O 66. THEORETICAL STUDIES ON LINEAR OPTICAL CHARACTERIZATION OF 4-NITROPHENYL CARBAMIC ACID ETHYLESTER

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ABSTRACT: To estimate the potential for linear optical properties, the dispersion-free dipole polarizability and maximum one-photon absorption (OPA) wavelength values have been determined by density functional theory (DFT) quantum chemical calculations at B3LYP level. Systematic investigations have provided adequate evidence for the potential of DFT methods in the calculations of electric properties. We rely on the widely used B3LYP which denotes the hybrid functional, a linear combination of the gradient functionals together with the Hartree-Fock local exchange function. In addition to linear optical properties, the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) energies have been also examined by DFT/ B3LYP method.

Keywords: UV-Vis Spectroscopy, Theoretical Studies, Dipole Polarizability, Vertical Transition Wavelength, HOMO-LUMO Band Gaps