



# Nonlinear optical properties investigation of a newly synthesised Azo-( $\beta$ )-diketone dye

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## ABSTRACT

Azo- $\beta$ -diketone compound is prepared via coupling reaction of dizonium salt of sulfanilamide with acetylacetone. The compound is characterized by FTIR, Mass and <sup>1</sup>H NMR spectroscopies. The optimization of synthesized azo- $\beta$ -diketone is carried out using B3LYP method 6-31G (d,p) basis sets. Nonlinear optical properties of synthesized azo- $\beta$ -diketone is investigated via some quantum chemical descriptors calculation using DFT/B3LYP method with 6-31G(d,p) basis set. The UV-vis spectrum of the synthesized azo- $\beta$ -diketone is also calculated using TD-DFT with same optimization method and level. The nonlinear index of refraction of the azo- $\beta$ -diketone at 473 nm is calculated using the spatial self-phase modulation and Z-scan techniques where as high as  $3.259 \times 10^{-7} \text{ cm}^2/\text{W}$  is obtained due to the first technique and  $2.4 \times 10^{-8} \text{ cm}^2/\text{W}$  due to the second technique. The compound optical limiting property is tested at the same wavelength with limiting threshold of 12 mW is obtained. The diffraction ring patterns are theoretically simulated based on the Fresnel-Kirchhoff diffraction integral with results agree well with experimental findings.

## 1. Introduction

During the last four decades materials having fast response times and large nonlinear properties such as the nonlinear refractive index,  $n_2$ , and the third order nonlinear susceptibility,  $\chi^{(3)}$ , attracted enormous interest for the possible potential uses such as optical power limiting, all optical switching, etc. [1–7]. The most promising materials that having such properties are organic materials, nanomaterials, polymers, inorganic materials, semiconductors, and so on [8–14]. Due to their large nonlinear index of refraction, nonlinear coefficients of absorption etc., organic materials are the proper candidate for the use in the above mentioned applications [15]. For the sake of obtaining the nonlinear optical parameters number of techniques have been established during the period 1967–1990 viz., spatial self-phase modulation [16], thermal lens [17] and the Z-scan [18,19].

Sulfanilamide and its derivatives have been synthesized and studied for different reasons such as its effect on <sup>13</sup>C fluxes [20], its biological evaluation as antimicrobial agents [21], its sorption to soil organic sorbents [22], characterization and spectral study [23], pharmacological screening of its substituted derivatives [24], evaluation of its

ciprofloxacin conjugates [25], as antimicrobial drugs [26], study of its antioxidant activity [27] etc. On the other hand acetylacetone and its derivatives have been studied for various reasons such as its ionization and isomerization, the chemistry of metal acetylacetonate complexes [28], its binary mixtures [29], its estimation of Fe (111) using substoichiometric isotope dilution analysis [30], thermal decomposition of calcium(11) bis(acetylacetonate) n-hydrate [31], composition and fluorescence by solvothermal method [32], synthesis of some symmetrical dioxime esters [33], effect of the titanium isoperoxide [34], etc. The only available nonlinear study of acetylacetonate is due to Henari and Henari in 2016 [35] where Z-scan technique was used in the medical image processing. Azo compounds are very interesting synthetic colorants compounds having versatile applications in different areas in the industry like textile and printing [36–38]. The azo dyes playing a crucial role in the control of the pigments and printing market [39]. Furthermore, azo compounds are important units in the field of nonlinear optics, media of optical storage, and devices of liquid crystalline and sensors [40,41]. Therefore they received the concern of researchers constantly [42–44]. Designing of new optical materials required the perform of a theoretical investigation and experimental measurements

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