

Photo Excited State Crystallography of Iodo-bridged Dicopper (I) Complex

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Luminescent dicopper(I) complex $[\text{Cu}_2\text{I}_2(\text{PPh}_3)_2(4,4'\text{-bpy})]_\infty$ (bpy=C₁₀H₈N₂) consists of {Cu₂I₂} planer units, which are bridged by diimine ligands constructing infinite chain structure. The assignments of intense emission bands of these oligo-copper compounds are complicate because weak interacted multi-copper centered (CC) charge transfer is often concurrent with common Cu(I) to ligand charge transfer. We have tried to observe direct geometrical distortion of the complex by photo excited state crystallographic technique in order to figure out this emission nature.

Single crystal X-ray diffraction experiments were performed by using the low-temperature vacuum X-ray camera at SPring-8 BL02B1 beamline. Full intensity data of both under light irradiated and non-irradiated conditions were collected by multiple-exposure method by using IP detector. Photo-difference Fourier syntheses show that a small portion of two I atoms in {Cu₂I₂} unit move toward close to each other, while two Cu atoms tend to move apart from each other toward N atom of the bipyridine ligand.

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