Theoretical calculations of second and third-order nonlinear susceptibilities and their corresponding hyperpolarizabilities of a styrylquinolinium dye

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Résumé en anglais	The second (Xexp(2)) and third-order (Xexp(3)) susceptibilities of a styrylquinolinium dye (1) have been determined utilizing second-harmonic generation (SHG) and third-harmonic generation (THG) techniques, respectively. The reported measurement findings on Xexp(2) and Xexp(3) have been compared with the theoretical data evaluated here by means of ab-initio quantum mechanical calculations. The electric dipole moments (μ), static dipole polarizabilities (a) and first hyperpolarizabilities (β) have been computed by density functional theory (DFT) at B3LYP/6-311+G(d, p) level. To reveal the frequency-dependent second and third-order microscopic nonlinear optical (NLO) behavior of the title compound, the dynamic dipole polarizabilities, first and second (γ) hyperpolarizabilities have been theoretically investigated using time-dependent Hartree-Fock (TDHF) method. According to the experimental and theoretical results, the values of susceptibilities and the corresponding microscopic coefficients with large non-zero responses make the examined dye promising candidate for NLO applications.
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Liens

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