Experimental and theoretical studies of the second- and third-order NLO properties of a semi-organic compound: 6-Aminoquinolinium iodide monohydrate

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Résumé en anglais	Abstract A new semi-organic compound, 6-aminoquinolinium iodide monohydrate (I), has been synthesized and characterized by single crystal X-ray diffraction, UV–vis absorption and fluorescence spectroscopy and nonlinear optical (NLO) measurements. The second- and third-order NLO responses were investigated with the second- and third-harmonic Maker fringes techniques, carried out on thin films at a fundamental wavelength of 1064 nm. From the molecular structure, the molecular hyperpolarizability tensors were determined with density functional theory and second-order Møller–Plesset perturbation method. The second- and third-order susceptibility tensors of the reported crystal were evaluated using the oriented gas model with the Lorenz–Lorentz and the Wortmann–Bishop local-field corrections. The calculations using the Wortmann–Bishop local-field were able to reproduce the correct order of magnitude of the experimental third-order susceptibilities. The value of $\chi^{(3)}$ obtained by summing the effective third-order polarizability calculated for the asymmetric unit surrounded by ESP-derived charges have also the same order of magnitude of the experimental.
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