FIRST MOLECULAR ELECTRONIC HYPERPOLARIZABILITY OF TWO OXAZOLES DYES IN SOLUTION

Baeceló, Ernesto; Navarro, María Camila; Gelves-Ospina, Melissa; Rodrigues, Fernando; Rosa, Pedro; Orozco, Erick; Benítez, Juan Camilo

Abstract

Two π -conjugated oxazoles compounds dissolved in toluene were characterized by the hyper-Rayleigh scattering technique in order to determine the value of the first molecular hyperpolarizability (β HRS). Quantum-chemical calculations using time-dependent density functional theory level were performed to calculate the static and dynamic β HRS theoretical values. Experimental β HRS have shown values of about $42 \times 10^{-30} \text{ cm}^4 \text{ statvolt}^{-1}$ and $31 \times 10^{-30} \text{ cm}^4 \text{ statvolt}^{-1}$ for both organic compounds, which are in a satisfactory accordance with the calculated results.

Keywords

Photonics, Quantum chemistry