

# Studies of the $g$ Factor for $\text{Cr}^{4+}$ Ion in $\text{Bi}_4\text{Ge}_3\text{O}_{12}$ Crystal from Crystal-field and Charge-transfer Mechanisms

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The complete third-order perturbation formulas of the  $g$  factors  $g_{\parallel}$  and  $g_{\perp}$  for  $3d^2$  ions in tetragonal  $\text{MX}_4$  clusters have been obtained by a cluster approach. In these formulas, in addition to contributions to the  $g$  factors from the crystal-field mechanism in the crystal-field theory, the contributions from the charge-transfer mechanism are included. From these formulas, the  $g$  factors  $g_{\parallel}$  and  $g_{\perp}$  for a  $\text{Cr}^{4+}$  ion in a  $\text{Bi}_4\text{Ge}_3\text{O}_{12}$  crystal are calculated. The results agree with the observed values. The calculated  $\Delta g_i (i = \parallel \text{ or } \perp)$  value due to the charge-transfer is opposite in sign and about 20% greater than that due to the crystal-field mechanism. So, for the  $3d^n$  ions having a high valence in crystals, a reasonable explanation of the  $g$  factors should take both the crystal-field and charge-transfer mechanisms into account.

*Key words:* Electron Paramagnetic Resonance; Crystal- and Ligand- field Theory;  
Charge-Transfer Mechanism;  $\text{Cr}^{4+}$ ,  $\text{Bi}_4\text{Ge}_3\text{O}_{12}$ .