Poster Presentation

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First steps towards time-resolved 'in-house' X-ray diffraction experiments

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High-intensity X-ray sources, such as synchrotrons or X-ray free electron lasers, providing up to 100 ps time-resolution allow for studying very short-lived excited electronic states in molecular crystals. Some recent examples constitute investigations of Rh…Rh bond shortening,[1] or metal-to-ligand charge transfer processes in CuI complexes.[2] Nevertheless, in cases in which the lifetime of excited state species exceeds 10 μs it is now possible, due to the dramatic increase in the brightness of X-ray sources and the sensitivity of detectors, to use laboratory equipment to explore structural changes upon excitation. Consequently, in this contribution we present detailed technical description of the 'in-house' X-ray diffraction setup allowing for the laser-pump X-ray-probe experiments within the time-resolution at the order of 10 μs or larger. The experimental setup consists of a modified Bruker Mo-rotating-anode diffractometer, coupled with the high-frequency Nd:YAG laser (λ = 355 nm). The required synchronization of the laser pulses and the X-ray beam is realized via the optical chopper mounted across the beam-path. Chopper and laser capabilities enable high-repetition-rate experiments reaching up to 100 kHz. In addition, the laser shutter is being directly controlled though the original diffractometer software, allowing for collection of the data in a similar manner as done at the synchrotron (alternating light-ON & light-OFF frames). The laser beam itself is split into two allowing for improved uniform light delivery onto the crystal specimen. The designed setup was tested on the chosen set of crystals exhibiting rather long-lived excited state, such as, the Cu2Br2L2 (L = C5H4N-NMe2) complex, for which the determined lifetime is about 100 μs at 90 K. The results shall be presented. Research is funded by the National Science Foundation (CHE1213223). KNJ is supported by the Polish Ministry of Science and Higher Education through the "Mobility Plus" program.

[1] *J. B. Benedict, A. Makal, J. D. Sokolow et al., Chem. Commun., 2011, 47, 1704-1706,* ***[2]*** *A. Makal, J. B. Benedict, E. Trzop et al., J. Phys. Chem., 2012, 116, 3359-3365*

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