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Synthesis, DFT, molecular docking and optical nonlinear studies of a new phthalimide derivative

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ABSTRACT

A new phthalimide derivative, 2-(2-methyl-5-nitrophenyl)isoindoline-1,3-dione (H8), is synthesized. Suggested structure of the synthesized phthalimide derivative (H8) is characterized by FTIR, NMR, and mass spectroscopies. The polarizability (α) and hyperpolarizability (β) of compound H8 has been calculated via density functional theory (DFT) with B3LYP and basis set 6-31G(d,p). The compound H8 is considered a candidate material for nonlinear optical (NLO) applications, based on theoretical calculations that show its performance to be comparable to that of urea. A molecular docking study is conducted between the compound H8 (ligand) and the (PDB ID: 3 pp0) receptor, which is associated with proliferation in cancer cells, especially breast cancer. Molecular docking results show that the prepared compound could be a candidate for the inhibition of breast cancer cells. The NLO properties of the compound H8 are studied via the calculation of the nonlinear refractive index (NLRI), n_2, under irradiation with (<1W), cw, visible (473 nm) laser beam using diffraction patterns (DPs) and the Z-scan techniques where as high as 8.081×10^{-11} m^2/W of n_2 value and change of the medium refractive index, value of 3.095×10^{-3} are obtained. The closed aperture Z-scan proved that compound H8 nonlinearity is of thermal character, while the open aperture Z-scan proved that compound H8 bare no nonlinear absorption coefficient at the beam 473 nm and power input used. The (static and dynamic) all-optical switchings (AOSs) are studied using controlling, 473 nm cw, low power laser beam, and controlled 532 nm cw, low power laser beam. The controlling beam seem to affect the DPs of the controlled beam via it's area, number of rings, and asymmetry.

1. Introduction

In recent years, large 3rd- order nonlinear susceptibility materials and short response time have attracted many researchers owe to their possible applications in light controlled phase, all-optical switching, optical limiting, frequency conversion, data storage, image processing, optical telecommunication, refractive index modulation and optical computing [1–9]. The induced changes in the refractive index (RI) of materials due to the optical fields lead to a large number of nonlinear phenomena. The interplay between the nonlinear optical (NLO) response of a medium and divergence of the propagating laser beam, in the spatial domain, elicits number of self-action behaviours, viz., spontaneous pattern soliton, formation of optical self- trapping [10–12] and modulation instability [13]. The effect of spatial self-phase modulation (SSPM) [14] occurs due to the RI power-dependent and it has been observed in several systems [15,16]. Such effect, SSPM, generates in the far field a nested array of concentric intensity rings, or diffraction patterns (DPs) [17–21]. These DPs can be used in the calculation of the nonlinear medium nonlinear refractive index (NLRI). The Z-scan is a technique used since 1989–1990 [22,23], by so many researchers in the calculation of the NLRI and the nonlinear absorption coefficient (NLAC), of all types of materials [24–33]. It is sensitive, simple, and accurate.

The preparation of new chemical compounds with different applications is an important challenge to chemists [34–39]. They have excelled in preparing variety of compounds that have been used in a wide range of industrial, medical, pharmaceutical, agricultural, and other fields. The field of optical studies and the preparation of compounds with NLO properties can be used in various optical applications viz., laser rangefinders, opto-electronic switches, etc., is one of the broadest fields of applications. For this purpose, many chemical compounds of different types were prepared. Azo compounds took the widest scope in various disciplines such as the corrosion inhibition,

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