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

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The nine spin-Hamiltonian (SH) parameters (g-factors g_i and hyperfine structure constants $^{147}A_i$ and $^{149}A_i$ for $^{147}Sm^{3+}$ and $^{149}Sm^{3+}$ isotopes, where $i = x, y, z$) for the Samarium(III) ion in monoclinic potassium yttrium tungstate [$KY(WO_4)_2$] 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 66×66 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.

Key words: Electron Paramagnetic Resonance (EPR); Crystal Field Theory; Diagonalization Method; $KY(WO_4)_2$; Sm^{3+}.