

Interpretation of ESR Spectra of Copper(II) Complexes

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The ESR spectra of Cu(II) complexes, $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$, $\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$, and $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$ were collected at room temperature employing x-band ESR spectrometer with 100kHz field modulation. The coordination numbers of the three Cu(II) complexes are 6, and regular geometries are known tetragonally distorted octahedral coordination. The reason for this is ascribed to the Jahn-Teller effect arising from the unequal occupation of the e_g pair of orbitals (d_{z^2} and $d_{x^2-y^2}$), when a d^9 ion is subjected to an octahedral crystal field. From the angular variation of the position of single resonance observed in the three Cu(II) compounds, we evaluated the g tensors. The direction of the Jahn-Teller distortion, compression of octahedron and elongation of octahedron, has been determined from g tensors. Interpretation of the g tensors resulted in $d_{x^2-y^2}$ orbital ground state for the three Cu(II) complexes. The effects of different ligands bonded Cu(II) on the degree of electron transition energy, ΔE_{xy} , ΔE_{xz} , and ΔE_{yz} , have been also discussed.