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CRYSTAL-FIELD AND EXCHANGE-INTERACTION PARAMETERS FOR MULTIFERROIC $ErFe_3(BO_3)_4$

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Trigonal borates $RFe_3(BO_3)_4$ (R = Y, La – Er) with structure of the natural mineral huntite (space group $R32$) are multiferroics. The research on magnetoelectric (ME) properties of $RFe_3(BO_3)_4$ single crystals has shown that the magnitude of electric polarization induced by a magnetic field of 10 kOe in easy-plane neodymium and samarium compounds reaches values 400 $\mu C/m^2$ and 500 $\mu C/m^2$, respectively, which are record values for iron borates. A significant ME effect was expected to occur in easy-plane holmium and erbium iron borates as well. However, the induced electric polarization in $ErFe_3(BO_3)_4$ appeared to be extremely small [1]. Two phase transitions were observed in $ErFe_3(BO_3)_4$ single crystals, namely, a first-order structural transition from the high-temperature $R32$ phase into a lower-symmetry $P3_121$ phase at $T_S = 431$ K and a second-order transition into an antiferromagnetic easy-plane phase at $T_N = 39$ K. In order to explain magnetic and ME properties of $ErFe_3(BO_3)_4$, the crystal-field (CF) and Er-Fe exchange-interaction parameters are required. The parameters can be obtained through an analysis of spectroscopic data. We present the results of spectroscopic research and calculations performed on its basis.

$ErFe_3(BO_3)_4$ single crystals were grown by solution-melt technique using bismuth trimolybdate based flux. Polarized broad-band temperature-dependent transmission spectra of oriented $ErFe_3(BO_3)_4$ single crystals were registered using a Bruker IFS 125HR Fourier spectrometer. The analysis of the spectra in the region of *f-f* transitions of the Er^{3+} ion in the paramagnetic phase of the compound allowed us to identify the CF levels of the ground multiplet $^4I_{15/2}$ and nine excited multiplets. The exchange splittings of Kramers doublets of the Er^{3+} ion in $ErFe_3(BO_3)_4$ were measured at 5 K. The value of the ground-state exchange splitting was found to be 6.3 ± 1 cm^{-1}. The CF parameters and the parameters of the Hamiltonian of anisotropic *f-d* exchange interaction between Er and Fe ions were determined on the basis of analysis of the acquired spectroscopic data. The calculated temperature dependences of the magnetic susceptibility tensor components, field dependences of magnetization and theoretical estimates of ME effects in the erbium iron borate are compared with published experimental data.

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[1] A.M. Kadomtseva, Yu.F. Popov, G.P. Vorob'ev, A.P. Pyatakov, S.S. Krotov et al., *Low Temp. Phys.,* **36 (**2010) 511.