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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 TN =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 Bloc =7.88 T and JFN =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 Jnn =-6.25 K (intrachain interactions) and Jnnn =-1.92 K (interchain interactions) obtained from fitting agree well with the experimental data. © 2007 The American Physical Society.

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