Studies of EPR Parameters and Local Structure for Cr^{3+} in $NaInS_2$ Crystal

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The EPR parameters (zero-field splitting D and g factors $g_{\|}$, $g_{\perp}$) of Cr^{3+} in a $NaInS_2$ crystal are calculated from high-order perturbation formulas based on the two spin-orbit coupling parameter model for the EPR parameters of $3d^3$ ions in trigonal octahedral sites. In the calculations, both the contribution to EPR parameters from the spin-orbit coupling parameter of the central $3d^3$ ion and that of ligands are considered. From the calculations it is found that, to explain reasonably the EPR parameters, the local structure (in particular the local trigonal distortion angle θ) in the vicinity of the Cr^{3+} impurity is different from the corresponding structure in the host crystal. The change of the local angle θ with temperature is also obtained from the temperature dependence of zero-field splitting. The results are discussed.

Key words: Electron Paramagnetic Resonance; Defect Structure; Crystal- and Ligand-field Theory; Cr^{3+}; $NaInS_2$.