3rd Workshop on the Simultaneous Combination of Spectroscopies with X-ray Absorption, Scattering and Diffraction Techniques



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Using in situ single-crystal UV-vis and Raman spectroscopy to study the effect of X-ray radiation damage on the crystal structures of haem proteins

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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 of combining protein crystallography with in situ single-crystal spectroscopy when redox and metalloproteins are studied.

[1] H.-P. Hersleth, K.K. Andersson, Biochim. Biophys. Acta 2011: 1814, 785

- [2] Å.K. Røhr, et al., Angew. Chem. Int. Ed. 2010, 49, 2324
- [3] H.-P. Hersleth et al. Chem. Biodiv. 2008, 5, 2067

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