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DFT Simulation of UV-Visible Spectra and NLO Characteristics of 2, 5- and 2, 6-Dihydroxytoluenes

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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 speculationwas used for computations of 5DHT and 6DHT.

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.

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[21-24] of selected compounds.

RESULTS AND DISCUSSIONS

Most stable conformer

Geometryof chosen samples was optimized with the above selected method, and their minimum energy monomers depicted in figure 1.

UV-VISIBLE PEAKS

Calculated Ultraviolet-Visible absorption signals are due to the electronic transitions. The FMO are recognized as HOMO and LUMO, and they determine the reactivity of the selected compounds.[25] Electron donor is HOMO and acceptor is LUMO.[26,27] 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 λ_{max} = 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.
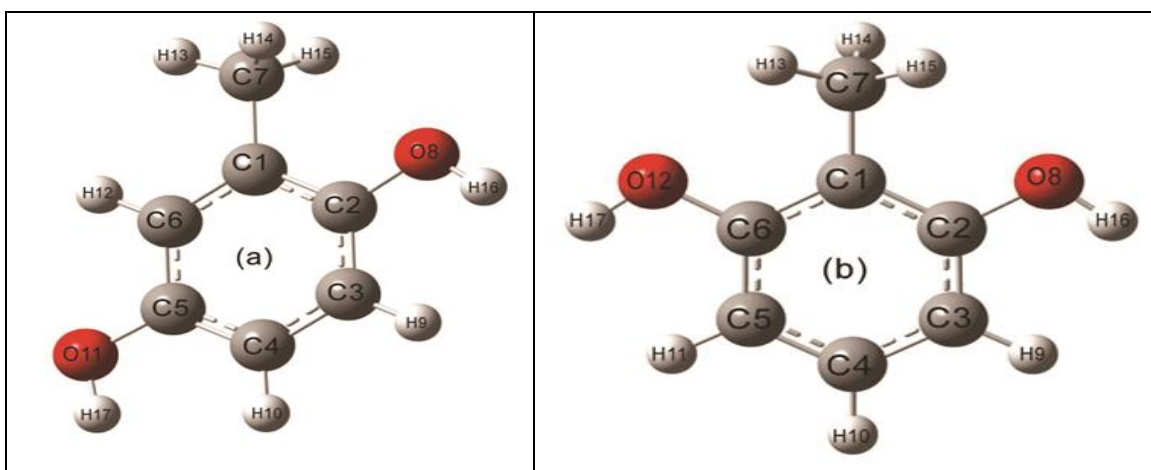

Figure **1.** Optimized geometrical structure of **(a)** 5DHT and **(b)** 6DHT.
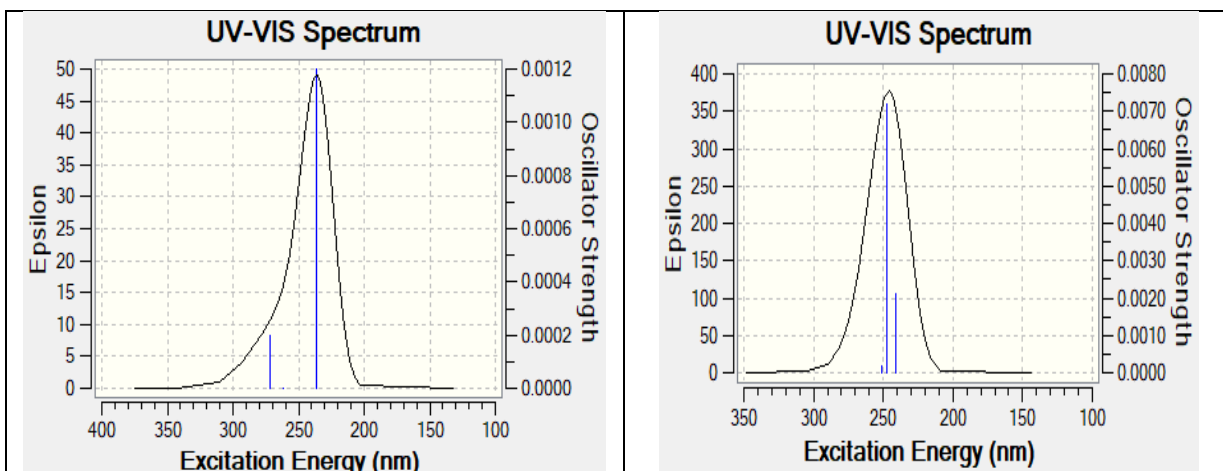

Figure 2. UV-Vis peaksof 5DHT and 6DHT.

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. Further, the calculated energy gap between the H and L values for 5DHT and 6DHT are 3.636eV and 4.404 eV. Their chemical potentials (μ = -6.862 eV and -7.000eV) are negative for both the molecules, and are chemically stable.[28,29] These parameters describes, the aspects like drug design and toxicological behaviour of eco system.

NLO PROPERTIES

When Electromagnetic radiation interacts with NLO material, then change occurse in phase, amplitude, frequency, or gives the new propagation field characteristics.[30] If this change is significant then the NLO material used in signal processing, optical inter-connections, telecommunications and optical memory.[31-33]

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.

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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