Studies of the EPR g Factors and Hyperfine Structure Constants for Yb^{3+} Ions in Single Crystals of Zircon-structure Orthophosphates

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The EPR g factors $g_{\parallel}$ and $g_{\perp}$ of Yb^{3+} and the hyperfine structure constants $A_{\parallel}$ and $A_{\perp}$ of $^{171}Yb^{3+}$ and $^{173}Yb^{3+}$ in crystals of the zircon-structure orthophosphates YPO_4, $LuPO_4$, and $ScPO_4$ are calculated from the calculation formulas of the EPR parameters for a $4f^{13}$ ion in tetragonal symmetry. In these formulas, the contributions to the EPR parameters from the J-mixing between the ground $^2F_{7/2}$ and excited $^2F_{5/2}$ states, the admixtures between the lowest Kramers doublet $\Gamma\gamma$ and the other 6 Kramers doublets (or irreducible representations) via the crystal-field and orbital angular momentum (or hyperfine structure) interactions and the covalency reduction effect are included. The calculated values agree with the observed ones. In the calculations, the superposition model is used to estimate the crystal-field parameters. It is found intrinsic parameters $A(R_0)$ that the superposition model with the same R_0 for Yb^{3+} in various zircon-type compounds obtained by considering local lattice relaxation are not scattered as those obtained by using the structural data of pure zircon-type compounds. It appears that, in order to obtain suitable superposition model parameters, the local lattice relaxation should be taken in to account.

Key words: Electron Paramagnetic Resonance; Crystal-field Theory; Superposition Model; Yb^{3+}; YPO_4; $LuPO_4$; $ScPO_4$.