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EPR and optical spectroscopy of structural phase transition in a Rb 2NaYF6 crystal

Falin M., Gerasimov K., Latypov V., Leushin A., Khaidukov N.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

The structural phase transition has been observed for the first time in the Rb2NaYF6 crystal and studied by EPR and optical spectroscopy. EPR spectra of Dy3+ and Yb3+ ions present as unintentional dopants in the nominally undoped crystal and forming tetragonal paramagnetic centers have been identified. A characteristic splitting of some optical lines has been observed in the temperature dependence of the Yb3 + optical spectra. It indicates the splitting of the cubic quartet energy levels of Yb3+ ions by the tetragonal crystal field. The empirical schemes of the energy levels for cubic and tetragonal paramagnetic centers of Yb3+ ions have been established and parameters of the corresponding crystal fields have been determined. The latter have been used for analyzing the crystal lattice distortions occurring in the vicinity of the Yb3+ ion during the phase transition. It has been established using the superposition model that the nearest octahedral environment of the Yb3 + ion is distorted as follows: the fluorine ions are rotated by the angle of 2.1 around the fourfold axis; the F- ions located symmetrically in the plane perpendicular to the rotation axis approach the dopant by 0.0014 nm, whereas the F- ions located on the rotation axis move away by 0.0028 nm. It has been concluded that the studied phase transition includes the critical rotations of the octahedral F groups and noncritical displacement of atoms in the rotated fluorine octahedra. © 2013 American Physical Society.

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