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Linear and nonlinear optical susceptibilities and the hyperpolarizability of borate $LiBaB_9O_{15}$ single-crystal: theory and experiment

Abstract

The single-crystal borate $LiBaB_9O_{15}$ was synthesized by a high-temperature solution reaction and structurally determined by the single-crystal X-ray diffraction technique. It crystallizes in the noncentrosymmetric space group R3c and features a three-dimensional $\infty^3[B_9O_{15}]^{3-}$ anionic framework, with infinite channels in which the Li^+ and Ba^{2+} cations are located. The linear optical properties were investigated experimentally in terms of the absorption spectrum, which reveals an optical gap of 5.17 eV. In addition we have calculated the linear optical properties using state-of-the-art all-electron full potential linearized augmented plane wave method. The nonlinear optical susceptibilities, namely, the second harmonic generation and the hyperpolarizability of the single-crystal borate $LiBaB_9O_{15}$ are calculated and evaluated at a static limit and at λ = 1064 nm. The calculation shows there exists three second-order nonlinear optical susceptiblities tensors components. We present measurements of the IR spectra in the range 500-2000 cm^{-1}, and the second harmonic generation was performed using a Quantel 15 ns Nd:YAG laser operating at 1064 nm.

Keywords — Hyper-polarizability, linear optical properties, nonlinear optical susceptibilities, second-order nonlinear optical, single crystal x-ray diffraction