16. X–8 X-ray diffractometers with a multiwire proportional chamber for multiwavelength anomalous data collection.

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Two diffractometers, PENELOPE I & II, have been built at the Synchrotron Radiation Laboratory LURE in order to make optimised anomalous diffraction experiments in macromolecular crystallography; both systems use a spherical drift multiwire proportional chamber (MWPC) designed by the team of G. Charpak at CERN, Geneva.

PENELOPE I included a monolithic channel-cut monochromator, a fixed detector and a CAMAC-based data acquisition system under computer control. 2.4 Å data at three wavelengths close to the L_{III} edge of Tb have been collected in 27 hours for a crystal of Tb-parvalbumin from Opsanus Tau (in collaboration with O. Dideberg, J.P. Wery & P. Charlier, Université de Liège, Belgium). A single Tb site was located; then, for each reflexion, measurements were combined by pairs to give probability distributions; these were multiplied together to give the best estimate of the protein phase. The analysis of the electron density map is made in collaboration with J. L. Risler, CGM, CNRS, Gif sur Yvette & J. Janin,(c).

PENELOPE II is an upgraded version of the first instrument. The monochromator has two crystals and a fixed exit slit (a collaboration with M. Sauvage & J. Frouin, Minéralogie et Cristallographie, Université Paris VI, Paris). A 6-axis goniometer was built by Huber. The area detector, mounted on the horizontal arm of the goniometer, is a state-of-the art MWPC; the spherical entrance window is made of Be instead of Al, which improves the efficiency at long wavelengths (up to 2.5Å); the thickness of the conversion gap has been raised from 100 to 144 mm, so as to increase the efficiency at short wavelengths (down to 1 Å). The useful sensitive area has a diameter of 480 mm, at 600 mm from the crystal. The pixel size is 1x1 mm^2. The dead time of the digital position encoder is 150 ns. From preliminary tests with an X-ray tube, we expect that reflexions from crystals with cell edges of up to about 120xλ(Å) will not overlap.

16. X–9 The first six months of data-collection with the ENRAF-NONIUS FAST diffractometer.

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By the time the Congress is held, the FAST system will have been available to users for about six months. It is hoped that preliminary details about data collected both from crystals of known structure and from a new crystal of unknown structure will be announced. The performance of the instrument during normal data-collection will be discussed, placing special emphasis on its handling of technically difficult problems such as measuring very weakly diffracting specimens and making full use of the intensity of synchrotron beams.

In addition a brief resumé will be given of the behaviour of currently available software and the improvements that will be offered by the so-called "Phase-III" software which will be released in August.

16. X–10 PROTEIN AND VIRUS X-RAY DATA COLLECTION WITH A XENTRONICS AREA DETECTOR.

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Our laboratory has developed software for X-ray crystallographic data collection using a compact, commercially available electronic area detector manufactured by Xentronics Inc. The current detector has a 12 cm active surface with a resolution on the face of 200 microns. At a specimen-to-film distance of 18 cm, X-ray reflections from Tomato Bushy Stunt Virus (I23, a=383.3 Å, 750,000 dalton/asymmetric unit) have been resolved to 2.6 Å resolution.

Data on a number of crystals have been collected from a series of 5 minutes-of-arc oscillation exposures ("frames"). Analysis of reflection centroids in three dimensions from a small number of strong spots is used to determine the crystal setting parameters and camera constants, from which reflection positions and shapes are predicted prior to integration.

Partial high resolution data sets have been collected on the influenza virus HA ($P4_1$, a=163.2, c=177.4, 200,000 dalton/asymmetric unit) and the 434 repressor-DNA operator complex (Anderson, J. and Harrison, S. C., unpublished) (I422, a=b=166, c=139 Å, 35,000 dalton/asymmetric unit) and compared to data collected by oscillation photography. Symmetry R factors are comparable or better than those observed for these crystals using film data collection.

Both native and mercury isomorphous heavy atom derivative data sets have been collected from crystals of the variable surface glycoprotein from the trypanosome parasite ($P4_12_12$, a=96.3, c=111.3, 43,000 dalton/asymmetric ~~unit~~). (Metcalf, P., Freymann, D., Turner, M., and Wiley, D. C., unpublished). The quality of this data relative to 6 Å data sets collected on a Syntex 4-unit diffractometer has been compared. A 6 Å resolution difference Patterson calculated from the data sets collected on the area detector is readily interpretable in terms of a single Hg site, and comparable to a difference Patterson calculated from data collected by diffractometer.