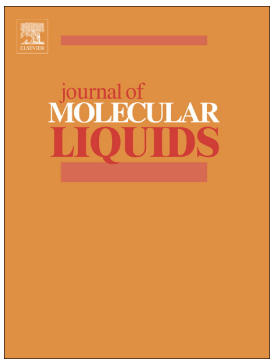

Theoretical investigation of nonlinear optical and vibrational properties of two liquid crystalline compounds

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Theoretical investigation of Nonlinear Optical and Vibrational Properties of two liquid crystalline compounds

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Abstract: This article is mainly focused on studying the different physical properties of liquid crystalline compounds using density functional theory (DFT) method. The compounds were found to be bent-core calamitic liquid crystals. The theoretical calculation has been used to find the different parameter such as reactivity parameters and structural parameters of these compounds. Dipole moments and Non-Linear Optical (NLO) properties are essential to understanding the physical behaviour of the liquid crystals and also reported in this article. The NLO properties of both the compounds possess a large number of activities which might be useful for NLO based applications. Theoretically, generate a FT-IR spectrum of both compounds helps to analyze the different vibrational modes. Vibrational Energy Distribution Analysis (VEDA), the software was used to interpret the Potential Energy Distribution (PED) function of FT-IR spectra. Detailed vibrational assignments of the wave numbers using VEDA were carried out on the basis of potential energy distribution with good agreements.

Keyword: Bent core LC, Density Functional Theory (DFT),Non-linear optics, Hyper-polarizability, Vibrational Spectroscopy

Introduction: Liquid crystals are partially ordered fluids and this phase lies between crystalline solid and isotropic liquid. This phase is also known a mesophase. Liquid crystals are anisotropic in nature and due to this anisotropy,it has unique optoelectrical properties relative to othermaterials[1-9].This unique nature of the compound has drawn the attention of the researchers to explore the properties of liquid crystals. In general, most of the calamitic liquid crystalline compounds are uniaxial but recently some researchers are working on bent-core or biaxial liquid crystalline compounds [10, 11, 12].

In the present article, the compounds used in our study were two bent-core mesogenic liquid crystals. One terminal of the benzene ring of both the compounds are connected by fluorinated atoms. The prime focus of our study was to observe different properties using the theoretical computational method. The computational approaches applied in the study of liquid crystal compounds have increased significantly in the last two decades. Different computational approaches and basis sets have been used during these years. It has been found that density functional theory (DFT) with B3LYPfunctionaland standard basis set of 6-31G gives sufficiently good and appropriate results for such liquid crystals [1, 13, 14].

Quantum mechanical density functional theoretical (DFT) methods have been used to study the different physical properties of our compounds. HOMO and LUMO energy gap describes the