EPR Investigation of the Structure of a Rhombic Co^{2+} Center in an NaF Crystal

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The local structure of the rhombic Co^{2+} center in NaF crystal is investigated by using the perturbation formulas of electron paramagnetic resonance (EPR) **g** factors $g_i\,(i = x,y,z)$ and hyperfine constants A_i for a $3d^7$ (Co^{2+}) ion in rhombic octahedral symmetry based on a cluster approach. In these formulas, the contributions from the admixture among different states, covalency effect as well as rhombic crystal field are included. By studying the EPR data of the rhombic Co^{2+} center, one can reasonably obtain the local structural (or rhombic distortion) parameters $\Delta R_c (\approx 0.268$ Å) for the central Co^{2+} and $\Delta R_p (\approx 0.181$ Å) for the two F^- ions along [100] and [010] axes closest to the Na^+ vacancy V_{Na}. The reasonableness of the results is also discussed.

Key words: Local Geometry; Electron Paramagnetic Resonance (EPR); Crystal- and Ligand Field Theory; NaF; Co^{2+}.