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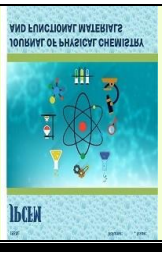

Investigation of Electronic Properties of Poly(Deamst0.70-Co-BMA) Copolymer: ab-initio Approach

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ABSTRACT

The theoretical molecular structure of Poly (DEAMSt0.70-co-BMA) copolymer molecule was performed by using the Gaussian 09 program. For the theoretical calculations, the Hartree-Fock (HF) theory with 6-31G (6D, 7F) basic set was used. In addition, the highest occupied molecular orbital (HOMO), the lowest unoccupied molecular orbital (LUMO) energies, the electronic properties (total energy, electronegativity, chemical hardness and softness) were investigated.

ARTICLE INFO

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HOMO and LOMO energies
electronic properties.

1. Introduction

In order to support experimental studies or to predict the results without performing experimental studies, computer-aided quantum chemical calculations are increasing with the development of computer technology. Computer-aided quantum chemical calculations are performed using molecular modeling programs. Quantum mechanics forms the basis of such calculations and the theoretical calculations provide optimized geometry, spectroscopic and electronic properties of the molecule. In this study, some electronic properties of Poly (DEAMSt0.70-co-BMA) copolymer molecule were calculated by Hartree Fock method 6-31G (6D, 7F) base set.

2. Theory

Hartree Fock theory, which is one of the ab initio methods, is an ideal method for determining the structure of molecules, spectroscopic, electronic and non-linear optical properties [1]. Gaussian 09W [2] and GaussView [3] package program is used in computer-aided quantum mechanical calculations, which includes molecular mechanics, quasi-experimental and ab initio methods and has a wide range of theories and basic set options. With these programs, the energies of atoms and molecules can be calculated, geometric optimizations can be made and energy-dependent vibration frequencies, force constants and dipole moments can be calculated. In addition, IR and Raman spectra, thermochemical properties, atomic charges, multipolar moments, NMR and magnetic sensitivity vibrational intensities, electron affinity and ionization energies, polarity, electrostatic potential, and electron density allows for the calculation of many properties for atoms and molecules. All these properties can be calculated in the gas phase, in solution, and in crystal structures. For this purpose, geometric properties, electronic properties (HOMO-LUMO energies, total energy, electronegativity (χ), chemical hardness (η)) [4] of Poly (DEAMSt0.70-co-BMA) copolymer molecule were obtained in this study.

3. Results

The geometry of a molecule is related to the bond angle and bond length between the atoms of that molecule and is one of the most important factors that directly affect the magnitude of the molecule's dipole moment [5]. The entitled compound has been optimized at HF/6-31G (6D, 7F) level in the gas phase and optimized structure of a mentioned molecule are given in Figure 1.

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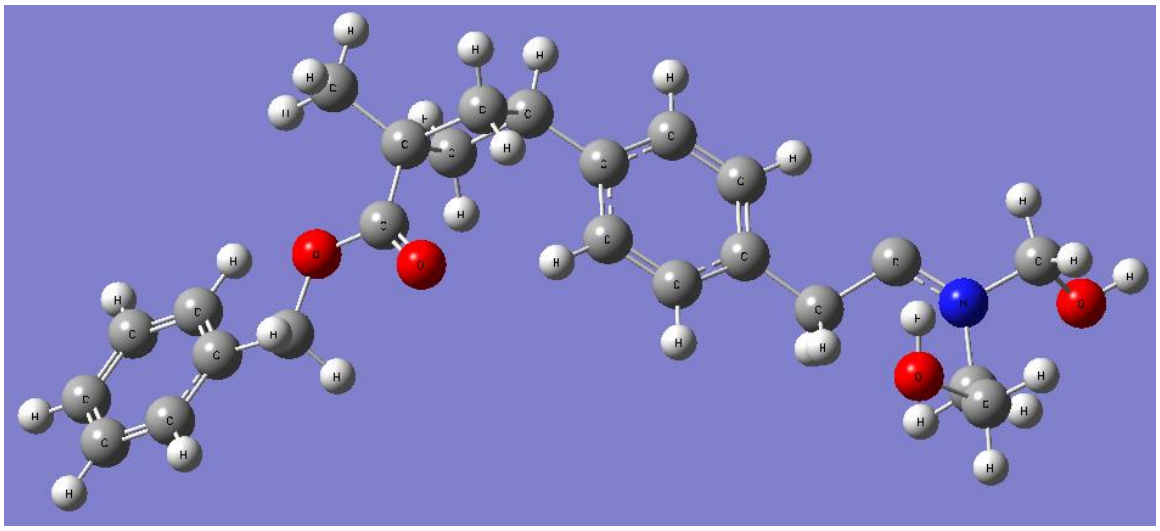

Figure 1. The optimized geometry structures of Poly(DEAMSt0.70-co-BMA) polymer

According to molecular orbital theory; all molecules have the highest filled molecular orbital HOMO (Highest Occupied Molecular Orbital), and the lowest empty molecular orbital LUMO (Lowest Unoccupied Molecular Orbital). HOMO, the outermost molecular orbital occupied by electrons, acts as an electron donor. LUMO is the first empty molecular orbital not occupied by electrons and acts as an electron acceptor [6,7,8,9]. HOMO energy is therefore directly related to the ionization potential and represents the molecule's ability to deliver electrons. LUMO energy is directly related to electron affinity and represents the molecule's ability to receive electrons. The difference between HOMO and LUMO energy values can be defined as the chemical stability of the molecule. The closer the energy levels of the interacting molecular orbitals are, the smaller the ΔE energy difference, the easier the interaction and reaction of the reactants will be. The HOMO and the LUMO energies of Poly(DEAMSt0.70-co-BMA) copolymer molecule and the energy difference between these have been shown in Figure 2. In the obtained results, the energy difference between the boundary orbitals of HOMO and LUMO of the molecule is calculated as 12.115 eV and this large energy range shows that the molecule is very stable. As shown in the figure, the red points are rich in electrons and the location of the HOMO orbitals also indicates the effectiveness of the molecule.

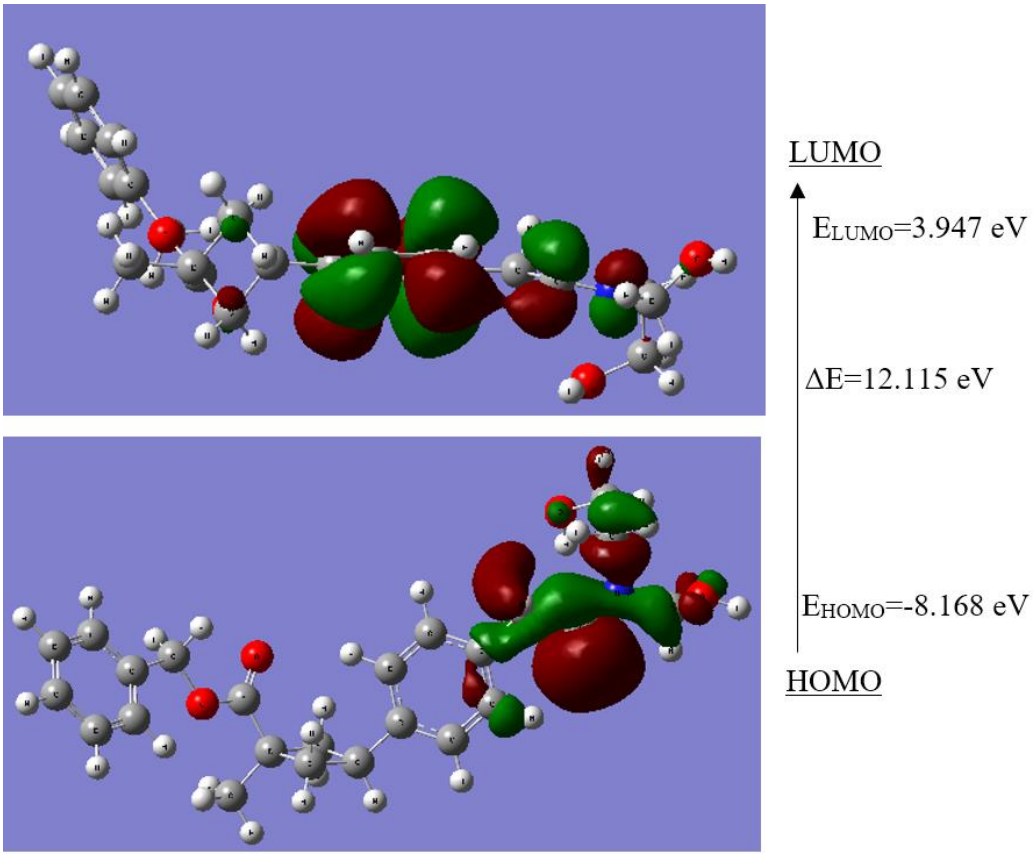

Figure 2: HOMO and LUMO energies calculated for poly(DEAMSt0.70-co-BMA) polymer

If the HOMO and LUMO energy values of a molecule are known, the following parameters can be found using them [6-10]: The ionization potential ($I = -E_{HOMO}$) is the minimum energy required to remove an electron from the molecule in the gas phase. Electron affinity ($A = -E_{LUMO}$) is defined as the amount of energy that increases when an electron is added to the molecule in the gas phase. Electronegativity ($\chi = (I+A)/2$) refers to the power of an atom in the molecule to attract electrons. Chemical hardness ($\eta = (I-A)/2$) is a measure of inhibition of charge transfer within the molecule. Molecules with high chemical hardness values have little or no intermolecular charge transfer. If the chemical softness ($S = 1/2\eta$), the charge density is low, i.e. the intra-molecular charge transfers are high. The calculated parameters for the title molecule are given in Table 1.

Table 1: Electronic properties calculated for Poly (DEAMSt0.70-co-BMA)

Parametre	**HF/6-31G (6D, 7F)**
E_{HOMO} (eV)	-8.168
E_{LUMO} (eV)	3.947
ΔE (eV)	12.115
I (eV)	8.168
A (eV)	-3.947
χ (eV)	2.1075
η (eV)	6.0575
S (eV^{-1})	0.0825

4. Conclusion

The geometry of poly (DEAMSt0.70-co-BMA) was optimized by HF-based 6-31G (6D, 7F) methods. The molecular structure, HOMO and LUMO energies, and some electronic properties have been studied. The present investigation provides structural information and electronic properties of the compound which may be useful to upgrade further knowledge on poly (DEAMSt0.70-co-BMA).

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