## P 32. QUANTUM CHEMICAL CALCULATION OF SECOND-ORDER NONLINEAR OPTICAL PROPERTIES OF 2-FURYL METHACRYLIC ANHYDRIDE

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**ABSTRACT:** The search of new materials with second-order optical nonlinearity is an important research field. So, the second-order nonlinear optical (NLO) materials have been extensively studied for many years. The basic structure of organic second-order NLO materials is based on the pi-bond system and due to the overlap of pi-orbital delocalization the electronic charge distribution leads to a high mobility of the electron density. To estimate the potential for second-order NLO behaviour of 2-furyl methacrylic anhydride; the dispersion-free quadratic hyperpolarizability has been determined by quantum mechanical calculations (finite field). In addition to second-order NLO properties, to elucidate the linear optical phenomena in the context of molecular orbital structure; the highest occupied molecular orbitals (HOMO), the lowest unoccupied molecular orbitals (LUMO) and the HOMO-LUMO band gaps have been also evaluated by means of density functional theory.

*Keywords: Quantum Chemistry, Nonlinear Optical Phenomena, First Hyperpolarizability, HOMO-LUMO Band Gaps, Finite Field.*