

Universidade de São Paulo
Instituto de Física de São Carlos

XIV Semana Integrada do Instituto de
Física de São Carlos

Livro de Resumos da Pós-Graduação

São Carlos
2024

Ficha catalográfica elaborada pelo Serviço de Informação do IFSC

Semana Integrada do Instituto de Física de São Carlos
(13: 21-25 ago.: 2023: São Carlos, SP.)

Livro de resumos da XIII Semana Integrada do Instituto de Física de São Carlos – Universidade de São Paulo / Organizado por Adonai Hilário da Silva [et al.]. São Carlos: IFSC, 2023.
358p.

Texto em português.

1.Física. I. Silva, Adonai Hilário da, org. II. Título.

ISSN: 2965-7679

39

Contribution of excited states on molecular first hyperpolarizability dispersion of chalcone derivatives

PELOSI, André¹; VICTOR, Valverde João¹; SANTOS, Carlos Henrique dos¹; DUCAS, Eli²; GONÇALVES, Pablo²; MENDONÇA, Cleber Renato¹; DE BONI, Leonardo¹

andre.gasparotto.pelosi@usp.br

¹Instituto de Física de São Carlos - USP; ²Instituto de Química - UFG

The tunable femtosecond hyper-Rayleigh scattering technique (HRS) was applied to measure the first hyperpolarizability (β) dispersion of five chalcone derivatives with different electron-donating groups (-CH₃, -OCH₃, -CH₂CH₃, -OCH₂CH₃). (1) Results show a sevenfold increase in β values for excitation wavelengths near two-photon absorption (2PA) resonances compared to the static hyperpolarizability. The molecular group -OCH₃ was shown to play an essential role in the observed first hyperpolarizability, a twofold increase in relation to the non-substituted. Besides, it was also seen that nonlinear optical coefficients such as β and σ follow a linear increase with the Hammett constant. The phenomenological n-Level model (nLM) was used to simulate the experimental results, elucidating features of the electronic molecular structure by the experimental values of β . Such model was also compared with 2PA simulation (SOS model), such as present the similar input parameters revealed that the presence of excited states leads to an enhancement of β .

Palavras-chave: Hyper Rayleigh scattering; Chalcones derivatives.

Agência de fomento: Sem auxílio

Referências:

1 CLAYS, K.; PERSOONS, A. Hyper-Rayleigh scattering in solution. **Physical Review Letters**, v.66, n. 23, p. 2980-2983, 1991.