

عنوان مقاله:

Linear and nonlinear optical properties of stilbazolium derivatives

محل انتشار:

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خلاصه مقاله:

Molecular organic materials having nonlinear optical (NLO) properties are required for applications in emerging optoelectronic and photonic technologies. NLO are useful because they allow the manipulation of laser beams, e.g., in frequency doubling or second harmonic generation (SHG), a quadratic effect. Among known NLO compounds, stilbazolium salts are particularly attractive for use in devices. Stilbazolium chromophores have been incorporated into various macroscopic structures such as Langmuir-Blodgett (LB) films, intercalated layer materials, self-assembled superlattices, inclusion complexes and guest-host and side-chain polymer films. With the sole exception of a theoretical study on the N-alkyl stilbazolium salts only N-aryl stilbazolium salts have been previously studied for their NLO properties.[1] The present study is dedicated to perform a theoretical investigation about the linear and nonlinear optical (NLO) properties, represented as, dipole polarizability α , first hyperpolarizability β and second hyperpolarizability γ , respectively, trans- π - π' -(R)-N-methyl- π -stilbazolium (R = Bromo Br, methyl Me, Amino NH₂, Dimethylamino NMe₂, Hydroxy OH, Methoxy MeO). With this aim, we make a comparative study between the properties of these molecules to rationalize the differences in their properties in terms of the R group into the π -methyl- π -styryl-pyridinium

کلمات کلیدی:

.Nonlinear optical properties; stilbazolium ; Hartree-Fock; DFT

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