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Quantum Chemical Calculations on Molecular Structure, Spectroscopy and Non-Linear Optical Properties of Some Chalcone Derivatives

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Abstract : The chemistry of chalcones has generated intensive scientific studies throughout the world. Especially, interest has been focused on the synthesis and biodynamic activities of chalcones. The blue light transmittance, excellent crystallizability and the two planar rings connected through a conjugated double bond show that chalcone derivatives are superior nonlinear organic compounds. 3-(2-Chloro-6-fluoro¬phen¬yl)-1-(2-thien¬yl) prop-2-en-1-one, 3-(2, 4- Dichlorophenyl) – 1 - (4-methylphenyl) – prop -2-en-1-one, (2E)-3-[4-(methylsulfanyl) phenyl]-1-(4-nitrophenyl) prop-2-en-1-one are some chalcone derivatives exhibiting non linear optical (NLO) properties. NLO materials have been extensively investigated in recent years as they are the key elements for photonic technologies of optical communication, optical interconnect oscillator, amplifier, frequency converter etc. Due to their high molecular hyperpolarizabilities, organic materials display a number of significant NLO properties. Experimental measurements and theoretical calculations on molecular hyperpolarizability β have become one of the key factors in the design of second order NLO materials. Theoretical determination of hyperpolarizability is quite useful both in understanding the relationship between the molecular structure and NLO properties. It also provides a guideline to experimentalists for the design and synthesis of organic NLO materials. Quantum-chemical calculations have made an important contribution to the understanding of the electronic polarization underlying the molecular NLO processes and the establishment of structure–property relationships. In the present investigation, the detailed vibrational analysis of some chalcone derivatives is taken up to understand the correlation of the charge transfer interaction and the NLO activity of the molecules based on density functional theory calculations. The vibrational modes contributing toward the NLO activity have been identified and analyzed. Rather large hyperpolarizability derived by theoretical calculations suggests the possible future use of these compounds for non-linear optical applications. The study suggests the importance of π - conjugated systems for non-linear optical properties and the possibility of charge transfer interactions. We hope that the results of the present study of chalcone derivatives are of assistance in development of new efficient materials for technological applications.

Keywords : hyperpolarizability, molecular structure, NLO material, quantum chemical calculations
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