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D19: a neutron diffractometer for small proteins and chemical crystallography

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D19 is a monochromatic thermal neutron diffractometer for single crystal and fibre diffraction. With a wavelength selection of 0.8-2.4Å, and a large position sensitive detector, it is versatile and provides large solid angle coverage. D19 is optimized for the study of large chemical systems, small proteins and fibrous polymers but is also very efficient for texture analysis and accurate structures of smaller molecules.

In the recent past, D19 has produced remarkable results from a number of protein and chemical systems, yielding high impact publications. These studies have fully exploited the high flux of the instrument and the large solid angle of the detector. D19 has allowed the highest resolution protein structure ever determined with good completeness. This access to ultra-high resolution helped uncovering a world of structural detail below that visible by X-ray protein crystallography, with highly structured water, hydronium and Zundel ion networks that are likely to be of major importance in protein charge transfer processes [1]. The D19 diffractometer is unmatched for this scale of structural biology, and the availability of perdeuterated protein from the Life Sciences group offers highly optimized sample production. The use of D19, in combination with a crystal of perdeuterated protein has allowed the first practical use of macromolecular phasing by neutron diffraction to be demontrated [3]. Neutron anomalous dispersion was used to determine experimental phases of a protein crystal structure using standard crystallographic softwares. These results are likely to be of interest for use at existing and emerging spallation neutron sources where time-of-flight instruments provide inherent energy discrimination.

Here we will present the instrument as well as highlight some recent examples where data collected on D19 has brought unique insight to the structure. Ongoing instrument and software developments are likely to further broaden the scope of the instrument and allow larger systems to be studied.

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