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Society of Crystallographers in Australia

SCA

Newsletters

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FROM THE PRESIDENT

Of interest to scientific societies such as the SCA is the recent release of the FASTS Policy Document. FASTS stands for Federation of Australian Scientific and Technological Societies. It was established by senior scientists and technologists in 1985 to provide a lobby for science and technology (S&T) following the disastrous 1984 budget for science. The Federation is composed of 43 member societies, the SCA being one, who pay an annual subscription and nominate a representative to provide input to FASTS, through their office in Canberra or at the full Council meeting of the Federation. FASTS' major objectives are to increase solidarity within the S&T community, to enhance communication between the S&T community and Government, Industry and Commerce, and to promote a deeper understanding by the public of the importance of S&T. It has had some notable achievements, including making major contributions to the formation of the Science Council, to the establishment of an ACTU S&T policy and to the establishment of a separate Federal Government portfolio of S&T.

The development of a Policy Document represents a move by FASTS towards a more proactive role in the development of science and technology policy in Australia. The Document covers four broad areas - Education, Industry, Government Institutions/ National Facilities, and University Research/ Research Training. It represents as far as possible the consensus views of members of the forty-three societies that make up the Federation. In each of the four areas mentioned, the Document sets out the background, a FASTS' position statement and strategies that FASTS should undertake in relation to its position statement. Of interest to crystallographers is FASTS' position in relation to large national research facilities. The Document proposes that FASTS should lobby for the establishment of a government funded committee to finance large scale research which is outside the capacity of the present ARC system.

The Policy Document is in draft form. FASTS has requested input and comments that will improve the Document, so they can be incorporated at the next Council meeting at the end of November. Copies of the Document, and other information can be obtained from the FASTS Secretary, GPO Box 2181, Canberra, ACT 2601, Fax 06 249 6419. As a society we make a significant financial contribution to FASTS (~$4 of each member's SCA dues) and it's in our interests to ensure that FASTS effectively represents our views and policies in its submissions to the Australian Government and other bodies.

Word has just come through of a major achievement at the Australian National Beam Line at the Photon Factory, KEK, Tsukuba, with the successful installation and testing of a sagittal focussing monochromator. The monochromator passed the preliminary tests with flying colours achieving a 20 fold increase in the flux of the synchrotron beam. The monochromator was designed by Dudley Creagh, constructed in the Physics Department of the Australian Defence Force Academy, UNSW, and installed by Fred Johnson and Peter Scott. Testing was carried out by Richard Garrett and the ANBF PF staff, Gary Foran and David Cookson. The next critical stage of evaluation will occur in December when Mitch Guss and Jose Varghese test the application of the monochromator, with its higher photon flux, to protein crystallography problems.

The second circular for Crystal XIX is being distributed with this newsletter. The committee is delighted that Alec Moodie has agreed to give the after-dinner talk at the Conference Dinner. He will cover some history and personal reminiscences during his time at CSIRO's Division of Chemical Physics. Two other meetings of interest to crystallographers are being coordinated with Crystal XIX. The Bevan Fest, a meeting to celebrate the career and achievements of Professor "Judge"

Bevan starts at Ballarat University on the Friday afternoon, straight after Crystal XIX, and concludes with a dinner on the Saturday evening. On the Sunday and Monday, the AXAA is running a two day workshop for users of the Rietveld method at the Novatel Bayside Hotel in Melbourne. Further details and contact numbers are given in the Crystal XIX second circular.

SCA secretary, Max Taylor has just come out of hospital after over two months recovering from major surgery. He is happy to be back home regaining his strength and looking forward to re-establishing his interests and involvements. We wish him all the best for a continuing strong recovery.

Ian Grey

SKETCHES OF CRYSTALLOGRAPHY LABORATORIES

University of Queensland

Small Molecule X-Ray Diffraction Laboratory is housed on the sixth floor of the Department of Chemistry, The University of Queensland, St. Lucia. It was started in 1964 with an underground laboratory under the Great Court of the University. It has progressed to a typical modern laboratory with three generators, one still using valves.

The main equipment is an Enraf- Nonius CAD4 kappa diffractometer with a sealed tube, and graphite monochromator. There is a low temperature device which can control data collection from -100 to 100C. Other pieces of equipment include Weissenberg and Precession Cameras, Philips and Nonius Powder cameras. Powder data are collected on the latter and processed on a homemade densitometer (the old Stoe diffractometer from Mike Snow's Laboratory). In the corner and not being used is the first diffractometer that was purchased by Hans Freeman, an old Supper two circle diffractometer. The usual computer equipment and software is housed in a number of surrounding rooms.

These days most work is of a service nature to chemists within the Department and at the Centre for Drug Design and Development, Griffith University (Colin Raston), Queensland University of Queensland (Graham Smith), Central Queensland University and geologists at the James Cook University of North Queensland. Local work is centred around taking fibre photographs of spider silk, working on the structures of pesticides and herbicides, and related compounds.

A project involving the synchrotron is being developed in conjunction with Ian Gentle and Geoff Barnes of this University. It is to understand the structure of monolayers formed in a Langmuir balance or Langmuir-Blodgett films. So far data have been collected on beam line 16 at the Photon Factory in Tsukuba using grazing incidence diffraction. In the past, data were also collected on large crystals at 2 tan B, ANSTO neutron facility. Karl Byriel is the person responsible for the day to day running of the diffractometer with Colin Kennard in overall charge of the laboratory.

The newest addition to protein crystallography in Australia is the Protein Crystallography Laboratory within the Centre for Drug Design and Development (or 3D Centre) at the University of Queensland. This is the first protein crystallography laboratory in Queensland and was jointly funded by the Department of Primary Industry (DPI, Queensland), the Australian Research Council, the University of Queensland, Queensland University of Technology and Biosym Technologies. It is situated on Level 1 of the Gehrmann Laboratories and forms, with the Protein NMR Laboratory, the 3D Centre Biomolecular Structure Facility which was officially opened by Simon Crean on July 29, 1994.

The laboratory is equipped with an RU-200 rotating anode X-ray generator, RAXIS-IIC imaging plate area detector and Huber 205 precession camera. A mirror system will be installed in the near future to improve the X-ray intensity and a cryo-cooling system is currently being commissioned. A graphics room houses an SGI Indigo and Indy - used for electron density fitting, model building and structure refinement - and a wet laboratory and cold room are used for protein preparation, purification and crystallisation. Jenny Martin is the principal investigator and Wasa Wickramasinghe and Shuhong Hu are research officers in the Protein Crystallography Laboratory. The protein structure research that is undertaken within the laboratory includes team projects from the 3D Centre as well as collaborative work with groups in other departments of Queensland University, and with other tertiary institutes and research organisations, including the DPI. In addition, international collaborative projects have been set up with research groups in the US, Germany and Switzerland.

AUSTRALIA'S FUTURE NEEDS IN SYNCHROTRON RADIATION

On 29 April 1994 and under the auspices of the Australian Academy of Science the National Committee for Crystallography brought together a small group of protagonists for synchrotron radiation research in biology, protein crystallography, chemistry, atomic and molecular physics, materials science and surface science and polymer chemical physics to consider

future needs and options for synchrotron radiation research in Australia. A Draft Report from this meeting was presented to the Academy of Science in July and they encouraged and financially supported a second meeting of the Working Party held on 26 September 1994.

The meeting was called to review the information on options for Australian synchrotron beam use in the light of information gathered over the intervening months in response to questions posed after discussions on 29April 1994. The meeting's objective was to set a forward strategy for synchrotron access taking into account the current success and demand for the Australian National Beamline Facility at Tsukuba, Japan, the need for complementary high brightness facilities and further facts about small synchrotron possibilities for an Australian home-based facility. Following the "working party" meeting a brief report of the discussions was made to the scheduled Management Committee meeting for the Photon Factory on 27 September 1994.

Members of the working group have been requested to bring forward definite and costed proposals for future synchrotron access to another meeting of the group on 28 October 1994.

John White

SKETCHES OF CRYSTALLOGRAPHY LABORATORIES

Research School of Chemistry

Australian National University

The Research School of Chemistry (RSC) opened in 1967, but it was not until 1969 that the School appointed Dr Glen Robertson to head the Crystallography research group and also provide some capacity for crystal structure refinement for the School's synthetic chemists. Much of the group's early activity involved software development and adaptation, together with the study of transition metal hydrides using both single-crystal X-ray and neutron diffraction data.

The School's first automated single-crystal X-ray diffractometer was a Picker FACS-I which was commissioned in April 1970. This apparatus provided quality data for the School over many years. In 1978 the Group acquired a Philips PW1100/20 4-circle instrument with variable temperature (approx. -150o to +150oC) capability. Crystallographers who have worked in the Group included John Bell, Peter Whimp, Bruce Foxman, Bryan Anderson, Trevor Hambley, George McLaughlan, Wasantha Wickramasinghe and Jon White.

Dr Richard Welberry arrived at RSC in 1975 to establish a research group to study disordered crystalline materials. Richard's research has concentrated on the development of methods for recording, analysing and interpreting diffuse scattering from such materials. Initially his data collection was film-based, and modelling of diffuse scattering was achieved using optical transforms of 2-dimensional masks. Now he and his group record their data using position sensitive detectors mounted on purpose-built computer-controlled apparatus based on Weissenberg geometry. Modelling of disordered materials is now routinely performed using stand-alone workstations, and the 3-dimensional diffraction patterns corresponding to these materials are readily generated using the ANU’s super computing facilities. Disordered organic molecular crystals provided the subject of Richard's early research, but the scope has now extended to include non-molecular inorganic solids such as cubic stabilised zirconias and minerals such as cristobalite and mullite.

Professor John White was appointed in 1985 to establish a research group in the area of solid-state molecular science. A major part of the White group activity has centred on the use of high-resolution neutron and X-ray scattering for the study of a wide range of novel materials, including thin films, membranes, conducting copolymers, high-temperature superconductors, quasicrystals, fullerenes and their derivatives, graphite and clay intercalation compounds and mesoporous membranes.

In 1986 John's group began construction of a Small Angle X-ray Scattering (SAXS) Huxley-Holmes camera based on a GX13 rotating Cu anode for the study of coherent scattering phenomena. The source has now been upgraded to a GX18. More recently, work has continued on the development of 1-dimensional and 2-dimensional X-ray area detectors, and X-ray reflectometers for SAXS and the Australian National Beam Line at the Photon Factory. Through John the group has strong collaboration with a number of neutron scattering and synchrotron facilities throughout the world. Apart from involvement in the design and development of AUSANS at Lucas Heights, and the multipurpose camera on the Australian National Beam Line at the Photon Factory, the White group also collaborates with the Argonne National Laboratory and the Rutherford Appleton Laboratory.

Dr Tony Willis was appointed in 1985 to establish a crystal structure refinement unit for the School which was relatively

independent of Glen Robertson's research group. Tony, originally from the Allan White stable, arrived at RSC after many years working with Fred Einstein in Vancouver. With Tony's arrival there was a shift from using the home-grown software package ANUCRYS to the use of XTAL developed by Syd Hall and Jim Stewart.

Professor Bruce Hyde's solid-state inorganic research group, established in 1979, also had a strong interest in crystal structure. During the group's early years it had X-ray powder diffraction (XRD) and high-resolution transmission electron microscopy (HRTEM) as its principal analytical tools. During 1983 and 1984, John Parise added single crystal X-ray diffraction. With the appointment of Dr Ray Withers in 1986 electron diffraction in the TEM, and in particular the use of convergent-beam techniques, was added to the group's arsenal.

Upon the retirement of Bruce at the end of 1990, Ray Withers was appointed to head the solid-state inorganic group the following year. This saw a shift in the focus of the group's activity. In 1991 a strategic initiative entitled "New Generation Crystallography" was funded by the ANU's Strategic Developments Committee. The focus of this initiative was the study of modulated and other difficult crystal structures. To this end, David Rae was appointed to the group to provide the necessary single-crystal structure solving capability. David's appointment to RSC from the UNSW had followed five years of fruitful collaboration with the solid-state inorganic group. The funds from this initiative also enabled the appointment of Siggi Schmid (Research Fellow) and Klaus Futterer (PDF) to the group, with David Hockless being appointed to support Tony Willis in an expanded RSC crystallography unit. The other integral member of the group is Dr John Thompson whose expertise lies in novel synthesis as well as powder and single crystal X-ray diffraction.

The solid-state inorganic group has had long-standing collaboration with Drs Lindsay Davis, Chris Howard and Margaret Elcombe at Lucas Heights. Recent collaboration there has concentrated on the study of cubic stabilised zirconias. Over the past two years the group has also collaborated with Professor Nobuo Ishizawa of the Tokyo Institute of Technology in using the 4-circle diffractometer on the vertical wiggler Beam Line 14A at the Photon Factory, Japan.

In 1991 Dr David Ollis was appointed to establish and lead a Protein Crystallography and Engineering group at RSC. This followed the successful bid for a Centre for Molecular Structure and Function (CMSF) proposed jointly by three of the research schools as an Institute strategic initiative in the 1989 round. In just over two years David has created a fully operational protein crystallography laboratory, with the appointment of three postdoctoral fellows, Paul Carr, Eong Cheah, Karen Edwards, and three graduate students. His laboratory was the first in Australia to commission a Rigaku R-AXIS II for routine protein data collection. In addition to this central item of equipment, the laboratory houses a Rigaku AFC6R 4-circle diffractometer with rotating Cu anode, and substantial computing hardware and software for data processing and display. So far two protein structures have been solved and a number of proteins are being subjected to crystallisation trials.

As part of the CMSF, the Ollis Protein Crystallography and Engineering group benefits enormously from the collocation of complementary groups in RSC and the other research schools, enabling the group to be actively involved in recombinant DNA and protein chemistry, as well as structure analysis. The group also participates in collaborative research projects with Professor Barry Davidson at Melbourne University and Dr Subash Vasudevan at James Cook University.

Soon after the commissioning of the protein crystallography equipment, a decision was taken to upgrade the PW1100/20 to PC control using the hardware/software package developed by Zwi Barnea and Mark Grigg of the University of Melbourne Physics Department. With the decommissioning of the Picker FACS-I a Rigaku AFC6S was purchased to support the increased demand for conventional data collection. With the addition of David Hockless to the team the crystallography software portfolio has expanded to include the TEXSAN structure solving and refinement package. The expanded capability of the crystallography unit both in terms of equipment and personnel, and other recent academic appointments, has enabled a significant increase in collaboration with research groups in state universities and other Australian organisations.

The future of crystallography in all its varied forms figures prominently in RSC's strategic plan for the next five years. The School is strongly committed to maintaining its strengths in synthetic organic and inorganic chemistry, and a modern, well-supported crystallography unit is fundamental to achieving this goal. There will also be expansion in biological chemistry research with the Protein Crystallography group expected to support many of the new activities. RSC's participation in the new ANU Centre for the Science and Engineering of Materials also requires ongoing commitment to RSC's present expertise in the study of the crystal structure of "Materials". Those research groups involved in instrument development for chemical research, the Welberry group in diffuse scattering data measurement, and the White group in small angle scattering experiments and area detection, are also guaranteed of the School's support.