P 34. ONE-PHOTON ABSORPTION WAVELENGTHS, ELECTRIC DIPOLE MOMENT AND FIRST HYPERPOLARIZABILITY OF BENZALBARBITURIC ACID DERIVATIVE WITH DONOR SUBSTITUENT

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ABSTRACT: Benzalbarbituric acid derivative with donor substituent hydroxy has been designed. Due to the shape of the molecule, the second-order nonlinear optical (NLO) properties are expectable and can be more or less accurately predicted. To reveal the potential for second-order NLO phenomena; the electric dipole moment and static first hyperpolarizability have been determined by density functional theory (DFT) quantum chemical computations at B3LYP level. According to the calculation results, the title compound exhibits non-zero dispersion-free first hyperpolarizability, and it might have relatively good second-order NLO behaviour. The one-photon absorption (OPA) characterizations of the examined molecule have been theoretically obtained by DFT method.

Keywords: Electric Dipole Moment, Density Functional Theory, One-photon Absorption, Nonlinear Optics, Benzalbarbituric Acid.