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

Chuan-Ji Fu[a], Shao-Yi Wu[a,b], Yue-Xia Hu[a], Xue-Feng Wang[a], and Wang-He Wei[a]

[a] Department of Applied Physics, University of Electronic Science and Technology of China, Chengdu 610054, P. R. China
[b] International Centre for Materials Physics, Chinese Academy of Sciences, Shenyang 110016, P. R. China

Reprint requests to S.-Y. W.; E-mail: shaoyi_wu@163.com

Z. Naturforsch. **64a,** 387 – 392 (2009); received May 5, 2008 / September 25, 2008

The EPR parameters g factors $g_{\|}$, $g_{\perp}$ and the hyperfine structure constants $A_{\|}$ 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 $3d^9$ 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 Ds and Dt 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).