Universidade de São Paulo
Instituto de Física de São Carlos

XII Semana Integrada do Instituto de Física de São Carlos

Livro de Resumos

São Carlos
2022

Semana Integrada do Instituto de Física de São Carlos

SIFSC 12

Coordenadores

Prof. Dr. Osvaldo Novais de Oliveira Junior
Diretor do Instituto de Física de São Carlos – Universidade de São Paulo

Prof. Dr. Javier Alcides Ellena
Presidente da Comissão de Pós Graduação do Instituto de Física de São Carlos – Universidade de São Paulo

Profa. Dra. Tereza Cristina da Rocha Mendes
Presidente da Comissão de Graduação do Instituto de Física de São Carlos – Universidade de São Paulo

Comissão Organizadora

Adonai Hilario
Arthur Deponte Zutião
Elisa Goettems
Gabriel dos Santos Araujo Pinto
Henrique Castro Rodrigues
Jefter Santiago Mares
João Victor Pimenta
Julia Martins Simão
Letícia Martinelli
Lorany Vitoria dos Santos Barbosa
Lucas Rafael Oliveira Santos Eugênio
Natasha Mezzacappo
Paulina Ferreira
Vinícius Pereira Pinto
Willian dos Santos Ribela

Normalização e revisão – SBI/IFSC

Ana Mara Marques da Cunha Prado
Maria Cristina Cavarette Dziabas
Maria Neusa de Aguiar Azevedo
Sabrina di Salvo Mastrantonio

Ficha catalográfica elaborada pelo Serviço de Informação do IFSC

Semana Integrada do Instituto de Física de São Carlos
(12: 10 out. - 14 out. : 2022: São Carlos, SP.)
Livro de resumos da XII Semana Integrada do Instituto de Física de São Carlos/ Organizado por Adonai Hilario [et al.]. São Carlos: IFSC, 2022.
446 p.
Texto em português.
1. Física. I. Hilario, Adonai, org. II. Titulo

ISBN: 978-65-993449-5-4 CDD: 530

PG5

Using one- and two-photon absorption effects for molecular first-order hyperpolarizability dispersion measurements in organic molecules

SCIUTI, Lucas; ABEGAO, Luis; COCCA, Leandro Zucolotto; SANTOS, Carlos Henrique D. dos; COSTA, Rafaela da; LIMBERGER, Jones; MISOGUTI, Lino; MENDONÇA, Cleber

lfsciuti@gmail.com

The first-order hyperpolarizability (β) is a microscopic optical parameter associated with a hyper-Rayleigh scattering with the second-order electrical susceptibility (χ^2) as the macroscopic counterpart. The knowledge of both parameters is important for certain optical applications of organic molecules. For instance, the electro-optical coefficient (EO) is related with β and it is the quantity that characterizes the molecule as suitable for molecular EO modulators. (1) Further, the second harmonic generation (SHG) is connected to χ^2. (2) However, the direct experimental measurement of β for a particular wavelength and, in particular, its dispersion $\beta(\lambda)$ is a complex and expansive task still nowadays. Therefore, we investigate the application of a complete phenomenological model for calculate $\beta(\lambda)$ (3) for arylated chalcone derivatives dissolved in dichloromethane (DCM). The central frequencies, linewidth and the transition electric dipole moment of the molecule's electronic excited states were measured through one-photon absorption spectra. Permanent electric dipole moment differences between the excited states and the ground one were obtained by fitting the Sum-over-States (SOS) model for the two-photon absorption spectrum measured with the absorptive Z-Scan technique. The molecules showed three experimental decomposed electronic excited states which leads to a four-level phenomenological model. The results of the phenomenologically calculated $\beta(\lambda)$ were compared to the vastly used quantum chemical calculations (QCC) for β. The values obtained from both models were equivalent for the static hyperpolarizability (β_0) and for the dynamic one in the spectral range considered. The application of the non-simplified phenomenological model revealed two-photon resonances and tend to be a fast tool to achieve the dispersion of β through easily obtained experimental parameters.

Palavras-chave: First hyperpolarizability. Chalcone molecules. Two-photon absorption.

Agência de fomento: Sem auxílio

Referências:

1 BALE, D.H.; EICHINGER, B.E.; LIANG, W. ; LI,X.; DALTON, L.R; ROBINSON, B.H., REID, P.J. Dielectric dependence of the first molecular hyperpolarizability for electro-optic chromophores, **Journal Physical Chemistry B**. v.115, p. 3505–3513, 2011.Disponivel em: https://doi.org/10.1021/jp109870y.Acesso em: 29.08.22.

2 MINIEWICZ, A. *et. al.* Second harmonic generation in nonlinear optical crystals formed from propellane-type molecules, **Journal Material Chemistry C**. v.7, p. 1255–1262, 2019. Disponivel em: https://doi.org/10.1039/c8tc05268a.Acesso em:29.08.22.

3 ORR, B.;WARD, J. F. Perturbation theory of the non-linear optical polarization of an isolated system, **Molecular Physics** v.20, n.3, p.513–526, 1971. Disponivel em: https://doi.org/10.1080/00268977100100481.Acesso em: 29.08.22.