Theoretical Studies of the EPR Parameters of Nd^{3+} in $LiYF_4$

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The perturbation formulas of the electron paramagnetic resonance (EPR) parameters $g_\parallel$, $g_\perp$, $A_\parallel$ and $A_\perp$ for a $4f^3$(Nd^{3+}) ion in tetragonal symmetry are established in this work. In these formulas, the contributions to the EPR parameters arising from the second-order perturbation terms and the admixtures of different states are included. Then the above formulas are applied to a tetragonal Nd^{3+} center in $LiYF_4$, where the related crystal-field parameters are calculated from the superposition model and the local structural parameters of the Y^{3+} site occupied by the impurity Nd^{3+}. The EPR parameters and the optical spectra within the $^4I_{9/2}$ and $^4I_{11/2}$ states obtained in this work agree reasonably with the observed values.

Key words: EPR; Crystal-fields and Spin Hamiltonian; Nd^{3+}; $LiYF_4$.