Cu Kβ X-ray Emission Spectroscopy as a Probe of Coordination Environments of Cu(I) Sites

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Cu(I) sites are considered to be spectroscopically silent because they have d^{10} closed subshell configuration and do not show spectroscopic signatures in many conventional spectroscopic methods. Kβ X-ray emission spectroscopy (XES) probes transitions from the occupied states to the 1s core hole and thus is particularly useful for Cu(I) sites. The Kβ XES spectra of Cu(I) model complexes have been investigated to establish background theory and to identify analytically useful features. The density functional theory calculations which well reproduced the experimental spectra allowed for quantitative analysis. These results play an important role in analyzing Kβ XES applied to Cu(I) active sites in Cu enzymes.