DFT SIMULATION OF UV-VISIBLE SPECTRA AND NLO CHARACTERISTICS OF 2, 5- AND 2, 6-DIHYDROXYTOLUENES

Abstract

UV-Visible signals were simulated for 2, 5-dihydroxytoluene (5DHT) and 2; 6-dihydroxytoluene (6DHT), Frontier molecular orbital (FMO) technique was employed to understand the origin of Ultraviolet-Visible spectra and chemical reactivity of the samples. Non-linear optical parameters like dipole moment and hyperpolarizability were calculated. DFT/B3LYP/6-311++G (d,p) level of speculation was used for computations of 5DHT and 6DHT.

Keywords: FMO, dihydroxytoluene, UV-Visible Peaks, NLO materials.

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I. INTRODUCTION

2, 5- dihydroxytoluene (5DHT) and 2, 6- dihydroxytoluene (6DHT) are well-known in support of their employ in medicinal applications [1-5].It was revealed that cytotoxicity of 5DHToccurs from its methyl moiety [6]. Recently we reported DFT calculations of such biologically active molecules [7-15]. Hence, we undertook this work with the following aspects.

- Simulated UV-Visible spectra and,
- FMO and chemical reactivity parameters and Non-linear optical properties, to make the exploration complete.

II. COMPUTATIONAL ASPECTS

Using DFT/6-311++G (d,p) level of assumption and employed in Gaussian Window 09 program suit [16, 17] simulated UV-Vis spectrum [18-20]. We computed Chemical reactivity [21-26] of selected compounds.

III. RESULTS AND DISCUSSIONS

1. **Most Stable Conformer:** Geometry of chosen samples was optimized with the above selected method, and their minimum energy monomers depicted in figure 1.

2. **UV-Visible Peaks:** Calculated Ultraviolet-Visible absorption signals are due to the electronic transitions. The frontier molecular orbitals are recognized as highest occupied molecular orbital (HOMO) and (LUMO) lowest un-occupied molecular orbital, and they determine the reactivity of the selected compounds [27]. Electron donor is HOMO and acceptor is LUMO [28, 29]. The estimated peaks at λ_{max} = 235.97 nm, its oscillator strength, f = 0.0012 and another one observed at λ_{max} = 271.41nm with f = 0.0002 for 5DHT and λmax = 241.11 nm, its oscillator strength, f = 0.0021 and another one observed at λ_{max} = 247.37 nm with f = 0.0072 for 6DHT, and are shown in figure 2. The origin of the signals is mainly due to the shifts as of H→L+1, H→L+3 in 5DHT and H→L+1, H→L+2 in 6DHT.

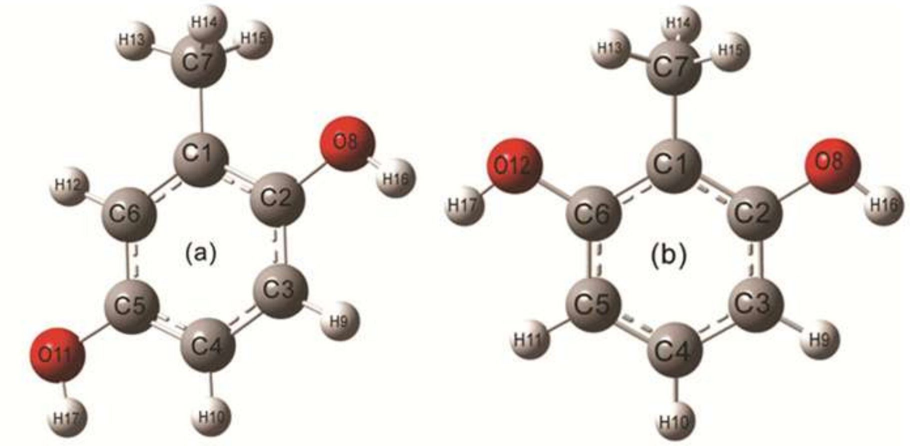

Figure 1: Optimized Geometrical Structure of (a) 5DHT and (b) 6DHT.

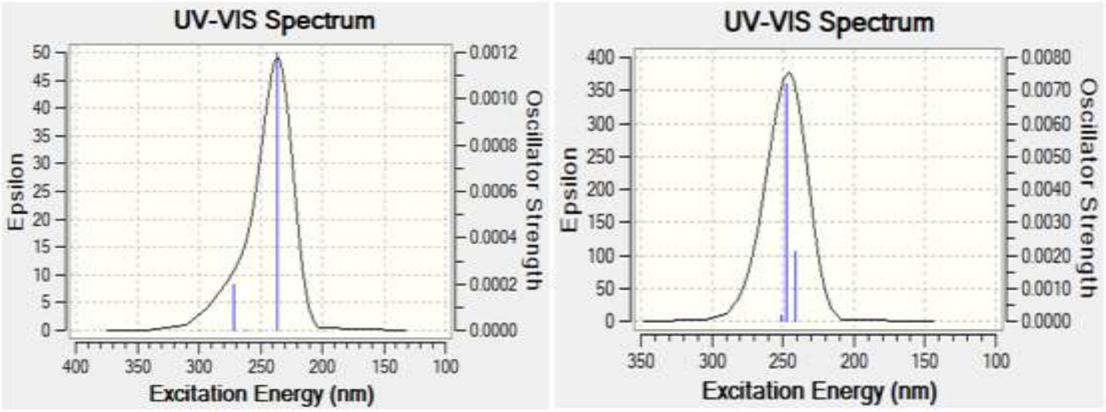

Figure 2: UV-Vis Peaks of 5DHT and 6DHT.

3. **Chemical Reactivity of the Molecules:** Frontier molecular orbital energy gap plays vital role in understanding the chemical reactivity such as reactants kinetic characteristics and chemical reactions of the molecule. The calculated energy gap between the H and L values for 5DHT and 6DHT are 3.636eV and 4.404 eV. Their chemical potentials ($\mu = -6.862$ eV and -7.000eV) are negative for both the molecules, and are chemically stable [30, 31]. These parameters describe the aspects like drug design and toxicological behaviour of eco system.

4. **NLO properties:** When Electromagnetic radiation interacts with NLO material, then change occurse in phase, amplitude, frequency, or gives the new propagation field characteristics [32]. If this change is significant then the NLO material used in signal processing, optical inter-connections, telecommunications and optical memory [33-36]. The NLO behaviour of selected compounds are judged by comparing the related quantities of Urea. For Urea, hyper polarizability (β_t) and dipole moment (μ_t) are 372.8×10^{-33} cm$^{5/}$esu and 1.3732 Debye, respectively. For 5DHT and 6DHT, these values are $\beta_t = 98.594 \times 10^{-33}$ cm$^{5/}$esu, 299.729×10^{-33} cm$^{5/}$esu, and $\mu_t = 0.938$ Debye, 0.792 Debye. The estimated values are less compared with that of Urea; hence titled compounds are not NLO materials.

IV. CONCLUSION

Theoretical UV-Visible peak values, FMO and chemical reactivity parameters computed for the selected compounds and these are not NLO materials.

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