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ORIGINAL RESEARCH ARTICLE

Visible Light-Assisted Photocatalyst-Free Synthesis, Characterization, Theoretical, and Nonlinear Optical Performance of a New 1,3,4-Oxadiazole Derivative

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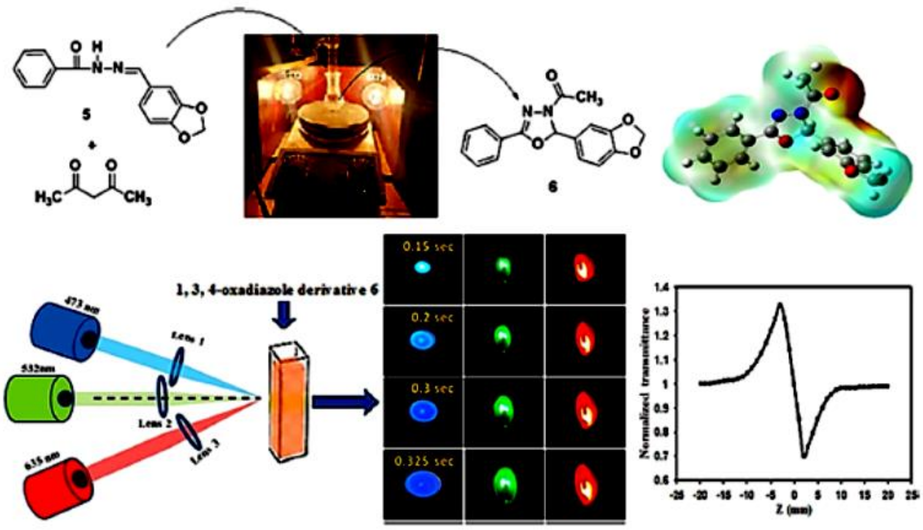
Abstract

A simple and efficient protocol was developed for the visible light-induced cyclization of a hydrazone derivative to afford a new 3-acetyl-2,3-dihydro-1,3,4-oxadiazole derivative **6**($C_{17}H_{14}N_2O_4$). The protocol proceeded smoothly, with high yield of the target product at room temperature in the absence of any photocatalysts under an air atmosphere. After structural optimization of the target derivative **6**, its efficiency was elucidated using density functional theory (DFT)-assisted calculations with two functional hybrids, B3LYP/cc-pVTZ and M062X/cc-pVTZ, to verify the important electronic descriptors including highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) as frontier orbitals, ΔE_{gap} ($E_{HOMO} - E_{LUMO}$), polarizability, and hyperpolarizability. The nonlinear optical (NLO) properties of the target derivative **6** were studied using the diffraction patterns (DPs) and Z-scan methods. DPs were formed due to the interference of beams emanating from enormous points on the laser beam wave front and on the semitransparent screen situated in the far field related to the sample cell. In the closed aperture Z-scan case, we observed the phenomenon of self-defocusing (SDF) of the laser beam transmitted from the target sample. The origin of the nonlinearity shown by the sample was thermal due to the use of a continuous-wave (CW) laser beam. At the maximum power input, the number of the formed rings and the Z-scan were utilized to obtain two values of the nonlinear refractive index (NLRI), n_2, i.e., 5.9949×10^{-7} and 0.344×10^{-7} cm^2/W, respectively. By applying 473 nm as the controlling beam and 532 and 635 nm as the controlled beams, both static and dynamic all-optical switching (AOS) were studied.

Graphical Abstract



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