Explanation of the *g*-factors and Hyperfine Structure Constants of Co^{2+} in Tetragonal K_2ZnF_4

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Z. Naturforsch. **55a,** 539–544 (2000); received January 19, 2000

The formulas of the *g*-factors $g_{\|}$, $g_{\perp}$ and the hyperfine structure constants $A_{\|}$, $A_{\perp}$ for $3d^7$ ions in tetragonal octahedral crystals are established from a cluster approach. Differing from previous formulas, in these formulas the role of configuration interaction (CI)- and covalency (CO)-effects is considered, and the parameters related to both effects are obtained from the optical spectra and the structural parameters of the studied crystal. From these formulas, the EPR parameters g_i and A_i for K_2ZnF_4:Co^{2+} are calculated. The results show good agreement with the observed values. The contributions to the EPR parameters g_i and A_i from the CI and CO effects, and the relationship between the sign of Δg ($= g_{\perp} - g_{\|}$) and the tetragonal distortion (elongated or compressed) of the ligand octahedron are discussed.