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Study of the effect of peripheral groups on the two-photon absorption cross-section in bromo-chalcone derivatives

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The two-photon absorption (2PA) has several practical applications, ranging from imaging by two-photon microscopy to microfabrication through, for example, two-photon photopolymerization, enabling higher spatial resolution. It also finds applications in photodynamic therapy (PDT), allowing the excitation of a photosensitizer at wavelengths outside the absorption window of living tissues. Thus, it is evident that the development of new devices and applications in Photonics requires the investigation of new nonlinear optical (NLO) materials with desired properties. Chalcones are a family of organic compounds with promising nonlinear optical properties, due to the presence of delocalized electrons. They also feature relatively simple synthesis, various interesting pharmacological properties and the potential to form photoproducts. (1) Therefore, this study aims to investigate the effect of substituents on the 2PA cross-section (2PACS) in some Bromo-Chalcone derivatives using the Z-scan technique. (2) The studied molecules share a bromine atom in the para-position of ring A (the aromatic ring attached to the carbonyl group) and different substituents in the para-position of the other ring (ring B). NLO experiments were performed using 150-fs pulses from a Yb:KGW laser system, which, coupled with an optical parametric amplifier (OPA), allow tuning the excitation wavelength from UV to near-infrared. Among the studied molecules, the one with an amine group (-N(CH3)2) as a substituent showed remarkable properties. In general, the samples have two characteristic absorption bands, non-characteristic fluorescence, and low 2PACS. However, the amine-substituted sample displayed a significant bathochromic shift (redshift), slower photoproduct formation dynamics, a high fluorescence quantum yield (around 14%), and a high 2PACS. This can be explained by the fact that, although nitrogen is more electronegative than carbon and tends to pull electrons from the single bond (σ) towards itself (inductive effect), it also possesses non-bonding pairs of electrons whose p orbitals overlap with the p orbitals of the aromatic ring, donating these electrons to the π-conjugated system (Mesomeric effect). Moreover, computational simulations of optimization of geometry using Density Functional Theory (DFT) were carried out and the results obtained corroborate this hypothesis. (3)

Palavras-chave: Chalcones; Z-scan; Two-photon absorption.

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