

Theoretical Investigations of the EPR Parameters of Ti^{3+} in Beryl Crystal

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The EPR parameters (g factors g_{\parallel} , g_{\perp} and hyperfine structure constants A_{\parallel} , A_{\perp}) of Ti^{3+} ion at the sixfold coordinated Al^{3+} site with trigonal symmetry in beryl crystal are calculated by the third-order perturbation formulas of $3d^1$ ions in a trigonal octahedron. In the calculations, the crystal-field parameters are obtained by the superposition model, and the impurity-induced local lattice relaxation (which is similar to that found for Fe^{3+} in beryl) is considered. The calculated EPR parameters (and also the optical spectra) are in reasonable agreement with the experimental values.

Key words: Electron Paramagnetic Resonance; Crystal- and Ligand-Field Theory;
Local Lattice Distortion; Ti^{3+} ; Beryl.