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

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### Abstract

High-resolution polarized broadband (180023000cm<sup>-1</sup>) optical absorption spectra of Tb<sup>3+</sup> in TbFe<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub> single crystals are studied between room temperature and 4.2K. The spectral signatures of the structural (R32P3 121, T<sub>S</sub>=192K) and magnetic (T<sub>N</sub>=41K) phase transitions are found and analyzed. Energies and symmetries of the Tb<sup>3+</sup> crystal-field (CF) levels were determined for both the high-temperature R32 and the low-temperature P3 121 structures of TbFe<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub> 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<sub>3</sub> point symmetry group for Tb<sup>3+</sup> in the R32 high-temperature structure. The CF calculations revealed the CF parameters and wavefunctions for Tb<sup>3+</sup> in TbFe<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub>. The value of the TbFe exchange integral and of the effective magnetic field created by the ordered Fe subsystem were estimated as J<sub>fd</sub>=0.26K and B<sub>eff</sub>=3.92T, using the observed splitting =32cm<sup>-1</sup> of the Tb<sup>3+</sup> 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<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub>. Lattice distortions below T<sub>S</sub> were evidenced by the observed changes of probabilities of the forced electric dipole transitions of Tb<sup>3+</sup>. © 2012 IOP Publishing Ltd.

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