

Experimental and theoretical study of the microscopic second- and third-order optical nonlinearities in dibenzylideneacetone derivatives

Francisco A. Santos, M. A. R. C. Alencar, J.J. Rodrigues Jr

Departamento de Física, Universidade Federal de Sergipe, 49100-000 São Cristóvão, SE, Brazil

Luis M.G. Abegão

Department of Radiology & Biomedical Imaging, Yale University, 330 Cedar St, New Haven, Connecticut 06520, USA

Ruben D. Fonseca

Universidad popular del Cesar, Departamento de Física, Barrio Sabana, 2000004, Valledupar, Cesar, Colombia

Aline M. Alcântara, Marcelo S. Valle

Departamento de Ciências Naturais, Universidade Federal de São João del Rei, 36301-160, MG, Brazil

Cleber R. Mendonça, Leonardo De Boni

Instituto de Física de São Carlos, Universidade de São Paulo, CP 369, 13560-970 São Carlos, SP, Brazil

Kenji Kamada

IFMRI, National Institute of Advanced Industrial Science and Technology, Ikeda, Osaka 563-8577, Japan

Materials with measurable second- and third-order nonlinear optical effects are of great interest for photonic applications and devices, such as photodynamic therapy, up-conversion lasing, optical-limiting, optical data storage, 3D microfabrication and two-photon excited fluorescence microscopy. Organic compounds are a class of materials particularly interesting, once they could stand out for the possibility of an ease nonlinear optical response optimization through molecular engineering, while compared with inorganic compounds. For example, molecular engineering could be used to increase the size of the π -bridge, adding planarity to the molecular structure, and adding donor and acceptor groups. Compounds made by dibenzylideneacetone derivatives has a straightforward and low-cost synthesis process, ultra-low molar absorptivity in the Vis-NIR region, which combined with a reasonable nonlinear optical response could be a promising nonlinear optical material. In this work, the first molecular hyperpolarizability (β) and two-photon absorption (TPA) cross-section (σ^{TPA}) of two dibenzylideneacetone derivatives in dichloromethane solution were studied. β was obtained by hyper-Rayleigh scattering technique with picoseconds pulses and the values were between 25 to $27 \times 10^{-30} \text{cm}^4 \text{statvolt}^{-1}$. The σ^{TPA} was studied by open-aperture Z-scan technique with femtosecond pulses, and the maxima TPA band values were 24 GM and 17 GM for both compounds. By delivering quantum chemistry calculations in Gaussian 09 software, employing the time-dependent density functional theory, the comparison between experimental and theoretical results are achieved, improving the discussion of results, suggesting that exists good accordance between simulated and experimental values.