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Phase transitions and crystal-field and exchange interactions in TbFe 3(BO 3) 4 as seen via optical spectroscopy

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Abstract

High-resolution polarized broadband (180023000cm 1) optical absorption spectra of Tb 3+ in TbFe 3(BO 3) 4 single crystals are studied between room temperature and 4.2K. The spectral signatures of the structural (R32P3 121, T S=192K) and magnetic (T N=41K) phase transitions are found and analyzed. Energies and symmetries of the Tb 3+ crystal-field (CF) levels were determined for both the high-temperature R32 and the low-temperature P3 121 structures of TbFe 3(BO 3) 4 and compared with the calculated ones. It follows unambiguously from the spectral data that the ground state is the 1+ 2 quasi-doublet of the local D 3 point symmetry group for Tb 3+ in the R32 high-temperature structure. The CF calculations revealed the CF parameters and wavefunctions for Tb 3+ in TbFe 3(BO 3) 4. The value of the TbFe exchange integral and of the effective magnetic field created by the ordered Fe subsystem were estimated as J fd=0.26K and B eff=3.92T, using the observed splitting =32cm 1 of the Tb 3+ ground quasi-doublet at the temperature 5K. The reliability of the obtained parameters was proven by modeling the literature data on the magnetic susceptibility of TbFe 3(BO 3) 4. Lattice distortions below T S were evidenced by the observed changes of probabilities of the forced electric dipole transitions of Tb 3+. © 2012 IOP Publishing Ltd.

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