

Optical spectra, crystal-field parameters, and magnetic susceptibility of multiferroic Nd Fe₃ (B O₃)₄

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Abstract

We report high-resolution optical absorption spectra for Nd Fe₃ (B O₃)₄ trigonal single crystal, which is known to exhibit a giant magnetoelectric effect below the temperature of magnetic ordering $T_N = 33$ K. The analysis of the temperature-dependent polarized spectra reveals the energies and, in some cases, symmetries and exchange splittings of Nd³⁺ 84 Kramers doublets. We perform crystal-field calculations starting from the exchange-charge model, obtain a set of six real crystal-field parameters, and calculate wave functions and magnetic g factors. In particular, the values $g = 2.385$ and $g = 1.376$ were found for the Nd³⁺ ground-state doublet. We obtain $B_{loc} = 7.88$ T and $J_{FN} = 0.48$ K for the values of the local effective magnetic field at liquid-helium temperatures at the Nd³⁺ site and the Nd-Fe exchange integral, respectively, using the experimentally measured Nd³⁺ ground-state splitting of 8.8 cm⁻¹. To check the reliability of our set of crystal-field parameters, we model the magnetic susceptibility data from literature. A dimer containing two nearest-neighbor iron ions in the spiral chain is considered to partly account for quasi-one-dimensional properties of iron borates, and then the mean-field approximation is used. The results of calculations with the exchange parameters for Fe³⁺ ions $J_{nn} = -6.25$ K (intrachain interactions) and $J_{nnn} = -1.92$ K (interchain interactions) obtained from fitting agree well with the experimental data. © 2007 The American Physical Society.

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