

Title: Theoretical investigations of nonlinear optical properties of two heterocyclic chalcones.

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Abstract: The emergence of the Optoelectronics together with the discovery in the decade of 60 of a new area of research named Molecular Modeling, stimulated the development of new materials whose properties provide its employment in the context of the Optoelectronics. We studied properties of the structure geometry, molecular electrostatic behavior and the nonlinear optical properties of the centrosymmetric heterocyclic chalcones (E)-1-(5-methylfuran-2-yl)-3-(5-methylthiophen-2-yl)prop-2-en-1-one (3) and the noncentrosymmetric heterocyclic chalcone (E)-1-(5-Chlorothiophen-2-yl)-3-(thiophen-2-yl)-2-propen-1-one (7), to provide insights of their linear and nonlinear optical properties in the static and dynamic cases. A new approach treating the supermolecule is employed in combination with an interactive electrostatic system in which the atoms of neighboring molecules are considered as point charges. The ab initio computational results of (hyper) polarizabilities are derived from an iterative process and confirm these crystals as good candidates for photonic devices, such as optical switches, modulators, pyrazoline derivatives and optical energy applications.

Key-words: Electrical Properties, Electrostatic iteration, Supermolecule approach.

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