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Quadratic crystal field tensors and spin Hamiltonian tensors of Fe3+ in Li2Ge7O15 above and below the phase transition temperature

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Abstract

Dopant Fe3+ ions in tetrahedral and octahedral positions of Ge4+ in the crystal Li2Ge7O15 were studied using EPR. Fe3+ substitutes for Ge4+ with a local charge compensation. The octahedral site and the tetrahedral sites significantly differ by the value of the invariant sum S(B4) of the B4 tensor of the spin Hamiltonian of Fe3+. The irreducible tensor products {V4⊗V4}4 and {V4⊗V4}2 the V4 tensor of the crystal field calculated using the point-charge model for octahedral and tetrahedral complexes provide the predominant contribution of the crystal field to the B4 and B2 tensors of the spin Hamiltonian of Fe3+, respectively. A comparison of the fourth-rank tensors B4 of the spin Hamiltonian and {V4⊗V4}4 of the crystal field determined at 300 K with those determined at 77 K supports the conclusion that the phase transition is accompanied by combined rotation of the [GeO4] tetrahedra with the [Ge(1)O6] octahedron almost unaltered. The spectrum lines are narrow and the variety of point defects in the vicinity of the paramagnetic impurity ions Fe3+, Cr3+ and Cu2+ is not detected. These facts are inconsistent with the statistically distributed model for the Li(2) atom. In specific cases at 300 K, when the wings of the two spectrum lines of the M→M+1 and the M+2 →M+3 transitions of Fe3+ ions belonging to one system of translationally equivalent positions overlap an extra line appears in the center between these lines. It is suggested that this effect is due to the soft phonon mode above the phase transition temperature. © 1996 Springer.

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