World Academy of Science, Engineering and Technology
International Journal of Physical and Mathematical Sciences
Vol:10, No:09, 2016

Vibrational Spectra and Nonlinear Optical Investigations of a Chalcone Derivative (2e)-3-[4-(Methylsulfanyl) Phenyl]-1-(3-Bromophenyl) Prop-2-En-1-One

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Abstract : Nonlinear optical (NLO) materials are the key materials for the fast processing of information and optical data storage applications. In the last decade, materials showing nonlinear optical properties have been the object of increasing attention by both experimental and computational points of view. Chalcones are one of the most important classes of cross conjugated NLO chromophores that are reported to exhibit good SHG efficiency, ultra fast optical nonlinearities and are easily crystallizable. The basic structure of chalcones is based on the π-conjugated system in which two aromatic rings are connected by a three-carbon α, β-unsaturated carbonyl system. Due to the overlap of π orbitals, delocalization of electronic charge distribution leads to a high mobility of the electron density. On a molecular scale, the extent of charge transfer across the NLO chromophore determines the level of SHG output. Hence, the functionalization of both ends of the π-bond system with appropriate electron donor and acceptor groups can enhance the asymmetric electronic distribution in either or both ground and excited states, leading to an increased optical nonlinearity. In this research, the experimental and theoretical study on the structure and vibrations of (2E)-3-[4-(methylsulfanyl) phenyl]-1-(3-bromophenyl) prop-2-en-1-one (3Br4MSP) is presented. The FT-IR and FT-Raman spectra of the NLO material in the solid phase have been recorded. Density functional theory (DFT) calculations at B3LYP with 6-311++G(d,p) basis set were carried out to study the equilibrium geometry, vibrational wavenumbers, infrared absorbance and Raman scattering activities. The interpretation of vibrational features (normal mode assignments, for instance) has an invaluable aid from DFT calculations that provide a quantum-mechanical description of the electronic energies and forces involved. Perturbation theory allows one to obtain the vibrational normal modes by estimating the derivatives of the Kohn−Sham energy with respect to atomic displacements. The molecular hyperpolarizability β plays a chief role in the NLO properties, and a systematical study on β has been carried out. Furthermore, the first order hyperpolarizability (β) and the related properties such as dipole moment (μ) and polarizability (α) of the title molecule are evaluated by Finite Field (FF) approach. The electronic α and β of the studied molecule are 41.907×10-24 and 79.035×10-24 e.s.u. respectively, indicating that 3Br4MSP can be used as a good nonlinear optical material.

Keywords : DFT, MEP, NLO, vibrational spectra
Conference Title : ICOLS 2016 : International Conference on Optics, Lasers and Spectroscopy
Conference Location : Paris, France
Conference Dates : September 26-27, 2016