

Theoretical Investigation of the g Factors for Copper (II) Ion in an Orthorhombic Crystal and its Application to $(\text{CuCl}_4)^{2-}$ Cluster

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On the basis of the crystal- and ligand-field theory, the high-order perturbation formulas of the g factors (g_x , g_y , g_z) are established for Cu^{2+} ions in an orthorhombic tetrahedral field with D_2 symmetry, including the central cationic and ligand anionic spin-orbital coupling interactions. By using these formulas, the anisotropic g factors of Cu^{2+} ion in $(\text{CuCl}_4)^{2-}$ cluster are calculated. The results are consistent with the experimental values. The calculations show that the contribution from covalency of the central ion and the 3p orbital ligand can not be neglected.

Key words: Crystal- and Ligand-Field; Electron Paramagnetic Resonance; Spin Hamiltonian;
 $(\text{CuCl}_4)^{2-}$ Cluster.