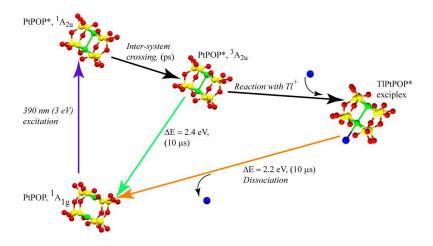
Structural Tracking of Chemical Reactions in Solution by Time-Resolved X-Ray Scattering

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Every photochemical reaction starts with an electronically excited state and ends with a ground state molecule. The pathway taken of the atomic nuclei, while molecules are partaking in such reactions, and hence their intermediary molecular structures, is a fundamental question in chemistry, and a host of systems have been studied by laser spectroscopy down to the femtosecond time scale. However, while spectroscopic methods provide information on energy levels, direct structural information is in general not available. In the last few years, this gap of information has been bridged by X-ray scattering experiments on time scales down to picoseconds. Initially this has been made for crystalline systems with their inherent amplification of the scattered intensity and recently also for liquid systems, the natural environment for most chemical reactions. We present results, based on which we have successfully determined key structural parameters directly for the highly reactive excited state of the square-planar platinum compound PtPOP (Pt2(P2O4H2)4(4–)) in aqueous solution [1]. Furthermore we were able to obtain the first direct structural fingerprint of a bimolecular reaction between the excited state PtPOP and Tl⁺ ions in solution [2].



- [1] Morten Christensen, Kristoffer Haldrup, Klaus Bechgaard, Robert Feidenhans'l, Qingyu Kong, Marco Cammarata, Manuela Lo Russo, Michael Wulff, Niels Harrit, and Martin Meedom Nielsen, Time-resolved X-ray scattering of an electronically excited state in solution. Structure of the 3A2u state of tetrakis-µ-pyrophosphito-diplatinate(II), J. Am. Chem. Soc., 131, 502-508, (2009).
- [2] Kristoffer Haldrup, Morten Christensen, Marco Cammarata, Qingyu Kong, Michael Wulff, Simon O. Mariager, Klaus Bechgaard, Robert Feidenhans'l, Niels Harrit, Martin M. Nielsen, Structural Tracking of a Bimolecular Reaction in Solution by Time-Resolved X-ray Scattering, Angew. Chem. Int. Edit., **48**, 4180-4184 (2009)