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All optical switching and the optical nonlinear properties of 4-(benzothiazolyldiazenyl)-3-chlorophenyl 4-(nonylthio)benzoate (EB-3Cl)

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ABSTRACT

Chemical computational calculations are carried out to investigate the molecular structure of 4-(benzothiazolyldiazenyl)-3-chlorophenyl 4-(nonylthio)benzoate (EB-3Cl) via the density functional theory (DFT) method. The B3LYP method is used to optimize the geometrical structure of the EB-3Cl compound with 6–31G(d,p) basis set level. HOMO-LUMO energies and some nonlinear optical (NLO) properties are calculated via the same method used in geometry optimization. The results show that the synthesized compound has good optical properties. Good agreement correlations of experimental and theoretical findings are found. The index of nonlinear refraction (INR) of EB-3Cl is determined via two methods, the diffraction ring pattern (DRP) and the Z-scan. High INR value of 5.92×10^{-7} cm^2/W is obtained via the first method. Optical limiting (OLg), of the synthesized compound is studied with OLg threshold value of 8 mW is obtained. All optical switching technique is tested in the prepared compound with good results are obtained and DRPs are simulated numerically based on the Fresnel-Kirchhoff integral.

1. Introduction

The passage of a continuous wave, cw, laser beam with Gaussian intensity distribution through a nonlinear medium can enhance many effects in the transverse directions viz., self-focusing (SF), self-defocusing (SDF) [1], light controlled phase, optical power limiting [2,3], index of refraction (IR) modulation, all optical switching [4], optical data storage [5,6], phase conjugation [7], self-phase modulation (SPM) etc. [8–11]. SPM is the result of IR deference at different positions radially i.e. spatial self-phase modulation (SSPM) due to laser beam nonuniform Gaussian spatial intensity distribution. SSPM leads to the generation of ring patterns which can be used in the determination of the total change of the linear index of refraction (LIR) of the nonlinear medium, and the index of nonlinear refraction (INR) based on the total rings number generated. By tightly focused a laser beam onto a nonlinear medium, the beam wave front can be diffracted transversely i.e. in the (x-y) plane. When the relation between the transmitted beam power measured by a power meter covered with a narrow circular aperture versus the sample position (±z) is drawn, two types of relations appeared. When the result is a peak followed by a valley the change in INR is negative i.e., SDF phenomena occur. While when the result is a valley followed by a peak the change in INR is positive i.e., SF phenomena occur. The Z-scan technique allows the

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