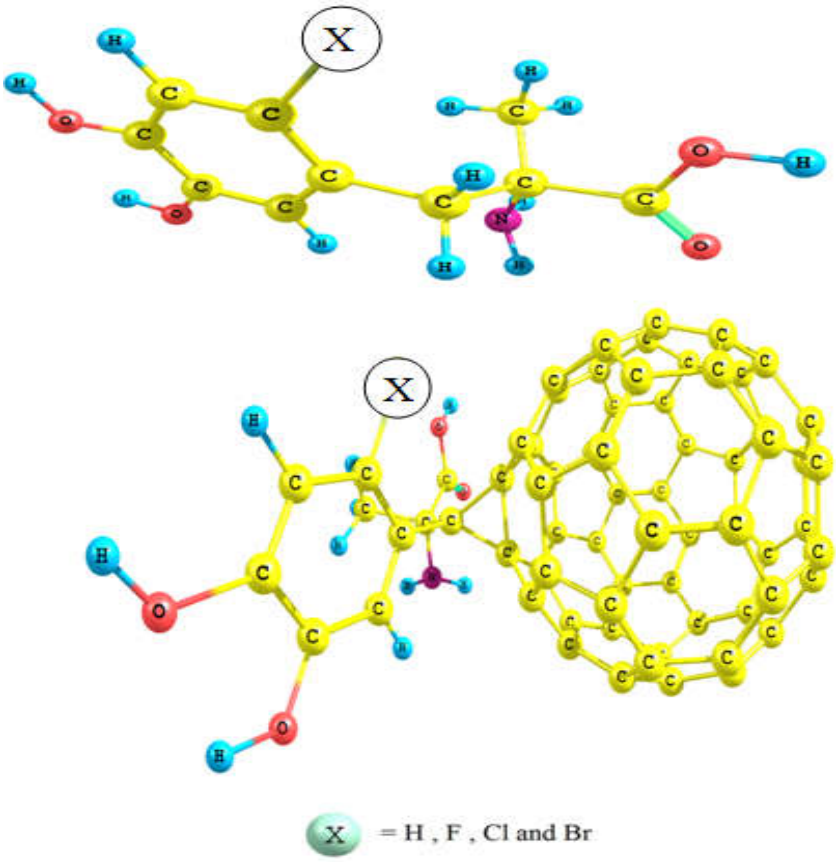

Fig.1. Show of MD and FMD obtained by B3LYP/6-31G level of theory

2. Computational details

The structures of methyle dopa (MD) and Fulleromethyle dopa (FMD) were designed primarily using of Gauss View 3.1 and nanotube modeler 1.3.0.3 soft wares (Fig.1). The optimization and natural bond

orbital (NBO) calculation were done in the gas phase. Finally obtained results were compared with each other. The optimization and NBO calculations of all systems are done by Hartree Fock (HF) and density functional theory (DFT) using B3LYP method and the standard 6-31G basis set, by Gaussian W98 suit of programs. Total computations were done under 1 atmosphere pressure and 298 Kelvin temperature [27-28].

3. Results

On the basis of these results, some separate issues such as energetic characters, electrophilicity, chemical potential, chemical hardness values were discussed of which results in this section.

Table 1. Calculated E HOMO and E LUMO (a.u), Chemical hardness η, chemical potential μ, electrophilicity values ω and maximum amount of electronic charge transfer ΔNmax in atomic units, for the methyle dopa (MD) and Fulleromethyle dopa (FMD) by B3LYP/6-31G* and HF/6-31G* levels of theory

Method	**HF/6-31G***							
Structure	**X**	**HOMO (a.u)**	**LUMO (a.u)**	**μ (a.u)**	**η (a.u)**	**(HLG) (a.u)**	**ΔN_{max} (a.u)**	**Dipole moment (Debye)**
MD	**H**	**-0.3051**	**0.1415**	**-0.0818**	**0.2233**	**0.4466**	**0.3662**	**4.3526**
	F	**-0.3159**	**0.1274**	**-0.0944**	**0.2217**	**0.4433**	**0.4259**	**3.0721**
	Cl	**-0.3179**	**0.1267**	**-0.0956**	**0.2223**	**0.4446**	**0.4301**	**2.7598**
	Br	**-0.3138**	**0.1284**	**-0.0927**	**0.2211**	**0.4422**	**0.8385**	**3.0397**
FMD	**H**	**-0.2786**	**-0.0136**	**-0.1461**	**0.1325**	**0.2650**	**1.1024**	**5.6772**
	F	**-0.2787**	**-0.0132**	**-0.1459**	**0.1328**	**0.2656**	**1.0990**	**5.4786**
	Cl	**-0.2788**	**-0.1316**	**-0.1460**	**0.1328**	**0.2656**	**0.9909**	**5.4192**
	Br	**-0.2780**	**-0.0133**	**-0.1457**	**0.1324**	**0.2647**	**1.1006**	**5.5639**
Method	**B_3LYP/6-31G***							
MD	**H**	**-0.2066**	**-0.0150**	**-0.1108**	**0.0958**	**0.1916**	**1.1563**	**3.7471**
	F	**-0.2120**	**-0.0173**	**-0.1146**	**0.0973**	**0.1947**	**1.1775**	**2.7990**
	Cl	**-0.2162**	**-0.0192**	**-0.1178**	**0.0985**	**0.1970**	**1.1954**	**2.4552**
	Br	**-0.2140**	**-0.0176**	**-0.1158**	**0.0982**	**0.1964**	**1.1791**	**2.8653**
FMD	**H**	**-0.2138**	**-0.1173**	**-0.1655**	**0.0483**	**0.0965**	**3.4305**	**5.6900**
	F	**-0.2144**	**-0.1168**	**-0.1656**	**0.0488**	**0.0976**	**3.3945**	**5.6428**
	Cl	**-0.2146**	**-0.1169**	**-0.1658**	**0.0488**	**0.0977**	**3.3939**	**5.6171**
	Br	**-0.2140**	**-0.1164**	**-0.1652**	**0.4879**	**0.0976**	**3.3866**	**5.6776**

3.1 Dipole moment

The results show that when structure of methyle dopa is linked to nano fullerene, the dipole moment in FMD increased. This parameter is an effective factor which has direct relationship with solubility and the more amount of this parameter, causes the more solubility inside the polar solvent (Table 1).

3.2. HOMO and LUMO indices

The FMD has band gap less than MD. A small HOMO-LUMO Gap (HLG) in atomic units automatically means small excitation energies to the excited states. Therefore FMD is more conductive than MD (Table 1).

3.3. Chemical potential

In order to compare the obtained results, consider them. The results show that when structure of Captopril is linked to fullerene, the chemical potential (a.u.) of FMD decreased, in the gas and liquid phase (Table 1).

3.4. Chemical hardness

FMD has chemical hardness less than MD. A concise definition of chemical hardness (a.u.) offers that a hard molecule has a large HOMO-LUMO gap and a soft molecule has a small HOMO-LUMO gap, so FMD is softer than MD. Soft molecules with a small gap, will have their electron density changed more easily than a hard molecule. So FMD is more reactive than MD (Table 1).

3.5. Electrophilicity index

Electrophilicity value (a.u.) in FMD increased. The electrophilicity index is a measure of electrophilic power of a molecule. When two molecules react with each other, one molecule behaves as a nucleophile system, whereas the other one acts as an electrophone system. A higher electrophilicity index shows higher electrophilicity of a molecule. So FMD has higher electrophilicity than MD, therefore FMD is a more strong Lewis acid (Table 1).

4. Conclusion

In this paper, the structural and electronic structures of MD and FMD have been investigated theoretically by performing DFT calculations at the B3LYP/6-31G level, in the gas phase and the liquid phase. The results show that FMD has band gap less than MD, also chemical hardness in FMD is lower than MD, so FMD with notice to electrophilicity and ΔNmax parameter, is more soft strong acid than MD. In terms of chemical reactivity we can conclude that soft molecules will be more reactive than hard molecules for unimolecular reaction such as isomerization and dissociation. This work can be useful for pharmaceutical researches because this action causes interesting medicinal properties.

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