A Theoretical Study on the Spin-Hamiltonian Parameters for Samarium(III) Ion in Potassium Yttrium Tungstate Crystal

Wei-Qing Yang\textsuperscript{a,b}, Wen-Chen Zheng\textsuperscript{b}, Ping Su\textsuperscript{b}, and Hong-Gang Liu\textsuperscript{b}

\textsuperscript{a} Department of Optics and Electronics, Chengdu University of Information Technology, Chengdu 610225, P. R. China
\textsuperscript{b} Department of Material Science, Sichuan University, Chengdu 610064, P. R. China

Reprint requests to W.-Q. Y.; E-mail: cdywq@cuit.edu.cn

Z. Naturforsch. \textbf{66a}, 139–142 (2011); received March 5, 2010

The nine spin-Hamiltonian (SH) parameters (g-factors $g_i$ and hyperfine structure constants $A_i$ for $^{147}\text{Sm}^{3+}$ and $^{149}\text{Sm}^{3+}$ isotopes, where $i = x, y, z$) for the Samarium(III) ion in monoclinic potassium yttrium tungstate [$\text{KY(WO}_4)_2$] crystal are calculated within the rhombic symmetry approximation from a diagonalization of energy matrix method. Differing from the conventional diagonalization method used in the calculation of crystal-field levels, in the present method, we attach the Zeeman (or magnetic) and hyperfine interaction terms to the conventional Hamiltonian and construct the $66 \times 66$ energy matrix for $4f^5$ ions in rhombic crystal field and under an external magnetic field by considering all the ground-term multiplets $4H_J$. The calculated results are in reasonable agreement with the experimental values.

\textbf{Key words:} Electron Paramagnetic Resonance (EPR); Crystal Field Theory; Diagonalization Method; $\text{KY(WO}_4)_2$; $\text{Sm}^{3+}$. 