

Society of Crystallographers in Australia



SCA

Newsletters

No 25, July 1994

The SCA homepage is located at <http://www.sca.asn.au>

FROM THE PRESIDENT

Due to the sustained dedicated effort since 1986 of some Australian crystallographers and the Australian Academy of Science's National Committee for Crystallography (ANCC), Australia now has its own National Beamline Facility (ANBF) at the synchrotron radiation source at Tsukuba in Japan. Excellent results have been obtained from EXAFS and powder diffraction experiments performed on the Australian designed and built diffractometer. The facility is clearly fulfilling an important role in Australia's *Big Science* requirements, but has its limitations, particularly in relation to beam intensity.

To build on the capabilities of the ANBF, and looking to Australia's future needs for synchrotron radiation, the ANCC established a working party (WP) which met on the 29-30 April. A number of papers were presented to the WP which dealt with present status and future needs in spectroscopy, surface science, solid state physics and crystallography. Various options for future developments were discussed. These included further developments at the Photon factory in Tsukuba, access as part of a consortium to one of the third generation synchrotron sources in France, USA or Japan, and an Australian based small synchrotron. There are many important technical matters to resolve in relation to the different options and these are being investigated prior to the WP meeting again. The study has got off to a good start by involving representatives from all the main synchrotron user groups.

Plans for Crystal XIX are progressing well. Ballarat University has been chosen as the venue. It is in a bushland setting about 10 km south of Ballarat. The University has excellent conference facilities, on-campus accommodation and its own catering service. Regular shuttle buses run from Tullamarine airport. The organising committee has negotiated with the University to keep costs to a minimum.

Michael Hart, Emeritus Professor of Physics, University of Manchester, will be the 1987 Fellow and present the Conference Lecture on the applications of synchrotron radiation. The first circular is being distributed with this *Newsletter*. The circular advises that applications will be invited from SCA student members for Studentships to help support their attendance at Crystal XIX, provided they present a paper or poster. Supervisors are encouraged to support their students to present their work at the conference.

In keeping with SCA policy to foster relationships with related professional organisations, we have coordinated with the Australian X-ray Analytical Association (AXAA) in relation to a workshop for Rietveld method users. The workshop will be held in Melbourne on the Monday and Tuesday (April 24-25) following Crystal XIX. This gives the opportunity for visitors from other states to attend both meetings, with an intervening weekend for relaxation. A first circular for the AXAA Rietveld workshop is included with the Crystal XIX circular.

Ian Grey

AUSTRALIAN NATIONAL BEAMLINE FACILITY

To commemorate the successful commissioning of the Australian National Beamline Facility at the Photon Factory, the following symposium will be organised at the 1994 annual meeting of the Crystallographic Society of Japan, which will be held from 24-26 November 1994 at Osaka University, Japan. The symposium, entitled *Impacts of Powder Diffraction in Advanced Materials Research*, intends to discuss the current status and future prospects of powder diffraction, bringing together Japanese and Australian diffractionists. This is the first Japan-Australia joint symposium in a CrSJ annual meeting. For further information contact:

Prof. B. O'Connor (Curtin University), e-mail: toconnorb@cc.curtin.edu.au or:

Prof. H. Hashizume (Tokyo Inst. Tech.), e-mail: hhashizu@nc.titech.ac.jp

Provisional Program

1. H. Hashizume Introduction
2. R. Hill Impact of Powder Diffraction in Advanced Materials Research.
3. D. Creagh BIGDIFF: the Multi-Purpose Diffractometer on the Australian National Beamline at the Photon Factory.
4. B. O'Connor Initial Applications and Prospects for BIGDIFF in Powder Diffraction.
5. H. Toraya Current Powder Diffraction Research Using Synchrotron Radiation in Japan.
6. C. Howard Neutron Powder Diffraction in Australian Materials Research.
7. F. Izumi Applications of TOF Neutron Powder Diffraction to High-Tc Superconductors.

Hiroo Hashizume

SKETCHES OF CRYSTALLOGRAPHY LABORATORIES

University of Sydney

The X-ray crystallography laboratory at the University of Sydney traces its beginnings to the School of Chemistry in the 1950's when Hans Freeman was still a graduate student. His own research work has maintained a consistent theme, focussing on the structural characterisation of biologically interesting molecules.

Most stages of the crystallographic technology have been represented in the Sydney laboratory in the last forty years. Generators have evolved from early low-power continuously evacuated models, through standard sealed tube generators to the direct drive rotating anode generators currently in use. Intensities were first measured by visual comparison on films. A Weissenberg geometry diffractometer was constructed from a commercially available mix of components in the 1960's. It has since been replaced by several standard four circle instruments. Computing facilities represent the most obvious improvement in technology. Hans Freeman was a pioneer in the use of computers with several publications in the 1950's describing the use of SILIAC one of Australia's first computers to calculate Fourier summations. The Sydney crystallographers were users over a period of time of mainframe computers at the Department of Defence in South Australia, the Atomic Energy Commission at Lucas Heights and the CSIRO in Canberra. Access to these machines involved decks of cards and the precursor of Australia Post. The Silicon Graphics workstations in use today perform least-squares refinement cycles in very nearly real time. Most importantly this revolution in technology has been matched by the complexity of structural problems being studied. The first structures of copper peptide complexes (some twenty or thirty non-hydrogen atoms) were sufficiently large in their day to comprise an entire PhD thesis project. The copper protein plastocyanin whose structure was solved in 1977 contained 929 non-hydrogen atoms in the asymmetric unit. Protein structures currently in progress have up to 130 KDa, 1400 amino acid residues or 7000 non-hydrogen atoms in the asymmetric unit.

In 1994 there are two X-ray crystallography laboratories at the University of Sydney. Hans Freeman and Trevor Hambley remain in the School of Chemistry and Mitchell Guss has established a new laboratory in the Department of Biochemistry. The Chemistry groups continue research into metal complexes of biological ligands. There is a common interest in metal amino-acid and metal peptide complexes. Trevor Hambley uses both crystallography and molecular mechanics modelling to study platinum complexes bound to DNA and DNA fragments, and carries crystal structure analyses as contributions to a number of drug design projects. In addition Trevor Hambley supervises a structure determination facility which carries out

more than 100 structure analyses per year for research groups in many departments throughout the University.

The new laboratory in the Department of Biochemistry is concerned entirely with protein structures. A collaboration with Professor Graeme Cox of the John Curtin School of Medical Research at the Australian National University has yielded crystals of several of the subunits of *Escherichia coli* adenosine triphosphatase (ATPase). A group under the direction of Professor John Hopwood at the Women's and Children's Hospital in Adelaide works on genetic diseases which result in excess storage of polysaccharides in lysosomes. One of these enzymes is being produced in large quantities by recombinant technology with the aim of its use in enzyme replacement therapy. We have crystallised this enzyme, N-acetylgalactosamine-4-sulfatase. The work on metalloproteins continues in collaboration with Hans Freeman, with the present emphasis being placed on a class of copper-containing amine oxidases. We have crystallised the protein isolated from pea plants and several crystallographic forms of the equivalent protein from a bacterium, *Arthrobacter globiformis*.

The equipment available in the two laboratories includes: in Chemistry, a Rigaku AFC-7 diffractometer on a Rigaku RU-200 rotating anode generator, and an Enraf-Nonius CAD-4 diffractometer on a sealed tube generator; in Biochemistry, a Rigaku R-Axis IIC imaging plate detector system, with mirror optics on a Rigaku RU-200 rotating anode generator and a second RU-200 with precession and oscillation cameras. Both laboratories are equipped with Silicon Graphics computing and graphics facilities for use in small molecule and macromolecule structure analysis and refinement. The small molecule crystal structure analyses are carried out using the teXsan system. SHELX-76 and the Enraf-Nonius MOLEN system are also available. The software for protein structure analysis includes: DENZO for data reduction, PROTEIN and CCP4 for standard crystallographic calculations, PROLSQ for restrained refinement and X-PLOR for refinement with simulated annealing.

Staff, in addition to the academics already mentioned, include Research Associates Dr Peter Turner and Dr Vinay Kumar, Research Assistants Vilma Zubak and Michael Costello and eight research students.

CRYSTAL XIX

April 18-21 1995

Crystal XIX, the next meeting of the Society of Crystallographers in Australia, will be held at the Ballarat University, Ballarat, Victoria. Contact: Lachlan Cranswick (Tel: 61-3-6470367) or Ian Grey (Tel: 61-3-6470211), CSIRO Division of Mineral Products, PO Box 124, Port Melbourne, Victoria 3207 Australia. Fax: 61-3-6463223, e-mail: lachlan@dmp.csiro.au or iang@dmp.csiro.au.

CRYSTAL XVIII

April 5-8, Medlow Bath, N.S.W.

Report of the Conference

Crystal XVIII was a success in terms of the attendance, the scientific program and the social events. There were more than 100 delegates as well as trade representation from nine companies. The atmosphere of the somewhat unusual but beautifully situated Hydro Majestic Hotel in the Blue Mountains of New South Wales, west of Sydney, provided the right mix of casual meeting facilities and organised functions to match the broad range of tastes in the Australian Crystallographic community.

The conference program was broadly based with significant contributions from the rapidly expanding protein community, materials science, diffraction physics and instrumental and computing techniques. An innovation at this meeting was a session devoted to oral presentations by graduate students.

Delegates arrived at the meeting on the afternoon of April 5. The convenient location of the Medlow Bath railway station simplified travel arrangement for those from interstate and overseas who did not have access to a car. Those who arrived early spent the afternoon drinking on the terrace or taking advantage of the fine weather for some short bushwalks into the valley. A champagne mixer was followed by dinner.

The scientific program commenced on the Wednesday morning with an opening session devoted to protein crystallography. Peter Colman preceded his presentation on the influenza protein, neuraminidase, with a brief history of protein crystallography in Australia. He detailed its progress from humble beginnings in the Department of Inorganic Chemistry at the University of Sydney to the present state, with six laboratories in three states and the Australian Capital Territory. Informal talk at the meeting suggested that there may be several more protein crystallography laboratories

established in the next few years. Protein crystallography featured prominently in the remainder of the first session and in the penultimate session on Friday morning. Recently solved structures were presented by Jenny Martin (Queensland, disulphide bond forming protein), Paul Carr (ANU, the PII protein), Matthew Wilce (St. Vincent's Institute, glutathione-S-transferase), Tina Izard (BRI, lyase), Tom Garrett (BRI, barley glucanase), and Shu-Hong Hu (St. Vincent's Institute, twitchin kinase). This relatively large number of new structures from a small community bodes well for the future growth of the field.

The more physically minded crystallographers were not to be outshone by their biologically oriented brethren. John Parise, one of a number of invited speakers from overseas, spoke on the use of pressure to modify structure. His work like many others described the integral use of synchrotron radiation. This interest in synchrotrons was especially timely given the recent opening of the Australian National Beamline Facility at Tsukuba in Japan as a powder diffractometer. In a later session Dudley Creagh and Richard Garrett described the latest developments at the Australian Beamline. There was a strong powder session led by Russell Morris who described the use of both neutron and synchrotron data to solve complex structures. Hiroo Hashizume gave a masterful and elegant presentation of the use of maximum entropy methods with powder data. John Helliwell from Manchester, the 1987 Fellow of the Society, explained the latest advances in synchrotron sources and how these very bright and intense beams would be used for complex biological structures. The rebirth of Laue diffraction with the advent of synchrotrons was especially interesting for the possibility it gives to do real time kinetic experiments with complete data sets collected in a millisecond or less.

The final scientific session returned to materials both ordered and disordered. Bill David from Oxford used C60 to show how state of the art instrumentation could be used to solve even very large structures with powder diffraction data. The meeting concluded with Richard Welberry's talk on modelling the diffuse scattering in cubic stabilised zirconias.

The social life of the meeting was lubricated with generous supplies of wine with the evening meals and at the opening mixer and poster session. These drinks were all provided from the generous support the meeting received from the trade sponsors. An undoubted highlight of the meeting was the speech by Sandy Mathieson following the conference dinner. He presented the story of Australian crystallography from the time of the Braggs up to the second World War with anecdotes of the many colourful characters, without notes or prompts of any kind. His easy style and genuine love of his subject captivated his audience. Sandy has promised to continue the story at the next meeting.

Trevor Hambley, Mitchell Guss

New Members

We welcome the following new members who have joined the Society in 1994.

Full Members

Dr Lachlan Cranswick, CSIRO Division of Mineral Products, Port Melbourne. Dr Jennifer Martin, Centre for Drug Design and Development, University of Queensland. Dr Andrei Nikulin, School of Physics, University of Melbourne. Dr Brian Usher, Telecom Research Laboratories, Clayton.

Student Members

Mr Mark Beuchat, Biomolecular Research Institute, Parkville. Mr Jeffrey Crass, Department of Chemistry, University of Technology, Sydney. Ms Jodieann Dawe, School of Chemical Technology, University of South Australia. Mr Gordon Dong, Department of Chemistry, University of Technology, Sydney. Ms Alison Green, School of Chemistry, University of Melbourne. Mr Aidan Heerdegen, Research School of Chemistry, ANU. Mr Damian Slizys, School of Chemistry, University of Melbourne.

CRYSTAL FRAGMENTS

- David Ollis (ANU) attended a meeting at Brookhaven from June 4-5 that was concerned with the future of the Protein Data Bank. It was entitled *From PDB to 3DB* and was organised by Joel Sussman and was attended by about 20 people.
- In May, Mark Spackman (University of New England) gave an invited lecture entitled *Estimating Molecular Properties and Interaction Energies from X-ray Diffraction Data* at a meeting called *CMCD4 - Computational Methods and Chemical Design - Molecular Modelling - Theory & Experiment*. held at Kloster Irsee in Southern Germany. He also

visited and gave a talk at the Free University of Berlin (Institute for Crystallography). At the European Synchrotron Radiation Facility (ESRF) in Grenoble he presented a talk and discussed possibilities of data collection on the Swiss-Norwegian Beam Line. At the University of Milan, Mark gave yet another lecture and discussed collaborative work with Prof. R. Destro. In August he returns to Europe to give an invited lecture on *Simple Representations of the Molecular Electrostatic Potential* at the Sagamore meeting in Brest and will also visit a few labs in the UK after the meeting.

- Syd Hall (University of Western Australia) was invited to speak at the ACA '94 meeting in Atlanta Georgia, June 25-July 1 in a session on *Enhancing Practical Electronic Communication*, a talk entitled *Use of the Star File for Data Exchange and Archiving*.

CAMBRIDGE STRUCTURAL DATABASE

The Australian Nuclear Science and Technology Organisation (*Ansto*) became the National Affiliated Centre (NAC) for the Cambridge Crystallographic Data Centre (CCDC) on July 1st. It succeeds the CSIRO Division of Chemicals and Polymers as NAC. The contact is Chris Howard. Previous users of the CSD will be contacted shortly since the agreements between academic users and the NAC will need to be rewritten before database and software updates can be supplied. Those whose requirements are urgent should not hesitate to contact Chris Howard (contact details elsewhere in this *Newsletter*) for immediate attention.

The CCDC has produced the first issue of what is intended as a regular newsletter, with information on such developments as the incorporation into the CSD of the Brookhaven Protein Databank, advances in search software, and the availability of the system on CD-ROM. Copies can be obtained from the NAC, or directly from The Administrative Secretary, Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK. Other enquiries should be directed to the NAC in the first instance.
