Theoretical Investigations of the Electron Paramagnetic Resonance g Factors for the Trivalent Cerium Ion in LiYF$_4$ Crystal

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The perturbation equations of the EPR parameters g$_\parallel$ and g$_\perp$ for the lowest Kramers doublet of a 4f^1 ion in tetragonal symmetry are established. In these equations, the contributions of the covalency effects, the admixture between $J = 7/2$ and $J = 5/2$ states and the second-order perturbation (which is not considered previously) are included. The crystal field parameters for the studied Ce^{3+} center are calculated from the superposition model. Based on the above perturbation equations and related parameters, the EPR g factors for the Ce^{3+} center in LiYF$_4$ crystals are reasonably explained. The results are discussed.

Key words: Crystal Field Theory; Electron Paramagnetic Resonance; Superposition Model; Ce^{3+}; LiYF$_4$.