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.