A Study of Spin-Hamiltonian Parameters and Defect Structure for Co$^{2+}$ Ion in the Tetragonal Zn$^{2+}$ Site of Ba$_2$ZnF$_6$ Crystal

Bang-Xing Li$^a$, Wen-Chen Zheng$^{a,c}$, and Wei-Qing Yang$^{a,b}$

$^a$ Department of Material Science, Sichuan University, Chengdu 610064, P.R. China
$^b$ Department of Optics and Electronics, Chengdu University of Information Technology, Chengdu 610225, P.R. China
$^c$ International Center for Materials Physics, Chinese Academy of Sciences, Shenyang 110016, P.R. China

Reprint requests to W.-C. Z.; E-mail: zhengwc1@163.com

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

The spin-Hamiltonian (SH) parameters ($g$ factors $g_\parallel$, $g_\perp$ and hyperfine structure constants $A_\parallel$, $A_\perp$) for the Co$^{2+}$ ion in the tetragonal Zn$^{2+}$ site of a Ba$_2$ZnF$_6$ crystal are calculated from the second-order perturbation formulas based on the cluster approach for the SH parameters of 3$d^7$ 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$_2$ZnF$_6$: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$_2$ZnF$_6$. 