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Structural, Electronic and Thermodynamical properties of 6-ethoxybenzo[d][1,3]oxathiol-2-one: A Theoretical Approach

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Abstract

This paper has presented a complete theoretical study of 6-ethoxybenzo[d][1,3]oxathiol-2-one with the help of combination of DFT/B3LYP method and 6-311++G(d, p) basis set. Electronic properties have been calculated with the help of HOMO-LUMO plot. The reactivity of molecule using various descriptors such as, local softness, electrophilicity, electronegativity, hardness, HOMO-LUMO gaps are calculated and discussed.

Keywords: *DFT, HOMO, LUMO, MESP, electronic property*

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INTRODUCTION

1,3-benzoxathiol-2-one and its derivatives have various biological properties including antibacterial, antimycotic, antioxidant, antitumor and anti-inflammatory activities [1]. They also act as inhibitors of carbonic anhydrase II [2] and monoamine oxidase [3]. The first synthesized 1,3-benzoxathiol-2-one, 6-hydroxy-1,3-benzoxathiol-2-one $C_9H_8O_3S$, also known as tioxolone or thioxolone, has been used for many years in the treatment of acne and other skin diseases (e.g. psoriasis) [4]. A recent study reported the syntheses and antifungal activities of some derivatives of tioxolone [5].

In this work, I present a detailed study of various aspects of 6-ethoxybenzo[d][1,3]oxathiol-2-one using Density Functional Theory (DFT). DFT offers a better compromise between computational cost and accuracy for medium size molecules. The molecular properties of title compound are discussed with the help of various chemical reactivity surfaces such as HOMO, LUMO and MESP etc. as well as a number of calculated electronic and thermodynamic parameters.

COMPUTATIONAL DETAILS

All calculations were done using G03 program package using combination B3LYP/DFT method and 6-311G++(d, p) basis set [6]. This basis set 6-311G++(d, p) with 'p' polarization functions on hydrogen atoms and 'd' polarization functions on heavy atoms is used for better description of polar bonds of molecule [7, 8]. Initial geometry is model with help of Gauss View 5.0 program package [9]. Geometry optimization is done without any symmetry constrains.

Optimized Parameters

The equilibrium geometry optimization of 6-ethoxybenzo[d][1,3]oxathiol-2-one are obtained by energy minimization, using DFT at the B3LYP/6-311++G (d, p) level. The optimized molecular structure of 6-ethoxybenzo[d][1,3]oxathiol-2-one is shown in Figure 1 with labeled atoms. Optimized geometry of title compound is further ensured by the absence of any imaginary normal mode frequency at the same level of theory.

Electronic and Thermodynamical Property

The HOMO represents the ability to donate an electron; LUMO as an electron acceptor represents the ability to obtain an electron. The HOMO and LUMO energy were calculated by DFT/B3LYP method. The electronic parameters, such as highest occupied molecular orbital (HOMO) energy (E-HOMO), lowest unoccupied molecular orbital (LUMO) energy (E-LUMO) and band gap

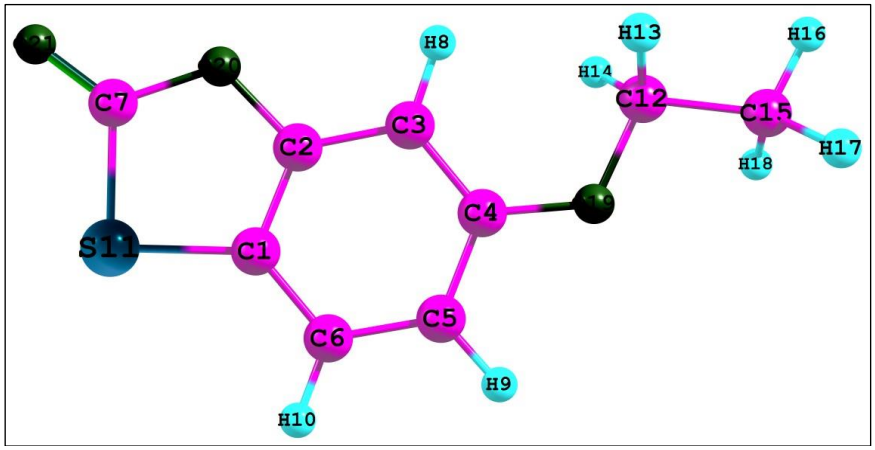

Fig. 1: *Optimized Geometry of 6-ethoxybenzo[d][1,3]oxathiol-2-one.*

energy (ΔE=ELUMO-EHOMO) were described through theoretical approach [10]. The energy (E_{gap}) between HOMO and LUMO of the present compound is found to be 5.25 eV. The molecular electrostatic potential (MESP) is a map of electrostatic potential over constant electron density of all molecules. It displays molecular size and shape as well as positive, negative and neutral electrostatic potential region in terms of color grading scheme. In this color grading scheme, the blue color represents the most electropositive i.e. low electron region, whereas the red color corresponds to the most electronegative center electron rich regions [11, 12]. The atomic orbital compositions of the molecular orbitals were obtained by Gauss-View software. On the basis of energy of frontier orbitals, the different global reactivity descriptors such as electronegativity (χ), chemical potential (μ) and global hardness (η) are computed using equations given below (Figures 2 and 3) [13]. The electronic parameters' ionization potential (I), electron affinity (A), absolute electro negativity (χ) and chemical hardness (η) etc. are calculated at B3LYP/6-311++G (d, p) level. I and A are calculated as the negative of energy eigen-values of HOMO and LUMO respectively. χ and η can be calculated by the following equation [14–16]:
$\chi=\frac{1}{2}(I+A)$ and $\eta=\frac{1}{2}(I-A)$.

Thermodynamical parameters zero point energy (ZPE), thermal energy at room temperature (E), heat capacity (C_v) and entropy (S) for title compound are calculated at the same level of theory and are useful in estimating reaction path of the molecules (Table 1).

Table 1: *Electronic and Thermodynamic Parameters Calculated at B3LYP/6-311++G (d, p) Level.*

Thermodynamical Parameters of the Molecule		**Electronic Parameters of the Molecule**	
Ionization Potential: I (eV)	6.30	Zero point energy (ZPE) (kcal/mol)	96.82
Electron Affinity: A (eV)	1.04	Thermal Energy E (kcal/mol)	104.10
E_g (eV)	5.25	Heat Capacity C_v (cal/mol-K)	43.19
Absolute Electro-negativity χ (eV)	3.67	Entropy S (cal/mol-K)	106.17
Chemical Hardness η (eV)	2.63		
Chemical Potential; μ (a.u)	4.69		

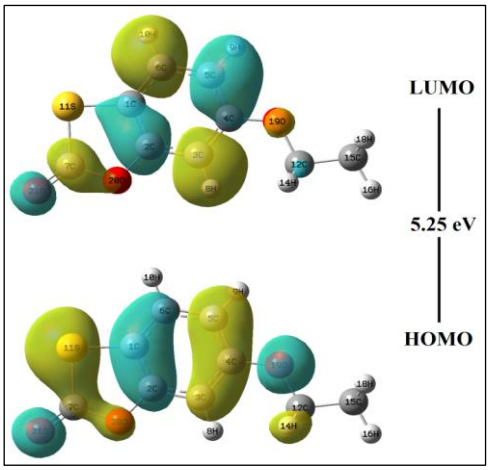

Fig. 2: *HOMO-LUMO Plots of Title Compound.*

CONCLUSION

The equilibrium geometries and other parameters of 6-ethoxybenzo[d][1,3]oxathiol-2-one were determined and analyzed at DFT/B3LYP level of theory using 6-311++G

(d, p) basis set. The chemical reactivity of title molecule is explained by energy gap and plot of lowest unoccupied molecular orbital-highest occupied molecular orbital (HOMO-LUMO). We have also calculated various electronic and thermodynamical parameters, which are very helpful in determining chemical reaction paths.

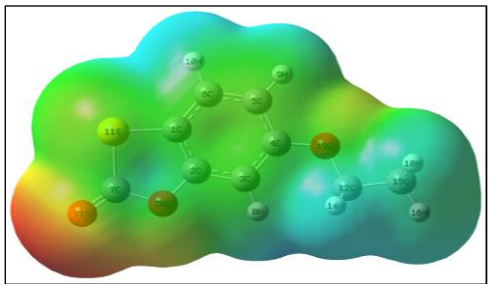

Fig. 3: *MESP Plot of Title Compound.*

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