P 9. QUANTUM CHEMICAL COMPUTATIONS ON LINEAR OPTICAL PHENOMENA OF 2,2'-(6-CHLORO-1,3,5-TRIAZINE-2,4-DIYL)BIS(AZANEDIYL)DIPYRIDIN-3-OL

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ABSTRACT: To provide an insight into the linear optical properties of 2,2'-(6-chloro-1,3,5-triazine-2,4-diyl)bis(azanediyl)dipyridin-3-ol, static linear polarizability and maximum one-photon absorption (OPA) wavelength values have been calculated by density functional theory (DFT) quantum mechanical computations at B3LYP level. Using DFT at B3LYP level, one can obtain a reasonably accurate description of the static dipole polarizability and optical spectrum of the examined structure. In addition to the linear optical properties, the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) energies have been evaluated by DFT/ B3LYP method.

Keywords: One-photon Absorption, HOMO-LUMO Band Gaps, Density Functional Theory, Linear Polarizability, Linear Optics.