A Study of Spin-Hamiltonian Parameters and Defect Structure for Co^{2+} Ion in the Tetragonal Zn^{2+} Site of Ba_2ZnF_6 Crystal

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Z. Naturforsch. **65a,** 877 – 881 (2010); received May 29, 2009 / revised September 8, 2009

The spin-Hamiltonian (SH) parameters (g factors $g_{\|}$, $g_{\perp}$ and hyperfine structure constants $A_{\|}$, $A_{\perp}$) for the Co^{2+} ion in the tetragonal Zn^{2+} site of a Ba_2ZnF_6 crystal are calculated from the second-order perturbation formulas based on the cluster approach for the SH parameters of $3d^7$ ions in tetragonal symmetry with the effective spin $S = 1/2$. In the calculations, a reduction factor due to the dynamical Jahn-Teller effect is used. The calculated results are in reasonable agreement with the experimental values, suggesting that the dynamical Jahn-Teller effect should be considered here. The defect structure of the Co^{2+} center in Ba_2ZnF_6:Co^{2+} is also obtained from the calculations. The results are discussed.

Key words: Electron Paramagnetic Resonance (EPR); Crystal- and Ligand-Field Theory; Defect Structure; Co^{2+}; Ba_2ZnF_6.