01. DETERMINATION OF MACROMOLECULAR STRUCTURES


Using the High Flux Reactor at the ILL a neutron data set has been collected to 3.5 Å spacing from a large partially deuterated crystal of a T-state haemoglobin (space group P212121; a=95.8, b=97.8, c=65.5 Å). Data were collected using the recently commissioned instrument D19 with its 3-d position sensitive detector (M. Thomas et al. in Position Sensitive Detection of Thermal Neutrons, P. Convert & J.S. Forsyth, eds., Academic Press, London, 1983).

The data have been processed using the programs developed for the instrument by R.D. Stansfeld based on a 3-d minimum C(1)/I method of integration (C. Wilkinson & H.W. Khamis in Convert & Forsyth, eds., loc. cit.). Starting from a carefully refined 1.5 Å X-ray model, joint refinement with the neutron data is in progress. This will be discussed in terms of the H/D exchange of amide hydrogen atoms. The non-crystallographic symmetry in these crystals will allow a comparison between the chemically identical but constitutionally distinct dimers of the haemoglobin tetramer.

01.7-2 ELECTRON MICROSCOPY STUDIES OF PROTEIN CRYSTALS FOUND IN VIVO. Sven Homvöllér, Da Neng Wang and Agneta Sjögren Structural Chemistry, University of Stockholm S-106 91 Stockholm, Sweden.

Protein crystals are known to be formed in vivo in many cases. These range from one-dimensional fibrillar crystals as for example in actin, over two-dimensional as in gap junctions and bacterial surface layers (5-layers) to three-dimensional crystals. However, only minor effects (i.e., ~a-1 Å elongation or ~a-3 Å distortion) of densities. The images were scanned in a microdensitometer and the Fourier transforms calculated. By this crystallographic approach we could conclude that there were two different crystal types, and not one as previously suggested. The large unit cell sizes clearly indicated that the crystals were composed of macromolecules, presumably proteins. Ref. Farrants, Homvöller & Stadhouders (1987) in press.