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RESEARCH

Synthesize of an Azo Compound: Investigation its Optical Nonlinear Properties and DFT Study

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Abstract
In the present work, a diazonium salt is prepared by a diazonium reaction of sulfamerazine in the presence of aqueous hydrochloric acid and sodium nitrate. Structural confirmation of azo compounds synthesize is achieved by mass spectrometry, infrared spectroscopy, and ^{1}H, ^{13}C nuclear magnetic resonance. The sample geometry is derived using Density Functional Theory (DFT) and DT-DFT applied to the basis set B3LYPL6-311 + G(d,p). An investigation is conducted on the optical nonlinear (ONL) properties of the azo compounds formed under the excitation with a low power 532 nm laser beam using diffraction patterns (DPs) and a typical Z-scan combined with optical limiting. The Fresnel-Kirchhoff integral provides numerically obtained boundary conditions in the sense of experimentally obtained values. As high as 2×10^{-7} cm^2/W of nonlinear refractive index (NLRI), n_2, 1.24×10^{-3} cm/W of the nonlinear absorption coefficient (NLAC), β, and 15.5 mW of the optical limiting (OL) threshold, T_H, are obtained.

Keywords Diazonium salt · Azo dye · DFT · Diffraction pattern · Z-scan · OL · Fresnel Kirchhoff integral

Introduction

With the advent of the widespread use of optical applications viz., phase conjugation [1], image processing [2], optical switching [3], etc., there has been the need for optical nonlinear (ONL) materials with large nonlinear refractive indexes (NLRIs) and fast response times.

When a laser beam traverses a material, an intensity-dependent refractive index in the medium can result. The large ONL susceptibility resulting from the nonlinear response of organic molecules has attracted much interest. During the last three years we have studied the ONL properties of so many materials [4–20]. Among the number of techniques developed to measure the NLRI, n_2, historically developed since 1965 viz., thermal lens [21], diffraction ring patterns (DPs) 1967 [22, 23], and the Z-scan (1989–1990) [24, 25]. In the first two, n_2 can be measured while in the third one n_2 and the nonlinear absorption coefficient (NLAC), β, can be obtained in simple and effective way. AZ_2 and AZ_o compounds have been studied in the past extensively [26–36]. The ONL properties of azo – dye have been studied too [37–53].

An important branch of chemistry that investigates the properties of compounds, is computational chemistry are very powerful tools to identify and give information about the electronic and structural properties of the materials [54, 53]. The relationship between azo dyes' structural and spectroscopic behaviors are the subject of this study. Photochromic and optical properties were monitored using Density functional theory (DFT) and TD-DFT by estimation optimized geometries and orbital energies. The current work aims to find a new material that responds nonlinearly to visible lower power laser beams and has high ONL properties. Therefore the ONL properties of an azo-dye are studied via the DPs and the Z-scan using visible, cw, laser beam of wavelength 532 nm. The optical limiting (OL) property of the prepared azo dye at the same beam is studied too. Theoretical model was used to study experimental diffraction patterns numerically.

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