P 35. DFT STUDIES ON VERTICAL TRANSITION WAVELENGTHS, ELECTRIC DIPOLE MOMENTS, FIRST AND SECOND FRONTIER MOLECULAR ORBITALS OF 4-AMINO-4-NITRO DIPHENYL SULFIDE

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ABSTRACT: 4-Amino-4-nitro diphenyl sulfide has been designed for the study of its linear optical properties. To reveal the linear optical characterization for the title compound; the electric dipole moment and one-photon absorption (OPA) wavelength values have been calculated using quantum mechanical procedure (density functional theory (DFT)). Besides, to obtain the structural characterization of the studied molecule; the highest occupied molecular orbitals (HOMO), the lowest unoccupied molecular orbitals (LUMO) and the HOMO-LUMO band gaps for first and second frontier orbitals have been theoretically determined by DFT/ B3LYP method.

Keywords: Linear Optical Properties, Quantum Mechanical Calculations, Density Functional Theory, B3LYP Functional, HOMO-LUMO Band Gaps.