CHAIRMAN'S MESSAGE

The CCP13 Newsletter continues to go from strength to strength, as befits an organisation that is healthy and making rapid progress in carrying through its aims. This edition, the fourth Newsletter, is not only bigger and meatier than ever before, but it has a new presentation format that makes it more attractive and readable and which we hope will help to promote the activities of CCP13 to a wider audience than before. Additional copies of the Newsletter have been printed so that it will go not only to people on the CCP13 mailing list, but also to places and people regarded as influential and potentially interested or supportive. In addition the Newsletters are being incorporated as part of the CCP13 World Wide Web pages (details elsewhere). The articles in the Newsletter illustrate some of the progress made in developing CCP13 fibre diffraction software in the past year, some ideas about the direction that CCP13 should take in the future, and application of the existing suite to a range of interesting biological and materials science problems. As detailed in the report by Geoff Mant, the 1995 Annual Workshop at Daresbury was, once again, a joint meeting of CCP13 and the UK Non-Crystalline Diffraction community, reflecting the considerable overlap of interests of the two groups. The meeting was very well attended and emphasises the importance of the topic. The success of the format means that the 1996 meeting will be structured in a similar way; we hope for an even larger audience. Remember not only that your poster could win a large cash prize (1st Prize - £100; 2nd Prize - £50), but also that abstracts will be included in the Annual Newsletter (also on the WWW) so that your work will be available to a much wider audience. There will be bursaries available for students and young scientists. Details of all these are given at the end of the Newsletter.

Reminder - What is a CCP?

CCP stands for Collaborative Computational Project. CCP13 is funded in the UK mainly by the Biotechnology and Biological Sciences Research Council (BBSRC) via its "Equipment and Facilities" office. An additional grant comes from EPSRC to help fund meetings and travel for the 'synthetic polymer' side of CCP13. CCP13 is one of 12 current CCPs. These are:

CCP1	Electronic structure of molecules
CCP2	Continuum states of atoms and molecules
CCP3	Computational studies of surfaces
CCP4	Protein crystallography
CCP5	Computer simulation of condensed phases
CCP6	Heavy particle dynamics
CCP7	Analysis of astronomical spectra
CCP9	Electronic structure of solids
CCP11	Biosequence and structure analysis
CCP12	Novel architecture computers in Fluid Dynamics
CCP13	Fibre diffraction
CCP14	Powder diffraction

Our current CCP runs to the end of September, 1998, with support from a recent BBSRC grant. The new grant will allow the continued employment of Richard Denny as the CCP13 RA and it will provide funds towards Workshops, Newsletter production and International interactions. The funding by BBSRC and EPSRC also allows CCP13 to carry out 'good works'. At the last CCP13 Workshop it was agreed that these would be to fund a small number of 'CCP13 Travelling Fellowships' and a 'CCP13 Visiting Scientist Program', details of which are given later.

Your Contribution

Interested groups or individuals are invited to contact any of the officers of CCP13 to obtain information about CCP13 Workshops, software developments, software standards and so on. Offers of home-written software that could be incorporated into the new CCP13 suite of programs would be much appreciated and will, of course, permanently carry the authors' attribution. Make sure that you are on the CCP13 mailing list and you will be kept informed.

Newsletter Editorial Policy

Articles for inclusion in the CCP13 Newsletter are welcome by the Editor at any time, but preferably items for the December 1996 issue should arrive before the end of November 1996. It is hoped that the Newsletter will become an Annual 'essential' for Fibre Diffractionists. This is the place to advertise your fibre diffraction or NCD meetings, to report on new software or 'hot' results obtained using the CCP13 Suite and to provide reports of meetings of interest, preferably together with one or two photographs. All technical articles will be scrutinised both for scientific content and presentational style by

the Editor (or his nominee) together with at least one other member of the CCP13 Steering Panel. In this way we hope to maintain high standards. Remember that the Newsletter not only goes to other Fibre Diffractionists, but also to various members of the Research Council Secretariats and to other funding agencies.

International Cooperation

Although these CCPs are UK funded projects, there is a very strong interest in making them international through cooperation with interested scientists in other countries. A natural link for CCP13, for example, exists with the Special Interest Group (SIG) in Fibre Diffraction of the American Crystallographic Association and possibly with some American synchrotron users (CHESS). Others exist with the ESRF at Grenoble and with the Photon Factory in Japan.

Retirements and New Elections

At the 1995 Annual Meeting, Trevor Forsyth and Mike Ferenczi were re-elected as committee members and Tim Wess was elected in place of Keith Meek who retired. The services of Keith during the start up phase of CCP13 have been much appreciated and it is a pleasure to record our thanks to him for his interest and enthusiasm.

Please note that the periods of office of John Squire (Chairman), Geoff Mant (Secretary) and Manolis Pantos (committee member) will finish at the May 1996 Meeting. Any nominations for election to these posts should be sent to the CCP13 Secretary, Dr. Geoff Mant before the May meeting. All three people are willing to continue in these roles for a further 3 year period. Elections will be held at the business meeting at the CCP13/NCD Annual Workshop in May, 1996.

John Squire

IF YOU ARE A FIBRE DIFFRACTIONIST STUDYING SYNTHETIC OR BIOLOGICAL POLYMERS. THIS CCP IS FOR YOU. PLEASE HELP TO MAKE IT WORK!

ACA MEETING - MONTREAL - JULY 23-28, 1995

The 1995 version of the annual ACA Meeting was held in the well-appointed Palais des Congres in Montreal, Canada. I was there as part of the session organised by the Fibre Diffraction 'Special Interest Group' (SIG) of the ACA. This was my first visit to Montreal and I had not realised until I got there quite how French it is. Although I soon realised that most people speak English, it obviously was diplomatic to exercise, at least initially, a little of the rather rusty schoolboy French that still remained. Fortunately I arrived in Montreal a day before the meeting started and was able to enjoy some of the splendid sites in this beautiful city, including a very pleasant, albeit short, cruise along the St. Lawrence River.

The Fibre Diffraction SIG meeting was divided into four sessions and was a good mix of synthetic and biological polymer work. Speakers or co-authors included some old friends from CCP13 meetings such as H. Zachmann, Watson Fuller, Alan Windle and Bill Stroud, together with some key US fibre diffractionists such as Gerald Stubbs, Rick Millane, Tom Hendrixson, John Blackwell, R. Chandrasekaran and Dan Kirschner. Another old friend, Don Caspar, also appeared in the audience for some of the sessions. Although it was a relatively small meeting for fibre diffractionists, many of the talks were very interesting and useful and it was certainly good to renew old contacts and to make new ones. At the same time, some other parallel sessions (e.g. on small-angle scattering, neutron scattering and macromolecular structure) brought other friends to Montreal, including Trevor Forsyth in the neutron scattering session.

This was the centenary ACA meeting of the discovery of X-rays by Røntgen, so one of the sessions paid tribute to the importance to all of us of this discovery. It was also the first ACA meeting since the deaths of two great crystallographers, Dorothy Hodgkin and Linus Pauling, so on the Tuesday evening there was a special tribute to them and to the enormous contributions that they made to the subject. Some of the families and long time friends of these two scientific giants were there and made their own contributions, the whole session being both fascinating and, at times, very moving.