Investigations on the EPR Parameters for the Square Planar Cu$^{2+}$ Centers in $K_2PdX_4$ (X = Cl, Br)

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The EPR parameters g factors $g_{\parallel}$, $g_{\perp}$ and the hyperfine structure constants $A_{\parallel}$ and $A_{\perp}$ for the square planar Cu$^{2+}$ centers in $K_2PdX_4$ (X = Cl, Br) are theoretically investigated from the perturbation formulas of these parameters for a 3$d^9$ ion under tetragonally elongated octahedra. In these formulas, not only the contributions from the conventional crystal-field (CF) mechanism, but also those from the charge-transfer (CT) mechanism are taken into account. The related molecular orbital coefficients are uniformly determined from the cluster approach, and the tetragonal field parameters $D_s$ and $D_t$ are obtained from the superposition model and the local structures of the systems. Based on only one adjustable parameter, the present results are in reasonable agreement with the observed values. Importance of the charge-transfer contributions is more significant for ligand Br than that for Cl due to the stronger covalency and much larger spin-orbit coupling coefficient of the former.

Key words: Crystal- and ligand fields; Electron paramagnetic resonance (EPR); Cu$^{2+}$; $K_2PdX_4$ (X = Cl, Br).