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Design considerations of UV-visible Microspectroscopy at single crystal neutron diffractometers

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Single crystal neutron diffraction experiments on protein crystals often require beamtimes of several days in order to measure a complete data set which leads to meaningful results on atom positions and occupancies. In case of room temperature measurements, the sample under investigation might change during that time. If one wants to study a radical intermediate state of the protein, often linked to a distinct UV-visible absorption of the crystal, one is often interested in the decay of the number of radicals in the crystal. Below a certain number, one would rather switch to another freshly prepared crystal. This would save precious neutron beamtime.
At synchrotron beamlines, UV-Visible microspectroscopy of the crystals mounted on the goniometer is readily available. The purpose of this set-up is to measure the UV-visible spectrum on an oriented crystal on the beamline without the need to take it off the beamline goniometer. This has the advantage that the crystal orientation relative to the light beam and polarization is known. Furthermore, a crystal unmounting step can be avoided for just measuring its UV-visible spectrum.
At neutron instruments, such microspectroscopy set-ups are usually not found. But this set-up could also be used to detect whether a ligand is present in a crystal, when the ligand has some optical absorption fingerprint. In this contribution I will discuss some design considerations of such a set-up.

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