Study of the Effect of Peripheral Groups on the Two-Photon Absorption Cross-Section in Bromo-Chalcone Derivatives

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The development of new devices and applications in Photonics requires the investigation of new nonlinear optical (NLO) materials with desired properties. Benzylideneacetophenones, commonly known as chalcones, are a family of organic compounds with promising NLO properties, despite their small molecular size, 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 characterize and investigate the effect of substituents on the two-photon absorption (2PA) cross-section in some Bromo-Chalcone derivatives, correlating the NLO response with their structures. 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). Initially, the samples were diluted in DMSO, and their linear absorption and fluorescence spectra were measured. Photo-irradiation with light at a lower-energy absorption wavelength systematically decreases the lower-energy band and increases the higher-energy one, with the presence of an isosbestic point indicating the formation of a photoproduct. The mean 2PA cross-section of the blend was measured using the Z-scan technique [2] with 150-fs pulses from a Yb:KGW laser system, which, coupled with an optical parametric amplifier (OPA), allows tuning the excitation wavelength from UV to near-infrared. Among the studied molecules, one in particular stood out: the one with the amine group as a substituent. The samples generally exhibit two characteristic absorption bands, non-characteristic fluorescence, and a low 2PA cross-section, on the order of 30GM. However, the sample with the amine group shows a significant bathochromic shift (redshift), slow dynamics in photoproduct formation, high fluorescence quantum yield (of about 14%) and a high 2PA cross-section, exceeding 80 GM for the lower-energy band. To support the experimental results, computational simulations were performed using Density Functional Theory (DFT) and the Sum-Over-States (SOS) approach.

References

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