

s8b.m1.p1 **Protons in Proteins - New insights from neutron diffraction.** D.A.A. Myles¹ & P.A. Timmins²
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Keywords: enzyme, neutrons, hydrogen.

Neutron protein crystallography offers unique advantages for molecular structural biology by enabling key and individual hydrogen atoms to be located in biological structures that cannot be seen by X-ray analysis alone. In the past, the relatively low flux of neutron beams has restricted such application to only a few projects of specific technical interest. Recently, decisive technical progress has allowed a new generation of advanced 2-D protein neutron diffractometers to be built. In Europe, the LADI Laue diffractometer provides the first dedicated facility for neutron protein crystallography at high-resolution. This instrument makes feasible studies of larger biological complexes and smaller crystals than previously thought possible. LADI is optimized for data collection to $>1.5\text{\AA}$ resolution from medium size proteins ($\sim 30\text{kDa}$), sufficient to locate individual hydrogen atoms of special interest, water structures or other small molecules that can be marked with deuterium to be particularly visible. Current studies aim to address specific questions concerning enzymatic mechanism, solvent effects, structure dynamics and their implications. The location of key catalytic hydrogen positions at enzyme active sites now provides a major theme. Details of these and other recent highlight studies will be presented.

s8b.m1.p2 **Data Collection and Phasing on One Data Set.** B. Schierbeek and F. van Meurs. *Nonius BV, Application Laboratory, Röntgenweg 1, 2624 BD Delft, The Netherlands.*

Keywords: anomalous scattering, CCD detectors, Kappa goniostat.

With the advent of new developments in sources and optics, the amount of photons coming from home laboratory sources is now approaching that of early version synchrotrons. The exposure times that can now be achieved are in the order of tens of seconds. So there is a clear need for CCD detector systems, that can do a quick survey of crystal quality or cooling conditions but at the same time can collect high quality data, at an affordable price.

Since the requirements for amount of disk space and memory is also getting less and less of a problem, researchers have investigated the effect of very high redundancy on data quality. The results show that collecting highly redundant data made it possible observe the weak effects of light atoms with a small anomalous scattering contribution, previously intractable in Patterson maps.

A high precision 4-circle Kappa goniostat allows obtaining data sets at different orientations of the sample, rather than collecting identical data in an identical manner. With this goniostat it is possible to scan the crystal with any axis along the rotation axis, to measure Friedel equivalents in the same image. Alternatively, it allows the collection of Friedel pairs at exactly the same position on the detector, by measuring at $\text{Chi} = 90^\circ$ and $\text{Chi} = -90^\circ$ and thus minimize systematic errors in the data set. This ability to produce accurate highly redundant data sets routinely in a day now provides the molecular biologist with a unique analytical tool, which can help to solve protein structures within a week, solely based on the results of one data set!