P 36. LINEAR AND SECOND-ORDER NONLINEAR OPTICAL BEHAVIOUR OF FLUORINE SUBSTITUTED THIENYL CHALCONE

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ABSTRACT: Among the materials producing linear and nonlinear optical (NLO) effects, organic materials are of considerable importance owing to their synthetic flexibility and large hyperpolarizabilities compared to inorganic materials. In view of the usefulness as potential linear and NLO materials, the chalcone having a substituted thienyl has been designed. The one-photon absorption (OPA) characterizations of the studied chalcone have been interpreted using computational chemistry. To provide an insight into the microscopic second-order NLO properties of the investigated molecule, the ab-initio calculations of the dispersion-free first hyperpolarizability have been performed by finite field (FF) method.

Keywords: Linear Optics, Vertical Transition Wavelength, First Hyperpolarizability, Second-order Nonlinear Optics, Chalcones.