Studies of the Spin Hamiltonian Parameters and the Local Structure of Tetragonal Zr^{3+} Centers in Orthophosphate MPO_4 (M = Sc, Lu, Y) Crystals

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Z. Naturforsch. **61a,** 688 – 690 (2006);
received June 7, 2006

The spin Hamiltonian parameters (g factors $g_{\|}$, $g_{\perp}$ and hyperfine structure constants $A_{\|}$, $A_{\perp}$) of Zr^{3+} on the tetragonal M^{3+} (M = Sc, Lu, Y) sites of zircon-type orthophosphate MPO_4 crystals are calculated by high-order perturbation formulas of d^1 ions in tetragonal symmetry. The crystal-field parameters are estimated by the superposition model and reasonable local structural data of impurity centers. The results show good agreement with the experimental values. It appears that in the case of size mismatch, the explanation of the spin Hamiltonian parameters of a paramagnetic impurity in crystals should take the impurity-induced local lattice relaxation into account.

Key words: EPR; Spin Hamiltonian Parameters; Crystal-Field Theory; Defect Structure; Zr^{3+}; MPO_4 (M = Sc, Lu, Y).