Current Topics in Biophysics (Zagadnienia Biofizyki Współczesnej) vol. 33(suppl.A), 2010, 195-198

Spectroscopic properties of Fe^{2+} (S=2) ions at tetragonal sites in K_2FeF_4 and K_2ZnF_4 Czesław Rudowicz, Danuta Piwowarska

Crystal field (CF) effects and energy levels $Fe^{2^+}(3d^6)$ ions in K_2FeF_4 with the ground state multiplet 5D split due to a tetragonal crystal field are considered. Microscopic spin Hamiltonian parameters, i.e. the zero field splitting (ZFS) and Zeeman electronic ones, within the orbital singlet ground state $^5B_{2g}$ with the spin S=2 are modeled for various ranges of the microscopic parameters, i.e. the spin-orbit coupling constant λ , the spin-spin coupling constant ρ , the CF energy level splittings Δ_i , and the mixing coefficient q, suitable for Fe^{2^+} (S=2) ions in K_2FeF_4 and K_2ZnF_4 . The results are compared with the available experimental data.