# Universidade de São Paulo
# Instituto de Física de São Carlos

# XII Semana Integrada do Instituto de Física de São Carlos

## Livro de Resumos

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## Femtosecond laser-induced hyper-Raleigh scattering: an frequency-resolved study of the first-order molecular hyperpolarizability of organic molecules

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Frequency-resolved nonlinear optical properties of materials are fundamental to identifying regions where the nonlinear response is more intense for use in developing photonic devices or biological applications. However, only a few studies in the literature report the first-order hyperpolarizability ($\beta$) dispersion (1), making it impossible to know the spectral behavior of molecules for possible applications, such as bioprobes and second-order nonlinear switches. Therefore, this paper describes a novel experimental optical setup of the femtosecond laser-induced Hyper Rayleigh Scattering (HRS) to determine the $\beta$ spectral dependence in organic molecules. As proof of concept, five new organic molecules of cinnamylidene acetophenone derivatives were investigated. A model derived from the time-dependent perturbation theory was used to simulate the behavior of the experimental results using photophysical parameters obtained from other spectroscopic techniques, such as one (1PA) and two (2PA) photon absorption. (2) Because the derivatives exhibit a similar conjugated structure with distinct electron donor and electron-withdrawing groups attached, the experimental spectra obtained for the first-order molecular hyperpolarizability dispersion vary according to the strength of the EW or ED group inserted at the structure, as expected. The highest $\beta$ value obtained near resonance was for molecule C4 $\beta$HRS (750 nm) = 295 cm5/esu, which is approximately twice as large as molecule C1 with no EW group. Furthermore, the experimental values for dispersion of $\beta$ for all molecules show excellent agreement with simulated ones using the photophysical parameters obtained from 1PA and 2PA, demonstrating the importance of computing all the components involved in the model used. Finally, through elaborating a figure of merit (FOM), it was possible to predict the values of first-order hyperpolarizability $\beta$ for the wavelengths studied for the same molecular structure but with different peripheral atoms (ED or EW groups).

**Palavras-chave:** Dispersion of the first order hyperpolarizability. Hyper rayleigh scattering. Two-photon absorption.

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**Referências:**

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