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EPR, ENDOR, and optical spectroscopy of the tetragonal Yb3+ center in KMgF3

Falin M., Latypov V., Kazakov B., Leushin A., Bill H., Lovy D.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

Electron paramagnetic resonance, electron-nuclear double resonance, and optical spectroscopy of the tetragonal Yb3+ center in KMgF3 are reported here. The results of these experiments allow us to conclude that a previously given structural model as well as the interpretation of the optical spectrum of this center are incorrect. A model is presented and experimentally and theoretically justified. In particular, the values of the hyperfine and transferred hyperfine interaction parameters were determined as well as an experiment-based energy-level scheme. Its parametrization is performed by including simultaneously the crystal field and the spin-orbit interaction within the 7F term. Furthermore, a theoretical analysis of the transferred hyperfine interaction (THFI) parameters is presented. It is further shown from optics and from microscopic calculations of the THFI parameters that g∥ and g⊥ have opposite signs and that the rule of correspondence between the cubic g factor and g̃=1/3 (gx+gy+gz) does not depend on the relative magnitude of the cubic and low-symmetry crystal field acting on the rare-earth ion.