Applied Magnetic Resonance 1998 vol.15 N2, pages 145-154

The analysis of spin hamiltonian and crystal field tensors for Fe3+ in crystals of LiCaAlF6 and LiSrAlF6

Nizamutdinov N., Khasanova N., Antonova I., Abdulsabirov R., Korableva S., Galeev A., Stepanov V.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

In single crystals of LiCaAlF6 and LiSrAlF6 doped with Fe3+ the trigonal EPR spectra with multiplicity KM = 1 were observed due to Fe3+ substituted for Al3+. The spin Hamiltonian parameters describing the fine structure and the superhyperfine structure were determined. It is argued that the tensors B2 and BA of the spin Hamiltonian for Fe3+ ions are essentially determined by the quadratic contributions of the crystal field at the substitution site. The signs and the relative values of the elements in the spin Hamiltonian tensor B4 of rank L = 4 for Fe3+ are determined by the irreducible tensor product [V4⊗V4]2 of the crystal field tensor V4 of rank L = 4 at the substitution sites. The ratio between the invariant sum of the spin Hamiltonian tensor B4 for Fe3+ in oxygen octahedra [FeO6] and that in fluorine octahedra [FeF6] is directly proportional to the fourth power of the ratio between the effective charges of surrounding ions. The sign of the spin Hamiltonian parameter B20 corresponds to the sign of the element [V4⊗V4]20 in the irreducible tensor product [V4⊗V4]2 of rank L = 2.