Journal of Electronic Materials
https://doi.org/10.1007/s11664-025-11758-1

ORIGINAL RESEARCH ARTICLE

Synthesis and Nonlinear Optical Studies of a New Azo Compound Derived from 4-Amino-2,3-Dimethyl-1-Phenyl-3-Pyrazol-5-One

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Received: 12 October 2024 / Accepted: 8 January 2025

Abstract

A novel azo dye is synthesized by reacting 4-hydroxy-3-methoxybenzoic acid with 4-amino-2,3-dimethyl-1-phenyl-3-pyrazol-5-one (azo dye N_1). The synthesized azo dye N_1 is characterized by Fourier transform infrared (FT-IR), mass, ^1H and ^{13}C nuclear magnetic resonance (NMR), and ultraviolet–visible (UV–Vis) spectroscopic techniques and melting point analysis. The B3LYP (Becke, three-parameter, Lee–Yang–Parr)/6-311+G(d,p) basis set is utilized to ascertain the sample geometry by density functional theory (DFT) and time-dependent DFT (TD-DFT) methods. Calculations of the quantum chemical descriptors are carried out to examine the sample's nonlinear optical (NLO) properties. The NLO properties of the sample are investigated under excitation with continuous-wave (CW) laser beams at 473 nm and 532 nm wavelengths. The nonlinear refractive index (NLRI) of the sample is ascertained using the 473 nm CW laser beam to obtain diffraction patterns (DPs) and Z-scan, where NLRI values of 3.698×10^{-7} cm^2/W and 0.25×10^{-7} cm^2/W are obtained. We found that the value of the refractive index of the azo dye N_1 calculated by the latter method is greater than its value for other materials. The all-optical switching (AOS) property of the azo dye N_1 is demonstrated when the controlling beam is at 473 nm and the controlled beam is at 532 nm.

Keywords Azo compound · DFT · NLO properties · DP

Introduction

The investigation of the nonlinear optical (NLO) properties of photonic materials is important, since the passage of intense laser beams through them may lead to self-focusing, self-defocusing, and spatiotemporal self-phase modulation. Several classes of materials have been explored with great interest, including organic materials, fullerenes, inorganic materials, semiconductors, polymers, and organometallic materials.[1–13] Over the last 40 years of laser technology, the significant NLO susceptibility resulting from the nonlinear response of organic materials has attracted considerable attention. Sharifi et al. published a series of articles concerning the enhancement of the linear and nonlinear properties of orythrosin,[14] the photo-physical properties of crocin,[15] and the optical study of xanthene-type dyes.[16] Thermal effects caused by absorption of a part of the laser beam energy passing through a material might modify the medium's refractive index (RI). The absorbed energy is transformed into heat following a Gaussian beam distribution within a thin medium. The heat gradient, initially confined to the irradiated volume, propagates to the non-irradiated area due to thermal conduction. This temperature profile produces a gradient in the RI. The spatial self-phase modulation that produces ring patterns from the interference of numerous laser beams originating from points on the beam wave front can be shown by the nonlinear response of materials interacting with the beam's divergence. The change in RI, Δn, of the medium, along with the nonlinear refractive index (NLRI), can be determined using these diffraction ring patterns. The Z-scan approach functions by positioning the sample at the focal point of a tightly focused Gaussian laser beam. The medium's interaction with the laser light changes when the sample is displaced. This results from the sample's fluctuating intensities, which depend on the sample's position (z) relative to the focus ($z = 0$). The Z-scan is a simple and

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