

Theoretical Investigations of the Spin Hamiltonian Parameters and the Local Structure of a Trigonal Co^{2+} Center in $\text{Bi}_4\text{Ge}_3\text{O}_{12}$

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Z. Naturforsch. **59a**, 563 – 567 (2004); received June 14, 2004

The spin Hamiltonian parameters anisotropic g factors g_{\parallel} , g_{\perp} and hyperfine structure constants A_{\parallel} and A_{\perp} , as well as the local structure of the trigonal Co^{2+} center in $\text{Bi}_4\text{Ge}_3\text{O}_{12}$ (BGO) are theoretically investigated by the perturbation formulas of the spin Hamiltonian parameters for a $3d^7$ ion in trigonal symmetry, based on the cluster approach. It is found that the impurity Co^{2+} substituting the host Bi^{3+} undergoes an off-center displacement $\Delta Z (\approx -0.132 \text{ \AA})$ away from the center of the oxygen octahedron along the C_3 axis. The spin Hamiltonian parameters based on the above displacement show reasonable agreement with the observed values. The results are discussed.

Key words: Electron Paramagnetic Resonance (EPR); Crystal-field Theory and Spin Hamiltonians; Defect Structure; Co^{2+} ; $\text{Bi}_4\text{Ge}_3\text{O}_{12}$ (BGO).