Studies on the EPR Parameters for the Rhombic Co^{2+} Center in Magnesium Acetate

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The electron paramagnetic resonance (EPR) g factors g_i ($i = x,y,z$) and the hyperfine structure constants A_i for the rhombic Co^{2+} center in magnesium acetate are theoretically studied from the perturbation formulas of these parameters for a $3d^7$ ion under rhombic symmetry. In these formulas, the contributions from the admixture among different states, covalency effect and rhombic crystal-fields are taken into account. The related crystal-field parameters are determined from the superposition model and the local geometrical relationship of the impurity center. The calculated results show reasonable agreement with the observed values. In addition, the nuclear quadrupole interaction constant Q is analyzed, and its negative sign is verified theoretically.

Key words: Electron Paramagnetic Resonance (EPR); Crystal- and Ligand-fields; Co^{2+}; Magnesium Acetate.