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Nonlinear optical (NLO) properties of donor-π-donor featuring diformyltriphenylamine chalcone derivatives

Abstract

This research was carried out to explore the impact of substituent groups with varying electron-donating strengths on the nonlinear optical (NLO) properties of four recently synthesized chalcone derivatives (DFC1–DFC4). Spectroscopic characterization was conducted via FT-IR and NMR, while thermal stability was assessed through TGA. Linear and third-order NLO behaviours were determined using a UV–Vis spectrometer and a Z-scan technique with 637 nm excitation. Density functional theory (DFT) with B3LYP functionals, focusing on nonlinear optical parameters including global reactivity descriptors, and photophysical properties including HOMO-LUMO energy levels. NLO properties, incorporating dipole moment, polarizability, and hyperpolarizabilities, were calculated using a numerically differentiated analytic method. Z-scan data revealed that DFC1–DFC4 NLO responses, significantly affected by electron-donating groups and intermolecular interactions, position them as promising materials for optoelectronic and NLO applications.

Keywords

D-π-d chalcone derivatives; extended π-conjugation; Nonlinear optical properties; Third-order nlo; Z-scan analysis