Studies of the Spin Hamiltonian Parameters for Cubic V^{2+}, Cr^{3+}, and Mn^{4+} Centers in MgO and CaO, based on Two Mechanism Models

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The high-order perturbation formulas of the spin Hamiltonian (SH) parameters g-shift $\Delta g\,(=g-g_s)$ and the hyperfine structure constant A for a $3d^3$ ion in cubic octahedra are established, based on the two mechanism model. In this model, not only the contributions from the conventional crystal-field (CF) mechanism, but also those from the charge-transfer (CT) mechanism are taken into account. These formulas are applied to the investigation of the SH parameters of cubic V^{2+}, Cr^{3+} and Mn^{4+} centers in MgO and CaO. Based on these studies, the sign of Δg due to the CT mechanism is opposite to that due to the CF mechanism, while the signs of the A factor due to the CF and CT mechanisms are equal. The theoretical results, including the contributions from the CF and CT mechanisms, agree better with the observed values than those containing only the conventional CF mechanism.

Key words: Crystal-fields and Spin Hamiltonians; Electron Paramagnetic Resonance (EPR); V^{2+}; Cr^{3+}; Mn^{4+}.