# Theoretical Investigations of the EPR Parameters for Three Tetragonal Centers in CsCl:$Cr^{3+}$ Crystal

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The electron paramagnetic resonance parameters zero-field splitting $D$ and $g$ factors $g_{\|}$ and $g_{\perp}$ of three tetragonal centers in CsCl: $Cr^{3+}$ crystal at room temperature have been investigated by a two-spin-orbit (S. O.)-coupling parameter model. In this model, the contributions arising from the S. O. coupling of the central $d^3$ ion and the ligands are included. For center III, the very small $D$ of the $[CrCl_6]^{3-}$ cluster may be due to the displacement ($\approx 0.506$ Å) of the two substitutional $Cl^-$ ions along the tetragonal ($C_4$) axis. For the centers I and II, the relatively larger $D$ results from the contribution of two or one water molecules, i. e., corresponding to $[CrCl_{6-n}(H_2O)_n]^{n-3}$ with, $n = 2$ or 1 along the $C_4$ axis, respectively. The reasonableness of the theoretical results is discussed.

*Key words:* Electron Paramagnetic Resonance (EPR); Crystal and Ligand-Field Theory; $Cr^{3+}$; CsCl.