

**MS40-O4** Direct observation of the excited state structure of a Ag(I)-Cu(I) complexRadosław Kamiński<sup>1,2</sup>, Katarzyna N. Jarzemska<sup>1,2</sup>, Bertrand Fournier<sup>2</sup>, Elżbieta Trzop<sup>2</sup>, Jesse D. Sokolow<sup>2</sup>, Yang Chen<sup>2</sup>, Robert Henning<sup>3</sup>, Philip Coppens<sup>2</sup>

1. Czocharalski Laboratory of Advanced Crystal Engineering, Biological and Chemical Research Centre, Department of Chemistry, University of Warsaw, Żwirki i Wigury 101, 02-089 Warsaw, Poland
2. Department of Chemistry, University at Buffalo, The State University of New York, Buffalo, NY 14260-3000, USA
3. The Consortium for Advanced Radiation Sources, University of Chicago, Chicago, IL 60637, USA

email: rkaminski@chem.uw.edu.pl

Heterodentate coordination complexes have been extensively studied because of their rich electronic and luminescent properties, which are of importance in the design of molecular devices. The short metal-metal contacts found in such complexes determine the nature of the lowest lying emissive states, and must be explored in order to understand their physical properties. Recent advances in time-resolved (TR) synchrotron techniques supported by specific data collection strategies and data processing procedures<sup>1</sup> allow for elucidation of molecular excited state geometries in the solid state. The approach has been so far successfully applied to several high-quality Laue-data sets collected at the 14-ID BioCars beamline at the Advanced Photon Source.<sup>2</sup>

In this contribution we present synchrotron TR experiment results obtained for a new solvent-free crystal form of a model complex containing Ag(I) and Cu(I) ( $\text{Ag}_2\text{Cu}_2\text{L}_4$ , L = 2-diphenylphosphino-3-methylindole ligand).<sup>3</sup> This system exhibits red solid-state luminescence with a lifetime of about 1  $\mu\text{s}$ . This is one of the shortest-lived excited states we have studied so far with the Laue technique. The relatively short lifetime goes along with significant structural changes observed upon irradiation, such as, the Ag...Ag distance shortening of about 0.26 Å for the excited state. The results clearly show strengthening of the Ag...Ag interactions suggesting a bond formation upon excitation.<sup>4</sup> The photocrystallographic findings are supported by spectroscopic measurements and quantum computations. The results confirm the triplet nature of the emissive state originating mainly from a ligand-to-metal charge transfer.

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**MS40-O5** Investigation of ultrafast dynamics of a molecular diode (PyDMA) using time-resolved Laue diffractionSreevidya Thekku Veedu<sup>1,2</sup>, Simone Techert<sup>1,2</sup>

1. Deutsches Elektronen Synchrotron (DESY), Hasylab, Notkestr. 85, Hamburg, Germany.
2. Max-Planck Institute for Biophysical Chemistry, Am Fassberg 11, Göttingen, Germany.

email: sreevidya.thekku.veedu@desy.de

Inspired by the electron transfer (ET) reactions as fundamental processes in chemistry and also in biology, we focussed on a promising model ie, donor-acceptor (D-A) systems which are synthetic molecules to understand the mechanism of photo induced electron transfer process. Light harvesting complexes are functional centers in plants where sunlight is converted into chemical energy. However, due to the complexity of the biological photo-reaction center, research has been focused on a smaller chemical model which share characteristic with their biological counter parts. Pyrene-N,N-dimethylaniline (PyDMA), a compound in which the electron donor N,N-dimethylaniline is covalently linked to the electron acceptor pyrene. Due to the small distance between the donor and the acceptor in PyDMA, a strong electronic interaction exists which manifests itself through femtosecond electron transfer processes. Knowledge of the geometry or mechanism of molecular excited states at atomic resolution is crucial for a full understanding of photo-induced chemical processes. Time-resolved X-ray diffraction (TR-XRD) using polychromatic synchrotron radiation allows a detailed study of the time evolution of structural intermediates and short living states of chemical systems at wide range of time-scales, drawing a complete picture of the photo-induced charge transfer process. Investigation of photo-excitation processes in molecular single crystals, where the initial photo-excitation processes occur on extremely short time-scales (femto-/picosecond time domain) have been in the focus of scientific investigations due to their possible applications, e.g. as optical switches. We investigated photo-induced structural changes of our system at 100 ps temporal resolution and will be discussed.

**Keywords:** Photo-induced electron transfer, PyDMA, Laue diffraction