

EPR of Gd³⁺ in single crystal colquiriite and analysis of the spin Hamiltonian tensors B₄ and B₆

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Abstract

In single crystal colquiriite LiCaAlF₆ doped with Gd³⁺ ions two EPR spectra of the Gd³⁺ ions with the Laue site-symmetry groups C_i and C_{3i} were observed. The spectrum angular dependence for trigonal Gd³⁺ centre was investigated in detail and corresponding spin Hamiltonian parameters were fitted. From analysis of the spin Hamiltonian tensors B₄ and B₆ it was established that Gd³⁺ with the Laue group C_{3i} substitutes at Ca²⁺ site with the excess charge compensation by an ion located along the threefold axis from this site. The transformation formulas for a sixth-rank irreducible Hermitian tensor under coordinate rotation are tabulated in an explicit form. By using the EPR data for Gd³⁺ substituted in a variety of host crystals, the fourth-rank and sixth-rank tensors of Gd³⁺ spin Hamiltonians were tabulated and correlated with structures of the coordination polyhedra at substitution sites. The results suppose a predominance of quadratic crystal field contributions into the spin Hamiltonian tensor B₄ of Gd³⁺. © Springer-Verlag 1997.
