On the EPR Parameters of Divalent Cobalt in ZnX (X = S, Se, Te) and CdTe

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The electron paramagnetic resonance (EPR) parameters g and the hyperfine structure constants A of Co^{2+} in ZnX (X = S, Se, Te) and CdTe are studied, using the perturbation formulas of the EPR parameters for a $3d^7$ ion in tetrahedra based on two mechanism models. In these formulas, both the contributions from the conventional crystal-field (CF) mechanism and those from the charge-transfer (CT) mechanism are taken into account. According to the investigations, the sign of the g-shift Δg_{CT} from the CT mechanism is the same as Δg_{CF} from the CF mechanism, whereas the contributions to the A value from the CF and CT mechanisms have opposite signs. Particularly, the contributions to the EPR parameters from the CT mechanism increase rapidly with increase of the spin-orbit coupling coefficient of the ligand and the covalency effect of the systems, i. e. $S^{2-} < Se^{2-} < Te^{2-}$.

Key words: Crystal-fields and Spin Hamiltonians; EPR; Co^{2+}; ZnX (X = S, Se, Te); CdTe.