

Theoretical Studies of Electron Paramagnetic Resonance Parameters for Cr⁴⁺ Ions in Ca₂GeO₄ Crystals

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Abstract: The electron paramagnetic resonance (EPR) parameters (zero-field splitting D and g factors $g_{||}$, g_{\perp}) of Cr⁴⁺ ions in Ca₂GeO₄ crystals have been calculated from the complete high-order perturbation formulas of EPR parameters for a 3d² ion in trigonal MX₄ clusters. In these formulas, in addition to the contributions to EPR parameters from the widely used crystal-field (CF) mechanism, the contributions from the charge-transfer (CT) mechanism (which are often neglected) are included. From the calculations, it is found that for the high valence state 3dⁿ ions in crystals, the reasonable explanation of EPR parameters (in particular, the g factors) should take both the CF and CT mechanisms into account.

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Key words: crystal- and ligand-field theory, electron paramagnetic resonance, charge-transfer mechanism, optical spectroscopy, tunable laser crystal

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