Studies of the EPR g-Shift of $[Cr(CN)_6]^{3-}$ Clusters due to Crystal-Field and Charge-Transfer Mechanisms

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The EPR g-shift Δg ($\approx g - g_e$) of the metal-cyanide cluster $[Cr(CN)_6]^{3-}$ is calculated by high-order perturbation formulas based on both the crystal-field (CF) and charge-transfer (CT) mechanisms (the latter is often neglected in the crystal-field theory). The result agrees with the experimental value. The sign of the g-shift Δg_{CT} due to the contribution of the CT mechanism is opposite to that of Δg_{CF} due to the contribution of the CF mechanism, and the absolute value of Δg_{CT} is about 34% of that of Δg_{CF}. It appears that for transition metal ions in a strong covalent cluster, a reasonable theoretical explanation of the g-shift should take both the CF and CT mechanism into account.

Key words: Electron Paramagnetic Resonance; Crystal- and Ligand-Field Theory; Charge-Transfer Mechanism; Cr^{3+}; $[Cr(CN)_6]^{3-}$.