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First-order hyperpolarizability dispersion on chalcone-based molecules

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The first-order molecular hyperpolarizability (β) dispersion was measured using tunable femtosecond hyper-Rayleigh scattering (tHRS) technique in seven chalcone-based molecules. (1) A theoretical model for β dispersion based on photophysical parameters was also applied. (2) Due to the different substitution patterns of the aryl/heteroaryl rings on the chalcones structure, different profiles of one and two-photon absorption spectra and β dispersion were observed. The applied model showed two important features for aiming high β values: (i) red-shifted one-photon and two-photon absorption bands and (ii) the number of absorption bands observed. To compare the results with other molecular structures, we employed the HRS figure of merit (FOM), which revealed that chemically engineered small chalcone molecules FOM is comparable to larger quadrupolar and octupolar ones. This clearly demonstrates that tunable femtosecond hyper-Rayleigh scattering measurements and its relationship with the absorptive photophysical parameters are essential for design and characterize nonlinear optical materials.

Palavras-chave: Tunable hyper-Rayleigh scattering. Chalcone-based molecules. Two-photon absorption spectra.

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