CCP13 visit to the Experimental Station at the DuPont R & D plant (July 19-20th 1998)

On July 19-20th 1998 Richard Denny and I (both wearing CCP13 hats) were invited to present seminars at the Experimental Station at the DuPont R & D plant near Wilmington, in Delaware. The visit was hosted by Kenn Gardner and Roger Leach of DuPont so that we could both present our work to the company and also heighten awareness amongst DuPont scientists of the CCP13 mission and of the software that is currently available in the CCP13 suite. Naturally the visit also allowed the two of us an opportunity to see the facilities that are available to research scientists working at DuPont. On the morning of the 20th July, Richard and I were shown around numerous laboratories devoted to structural work and in particular establishing the relationship between structure and physical properties using diffraction and other techniques. We also spent some time discussing with Kenn his own work on materials including the ether-ketone polymers, Kevlar, Nylon, as well as the unique properties of spider silk.

Richard's talk described the application of the CCP13 suite to typical (and non-typical!) fibre diffraction problems. He outlined the methods used in tackling these problems and the software that he had written to implement them. Included in this was a summary of the latest version of LSQINT and also of a recently developed version of F-XPLOR. F-XPLOR was derived from X-PLOR (Brünger *et al.*, *Science* (1987) **235**, 458) and was modified by Hong Wang and Gerald Stubbs (Vanderbilt) to cater for continuous fibre diffraction. Richard's modification now allows the treatment of polycrystalline diffraction data (see Denny, Shotton & Forsyth in last year's edition of *Fibre Diffraction Review*).

In my own talk I gave a description of the application of both X-ray and neutron fibre diffraction techniques in the study of nucleic acids, of the analytical methods used, and of the results that have been obtained. Part of this work illustrates the advantages that arise from availability of specifically and non-specifically deuterated polymer analogues in neutron diffraction. Although nucleic acids are somewhat outside DuPont's mainstream interests, the methodology that was used in this work is of general interest for structural studies of synthetic polymers as well as biological polymers. The isotopic replacement methods that have been used in neutron diffraction studies of DNA hydration can also be used to study the location of aromatic groups and of isolated hydrogen atoms in a wide variety of industrial polymers. Later on the three of us were able to discuss future collaborations in this area and it is pleasing that the first neutron experiments based on this collaboration have just been scheduled.

Before we left for Washington, Kenn treated us to a meal at his favourite restaurant. We ended up eating a large quantity of quite ferocious looking (although fortunately dead) crabs. You thought fibre diffraction was difficult? Just try eating a crab from first principles! There can have been few more entertaining sights than the two of us trying to work out the edible parts of the crustacean anatomy. I am by no means certain that I got it right.....

Trevor Forsyth
Institut Laue-Langevin & Keele University

7th Annual Fibre Diffraction/NCD Workshop

The 1998 joint Collaborative Computational Project for Fibre Diffraction and Non-Crystalline Diffraction Workshop was again held at CLRC Daresbury Laboratory from 12th - 14th May.

The first talk by Keiichi Namba (Matsushita Electric Industrial Co., Ltd.) got the meeting off to a fascinating start. Keiichi described the techniques involved in producing specimens of bacterial flagellum oriented to better than a spread of 1°, involving stages of liquid crystallisation, slow centrifugation and magnetic orientation. The excellent fibre diffraction data collected from these samples combined with phases from electron