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Study of the environment of Fe³⁺ in Na₂Cd(SO₄)₂ · 2H₂O by EPR

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Abstract

An EPR experiment on Fe³⁺ in a single crystal of Na₂Cd(SO₄)₂ · 2H₂O was carried out at Q band frequency and nitrogen temperature. The angular dependencies of the spectra were studied in the three crystallographic planes. In order to have a very precise orientation of the crystal, the experiment was done with a twinned crystal (superposition of two spectra in all three planes). The zero-field splitting of Fe³⁺ is of the same order of magnitude as the quantum $h\nu$, so that many $\Delta M=2$ transitions were observed. All spin-Hamiltonian parameters (20) were calculated using observed $\Delta M=1$ and $\Delta M=2$ transitions for 30 different orientations of the magnetic field. The pseudosymmetries of the fourth-order term of the spin Hamiltonian of Fe³⁺ are compared to those we calculated using the superposition model. It is seen that Fe³⁺ is substituted for Cd²⁺ and that the orientation of the octahedral environment of Fe³⁺ does not differ much in orientation from that of Cd²⁺. Differences between the distortions of the Cd-O₆ and Fe-O₆ octahedra are discussed. © 1985 American Institute of Physics.
