

PHOTOEXCITED STATE MOLECULAR STRUCTURES IN SOLUTION STUDIED BY PUMP-PROBE XAFS

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Knowing transient molecular structures during photochemical reactions is important for understanding fundamental aspects of solar energy conversion and storage. Fast x-ray techniques provide direct probes for these transient structures. Using x-ray pulses from the Advanced Photon Source at Argonne, the laser pulse pump, x-ray pulse probe XAFS (LPXP-XAFS) technique has been developed to capture transient molecular structures in disordered media with nanosecond time resolution. We have carried out pump-probe XAFS measurements on the MLCT state structure of Bis(2,9-dimethyl-1,10-phenanthroline) Copper(I) $[\text{Cu(I)(dmp)}_2]^+$ in toluene. The transient MLCT structure determined by x-ray absorption confirmed a whole charge transfer from the copper center to the ligand and the Cu coordination geometry change from tetrahedral to trigonal bipyramidal. The transient structural information combined with the kinetics data from transient optical absorption and emission spectroscopy established a new four-level energy diagram for the photophysics of $[\text{Cu(I)(dmp)}_2]^+$.

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