O 65. COMPUTATIONS ON STATIC LINEAR POLARIZABILITY, FIRST HYPERPOLARIZABILITY, FIRST AND SECOND FRONTIER MOLECULAR ORBITALS OF N-(4-AMINOBENZENESULFONYL) ACETAMIDE

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ABSTRACT: To investigate linear optical and microscopic second-order nonlinear optical (NLO) behaviour of N-(4-aminobenzenesulfonyl) acetamide; the electric dipole moment, static dipole polarizability and first hyperpolarizability tensor components have been computed using density functional theory (DFT). The calculated non-zero electric dipole moment value shows that the examined compound might have microscopic static dipole polarizability and first hyperpolarizability with non-zero values. In this talk, after a short introduction on the methodologies used for computing the examined properties; the results of theoretical studies performed on DFT quantum mechanical calculations of linear optical and nonlinear optical values for the title molecule will be explained. The first and second frontier molecular orbital energies have been also revealed by DFT at B3LYP level of theory.

Keywords: Optical Nonlinearity, Linear Polarizability, First Hyperpolarizability, Electric Dipole Moment, Density Functional Theory