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## Synthesis, characterization and the nonlinear optical properties of newly synthesized 4-((1,3-dioxo-1-phenylbutan-2-yl)diazenyl) benzenesulfonamide

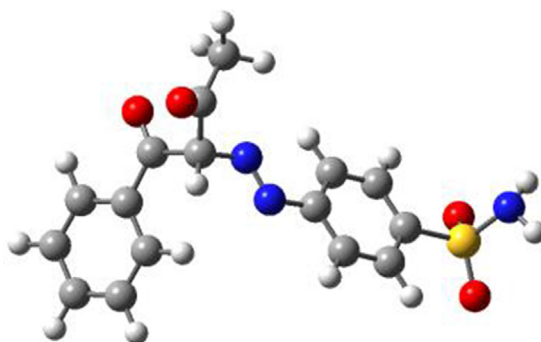
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### HIGHLIGHTS

- The azo compound was prepared by coupling reaction of dizonium salt of sulfanilamide with benzoylacetone.
- We studied the nonlinear optical properties of azo compound.
- The nonlinear refractive index of this sample is determined using diffraction ring patterns and Z-scan techniques.
- The sample exhibits self-diffraction ring patterns due self-phase modulation.

### GRAPHICAL ABSTRACT

Optimized structure of azo compound NA4.



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### ABSTRACT

The dye of azo compound is prepared by coupling reaction of dizonium salt of sulfanilamide with benzoylacetone. The product is characterized by FTIR spectroscopy, Mass spectroscopy and <sup>1</sup>H NMR spectroscopy. The geometries of the synthesized dye is optimized using B3LYP method and 6-31G (d,p) basis sets. Nonlinear optical properties are investigated theoretically by calculation of some quantum chemical descriptors using the DFT/B3LYP method with a 6-31G(d,p) basis set in comparison with urea as a standard. The UV-visible spectrum of synthesized azo dye are calculated using TD-DFT with B3LYP/6-31G(d,p) level. The nonlinear refractive index of the prepared dye is calculated via the diffraction ring patterns and Z-scan techniques using 473 nm visible, continuous wave laser light. The diffraction ring patterns are numerically simulated using the Fresnel-Kirchhoff theory with reasonable agreements. The property of optical limiting of the azo dye is tested.

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## 1. Introduction

During the last three decades the interest in finding or/ and synthesizing of new materials exhibiting nonlinear optical properties

such as having large nonlinear refractive indexes and fast response times grew almost exponentially. Such effects are of technological importance for the future use in applications viz., optical limiting, optical delay, optical switching, all-optical modulation, optical phase conjugation, in data storage [1–16], to name a few. To date, vast number of materials has been studied, shows excellent optical properties and proved their abilities use in number of photonic

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