

## **Electron paramagnetic resonance study of Fe<sup>3+</sup> ions at octahedral and tetrahedral mirror symmetry sites in the LiScGeO<sub>4</sub> crystal**

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### **Abstract**

An electron paramagnetic resonance (EPR) study of a synthetic single crystal of LiScGeO<sub>4</sub> doped with Cr ions carried out earlier at the X- and Q-bands at 300 K has indicated additional weak lines. A detailed analysis of these EPR lines, which were tentatively attributed to the Fe<sup>3+</sup> ions at two different mirror symmetry sites, is presented in this paper. The angular dependences in the three crystallographic planes were resolved by fitting the two distinct spectra denoted Fe<sup>3+</sup>(I) and Fe<sup>3+</sup>(II) with a spin Hamiltonian ( $S = 5/2$ ) of monoclinic symmetry. The rank-4 crystal field tensors at tetrahedral and octahedral sites were calculated with the point-charge model to determine the principal axis orientations of their cubic, tetragonal and trigonal components. A comparative analysis of the zero-field splitting tensors and the crystal field ones indicates that Fe<sup>3+</sup>(I) ions substitute for Sc<sup>3+</sup> at octahedral sites and Fe<sup>3+</sup>(II) ions substitute for Ge<sup>4+</sup> at tetrahedral sites with no significant distortion of the coordination polyhedra in the structure of LiScGeO<sub>4</sub>.

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