Poster Presentation

MS50.P07

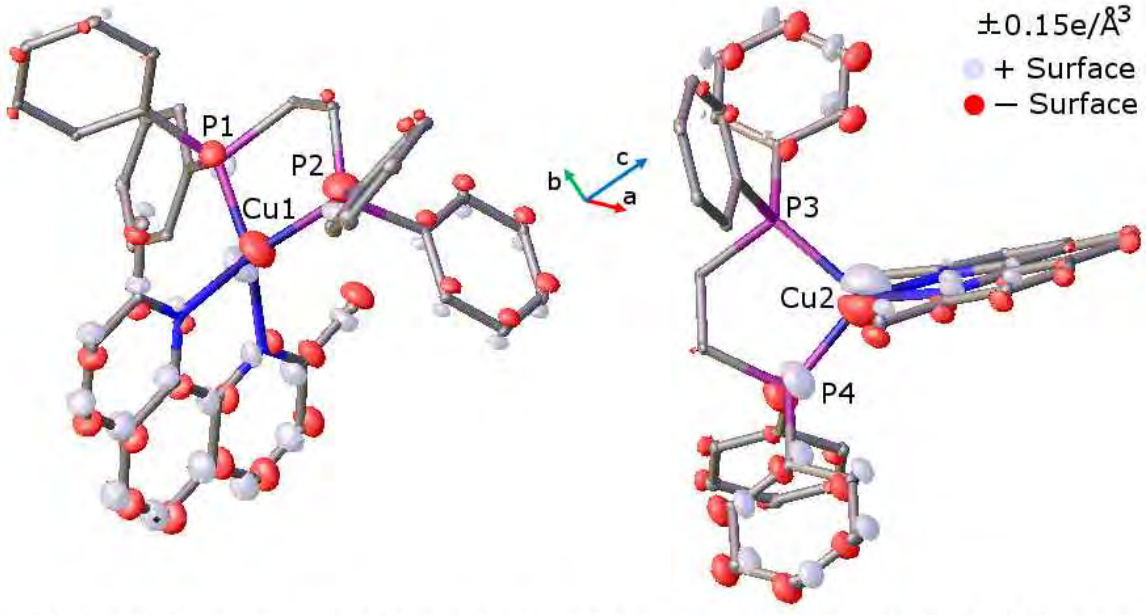
Selective time-dependent changes of Cu(DPPE)(DMP)·PF_6 on photoexcitation

E. Trzop[1], B. Fournier[1], K. Jarzembska[1,2], J. Sokolow[1], R. Kaminski[1], J. Benedict[1], Y. Chen[1], R. Henning[3], P. Coppens[1]

[1]University at Buffalo, Department of Chemsitry, Buffalo, USA, [2]University of Warsaw, Department of Chemsitry, Warsaw, Poland, [3]University of Chicago, The Consortium for Advanced Radiation Sources, Chicago, USA

Thanks to their potential applications as light-emitting devices, chemical sensors and dye-sensitized solar cells, heteroleptic copper (I) complexes have been extensively studied. Cu(DPPE)(DMP)·PF_6 (dppe= 1,2-bis(diphenylphosphino)ethane; dmp = 2,9-dimethyl-1,10-phenanthroline) crystallizes in the monoclinic system, $P2_1/c$, with two independent molecules in the asymmetric unit. Previous studies on this system [1,2] show strong temperature-dependent emission. The complex was studied at 90K under 355nm laser excitation. At this temperature, the luminescence decay for Cu(DPPE)(DMP)·PF_6 is biexponential with lifetimes of ~3µs and ~28µs. Two time-resolved X-ray diffraction techniques were applied for studies: (1) a Laue technique at BioCARS ID-14 beamline at the Advanced Photon Source, and (2) monochromatic diffraction at a newly constructed in-house pump-probe monochromatic facility at the University at Buffalo. Structural changes determined with the two methods are in qualitative agreement; discrepancies in position of the Cu and P atoms were observed. The molecular distortions were smaller than those determined at 16K in the earlier synchrotron study by Vorontsov et al. [2]. Photodeformation maps (see Figure below), in which the increase in temperature on photoexcitation has been eliminated, clearly illustrate the photoinduced atomic shifts for both data sets. Results will be compared with those obtained for other studied heteroleptic copper (I) complexes, for instance Cu[(1,10-phenanthroline-N,N') bis(triphenylphosphine)]·BF_4 [3]. The in-house pump-probe facility is discussed by Radoslaw Kaminski at this meeting. Research funded by the National Science Foundation (CHE1213223). BioCARS Sector 14 at APS is supported by NIH (RR007707). The Advanced Photon Source is funded by the Office of Basic Energy Sciences, U.S. Department of Energy, (W-31-109-ENG-38). KNJ is supported by the Polish Ministry of Science and Higher Education through the "Mobility Plus" program.

[1] *P. Coppens, I. I. Vorontsov, T. Graber, et al., J. Am. Chem. Soc. 2004, 126, 5980-5981,* ***[2]*** *I. Vorontsov, T. Graber, A. Kovalevsky, et al., J. Am. Chem. Soc. 2009, 131, 6566-6573,* ***[3]*** *A. Makal, J. B. Benedict, E. Trzop, et al., J. Phys. Chem. 2012, 116 (13), 3359-3365*



Photodeformation Map for In-House Pump-Probe 90K Data

Keywords: pump-probe techniques, heteroleptic copper (I) complex, luminescence