O 64. MOLECULAR STRUCTURE AND SECOND-ORDER NONLINEAR OPTICAL PHENOMENA OF 4-NITROPHENYLMETHYL-4-METHOXY BENZOATE

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ABSTRACT: To understand the linear optical and microscopic second-order nonlinear optical (NLO) behaviour of 4-nitrophenylmethyl-4-methoxy benzoate, the electric dipole moment and dispersion-free first hyperpolarizability values have been computed using density functional theory (DFT). There are rather strong relationship among the calculated electric dipole moment and first hyperpolarizability values. Therefore, the electric dipole moment value of the title compound may be responsible for enhancing and decreasing the first hyperpolarizability value. 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 evaluated by means of DFT.

Keywords: Second-order Optical Nonlinearity, Electric Dipole Moment, First Hyperpolarizability, Quantum Chemical Calculations, HOMO-LUMO energies