MS47-04 **Radiation damage in haem and flavoproteins studied by *in-situ* single-crystal spectroscopy.** Hans-Petter Hersleth,[a] Åsmund K. Røhr,[a] Wouter van Beek,[b] Guillaume Pompidor,[c] K. Kristoffer Andersson,[a] *[a]Departament of Molecular Biosciences, University of Oslo, Norway, [b]Swiss–Norwegian Beamlines at ESRF, France, [c]Swiss Light Source, Paul Scherrer Institute, Switzerland*
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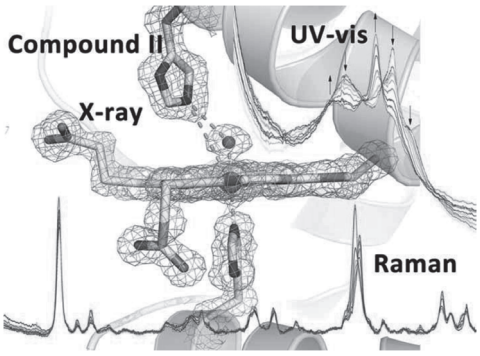
To be able to correctly interpret the crystal structure of redox- and metalloproteins caution must be employed. The influence of X-ray radiation damage to protein crystals is well known to occur even at cryogenic temperatures, and redox active sites like metal sites seem especially vulnerable for radiation-induced reduction [1,2,3]. We have used *in-situ* (online) UV-vis and Raman spectroscopy to study how different haem and flavoproteins are influenced by X-rays during crystallographic data collection [1,2]. The spectroscopic changes have been monitored as a function of X-ray exposure (dose absorbed), Our studies show that these redox states are very fast reduced by X-rays resulting in very short lifedoses. Structurally we have observed for haem proteins a lengthening of the Fe-O bond, and for flavoproteins a bending of the flavin ring during X-ray induced radiation damage, in agreement with DFT [1,2,3]. We have recently started to investigate if varying the doserates and wavelengths can increase the lifedoses. In general our studies show the need for combining protein crystallography with *in-situ* single-crystal spectroscopy when redox and metalloproteins are studied.



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MS47-05 **The Role of Hydrogen Abstraction in X-ray Radiation Damage.** Desiree Heintz,[a] Anja Burkhardt,[a] Resmi Raghunandan,[a] Matthias Gutmann,[b] Armin Wagner,[c] Edgar Weckert,[a] Alke Meents,[a] *[a]DESY, Germany, [b]ISIS Neutron Source, United Kingdom, [c]Diamond Light Source, United Kingdom,*
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X-ray radiation damage to biological samples is a major limitation in X-ray data collection, especially at highly brilliant 3rd generation synchrotron sources. In combination with highly advanced X-ray optics it has become possible to focus a large number of monochromatic photons into spots of a few microns. Such enormous flux densities allow structure determinations from large molecular complexes. The ultimately achievable resolution, however, is still limited by radiation damage as it alters the structure of the sample under investigation and ultimately destroys it.[1]

In order to mitigate X-ray radiation damage, the samples are conventionally cooled to 100 K.[2] However, recent studies have shown that this temperature might not always be ideal. [3] Radiation damage is still a major problem, especially in case of biological samples. Further mitigation or even prevention of radiation damage can only be achieved if the underlying mechanisms are understood. Recent results show that the abstraction of hydrogen from the molecules under investigation might play an important role in the damage process.[4] In a combined X-ray and neutron diffraction study, the influence of site-specific X-ray induced hydrogen abstraction on the global damage process in crystals has been investigated. Neutron diffraction experiments on previously X-ray irradiated crystals of the amino acid L-alanine and the nucleoside thymidine revealed that hydrogen abstraction is a main contributor to the global damage process. It could be shown that certain sites of a molecule are especially susceptible to site-specific hydrogen abstraction. Compounds possessing this site will be more susceptible to global radiation damage than compounds lacking it. Based on these experiments a model was proposed to describe the global damage process.

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