DFT Study of the Electronic Properties of Benzene and Hydroxylbenzene Molecule Group in Gas Phase

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Abstract

In this paper, theoretical study of Optimized geometry and Infrared (IR) Spectrum for Benzene and Hydroxybenzene molecule group by using Density Functional Theory (DFT) at Becke3Lee Yang Parr (B3LYP) level of theory with basis set 6-31G(d,p) in a gas phase have been studied. The optimized electronic properties of benzene and hydroxybenzene molecule group in gas phase have been performed using Gaussian 03 program. Benzene Molecule is the original Molecule before substituting Hydrogen by Hydroxyl (OH) radical. The substituting of hydrogen by Hydroxyl (OH) radical on Benzene molecule at different positions led/resulted in the study of eleven molecules. The electronic properties optimized include bond length, bond angle, total energy and energy gap. It was observed that the presence of the substituent's decreases the energy gap and 1,2,4,5-Tetrahydroxybenzene(TTHB) has the lowest energy gap from the studied molecules. Also the total energy decreases with the increase of hydroxyl radical, this means the molecules become more stable with increase of OH radical in the benzene ring. The IR Spectrum of the studied molecules has also been discussed.

Keywords: DFT, Bond length, Bond angle, IR spectrum, Energy gap