

Investigations of the EPR Parameters and Local Structures for Two Tetragonal Cr^{3+} Centers in NH_4Cl Crystal

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In this paper, the zero-field splittings D and g factors g_{\parallel} , g_{\perp} at room temperature for two tetragonal Cr^{3+} centers in $\text{NH}_4\text{Cl}:\text{Cr}^{3+}$ crystal have been investigated by a two-spin-orbit (S.O)-parameter model, in which both the contribution due to the S.O. coupling of central d^3 ion and that of ligands are considered. From the investigations, the signs of zero-field splitting and the local structures of both centers are obtained. The electron paramagnetic resonance parameters D , g_{\parallel} and g_{\perp} of both centers are also explained.

Key words: Spin-orbit Coupling; Electron Paramagnetic Resonance (EPR); Crystal-field Theory; Cr^{3+} ; NH_4Cl_4 .

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