

Society of Crystallographers in Australia



SCA

Newsletters

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

NEWS FROM THE NATIONAL COMMITTEE

The National Committee for Crystallography has been active on both national and international business over the last two months and this report covers both.

National Business

Developments in Australia's access to synchrotron radiation facilities have occupied a number of members of the committee. The Board of the Australian Synchrotron Radiation Program (ASRP) met in Melbourne on 3 April and received status reports on the experiments in progress at the photon factory and now at the SRICAT beam lines of the advanced photon source. First experiments for "friendly users" are expected this month at the BioCARS beamline for protein crystallography and it is expected that by the end of 1998 MAD experiments can be performed. Full operation of the BioCARS beamline is not expected until at least mid-1999. As the BioCARS beamlines are completed, technical effort will be switched to the ChemMatCARS beamline and the ASRP Sub-Committee concerned with this facility is monitoring progress. It is expected that the first "friendly user" experiments would occur in mid-1999 - probably with the single crystal spectrometer (which is now being installed) and the small angle scattering facility and the surface reflectometry to follow. There continues to be strong use of the Photon Factory as a result of the recent appointments. Beamline scientists for the Photon Factory, SRICAT, BioCARS and ChemMatCARS have been appointed.

These are Dr James Hester, Dr Anton Stampfl, Dr Harry Tong and Dr David Cookson (from the Photon Factory). The ASRP Fellowships Program has also been started with the appointment of Dr Stephen Holt and Dr Megan Maher.

The meeting also discussed the project for a national synchrotron radiation facility in the context of new instruments being planned for Switzerland and Canada and the proposal being developed in Victoria for purchasing an "off the shelf" industrial synchrotron suitable for X-ray lithography and soft X-ray/ultra violet

spectroscopic work. The ASRP Board has set up a strategy committee to consider the future of the major national research facility as the present funding goes only to 2001.

The replacement reactor for HIFAR at Lucas Heights has occupied the committee as has the unexpected gap that has appeared in the funding for Australian access to the ISIS neutron scattering facility in the United Kingdom. A number of members of the National Committee and of the Academies of Science and Science and Technology have participated in the specialist committee to define the instrument arrangements at the replacement reactor at Lucas Heights and a very interesting challenge has been offered to the design team to see if a reactor design and instrument configuration can be produced which will be truly innovative. It may be possible to use not only cold neutron guides but also thermal neutron guide tubes to take neutrons to instrument halls distant from the reactor and to have very few instruments located close to the reactor itself. This will greatly improve backgrounds and also the working conditions for experimenters. A major feature is the provision of an excellent cold source to ensure that experiments done at the replacement reactor will be complementary to those at other sources in the region. John White will be appearing before the Senate Committee of Inquiry into the replacement reactor in May 1998. The National Committee and the working party of the Australian Academy of Science has made a submission to the Senate Inquiry and copies of this should be available on the Web page.

International Developments

The National Committee has made nominations to the International Union of Crystallography following discussions of suitable persons at the last two meetings of the National Committee. These are nominations for positions in the Working Commissions and the Executive. John White is on the Program Committee for the Congress and General Assembly in Glasgow in 1999 and Mark Spackman, a member of the Program Sub-Committee, is working hard to develop a full program. Both would appreciate input from members of the Society for Crystallographers in Australia about program content.

A major development in neutron science has been foreshadowed in Japan. John White (as Chairman of the National Committee) and Dr Claudio Tuniz (ANSTO) were invited to the Japan Atomic Energy Research Institute (JAERI) Workshop and Advisory Committee on their new neutron project. This is a project to produce an accelerator which would deliver at least five megawatts of energy to a target from a proton accelerator working at about 1 GeV. The project is extremely large since present technology approaches only one tenth of this. Nevertheless the advisory group was convinced that the present working technology in Japan, if invested in the proposed way, might lead to the extremely intense proton beams foreseen and that the possibility foreshadowed by the Japanese colleagues of "spallation burning" of transuranic waste might be a possibility in the first thirty to forty years of the next century. This to us would also produce an extremely intense neutron source suitable for neutron scattering experiments. A parallel, though more modest, development is being made at the KEK in Tsukuba.

At the working group meeting the question of the formation of an Asia-Oceania Neutron Scattering Association was mooted. Such a development has been under discussion for about a year through the Neutron Scattering Commission of the International Union. Strong associations have been formed in Europe and in the United States and the time may be ripe to do this in the Asia-Australasia region. The matter will be taken up at the Asian Crystallographic Association Meeting in Malaysia in October this year. Another forum in which these matters will be discussed is the meeting in Fremantle, Australia (29th September - 3rd October 1998) of the Australian New Zealand Institute of Physics Congress. A broad program of discussion of Australia's involvement in synchrotron and radiation and neutron scattering facilities will be featured at that meeting.

John White

NEW DEVELOPMENTS IN SMALL ANGLE AND SURFACE SCATTERING

Facilities for small angle X-ray (SAXS) and neutron (SANS) scattering and reflectometry are about to become more generally available to Australian scientists it was learnt at the First Australian National University small angle and surface scattering meeting held in the Research School of Chemistry at ANU on the 15-16th April. Forty scientists whose interests ranged from biology through chemistry, physics and materials science to engineering heard about the new developments.

There are varied uses for these techniques which examine the detailed structure of condensed matter on scales from about 1 to 100 nanometres, in the supramolecular nanostructure range. By use of isotopic substitution or tuning the wavelength it is possible to selectively highlight different components in bulk materials and all types of surfaces (not only air/liquid or solid but also liquid/liquid etc.) and to follow chemical reactions and microstructure and texture formation at a scale inaccessible to ordinary microscopy or light scattering.

New instruments now available include an X-ray reflectometer at the Research School of Chemistry; two more SAXS machines at ANU and the University of South Australia; and a SAXS/Grazing incidence X-ray diffraction on "BigDiff" at the Australian National Beamline Facility, Tsukuba. These significantly improve access for local scientists previously mainly reliant on less convenient synchrotron and neutron facilities such as ISIS in the United Kingdom, Argonne and Brookhaven in the United States. Future developments include the SANS machine at Lucas Heights, which is now starting to produce data; a new neutron reflectometer, also at ANSTO; and, further in the future, new X-ray machines, such as ultrahigh resolution SAXS and millisecond timescale reflectometry, resulting from Australian participation in the APS 3rd generation synchrotron source at Argonne.

To exploit these new tools the Canberra meeting drew together many of the current practitioners. The first day was devoted to reviewing the field and sharing expertise so that newcomers and students were brought up to speed in these techniques which have recently become so much more important. Twenty five talks and posters on the second day illustrated the range of current interest already existing. Examples from the area of materials included studies on templated mesoporous silicates, titania/zirconia nanoparticles, composite films of silica and organic surfactants, colloidal silica, and quantum well semiconductor devices. More direct applications to petroleum geology, alumina crystallisation from Bayer liquors, domains in wood pulps, and activated carbons for water treatment were presented. The value of bringing together a wide range of people was illustrated by the back-to-back presentation of a fundamental study of protein positioning in surfactant/polymer/water mixed phases together with an applied food-science study of the emulsifying properties of proteins.

The meeting left a clear impression that with the new apparatus these techniques can provide a new view of structure in a range in the past thought too large for chemistry but too small for engineering.

Philip

Reynolds

CRYSTAL

FRAGMENTS

- At the Research School of Chemistry, ANU, Philip Reynolds has been promoted to Senior Fellow. Stephen Holt has been appointed Australian Synchrotron Research Project Fellow and Elliot Gilbert, Karen Edler, and Wilfred Fullagar have just been conferred with their Ph.D. degrees. Elliot is now an Orica-funded Postdoctoral Fellow at ANU; Karen is a Postdoctoral Fellow at Cornell University, and Wilfred is working with Phil Coppens at Brookhaven.
- Timothy White (formerly University of South Australia) has been appointed Senior Research Officer in the Environmental Technology Institute at the Nanyang Technological University of Singapore.

NOTICE OF BUSINESS MEETING OF THE SCA

Call for Nominations

A business meeting of the SCA will be held in conjunction with the Third Meeting of the Asian Crystallographic Association to be held in Bangi in the state of Selangor, Malaysia, from 13-15th October, 1998. The business meeting has been scheduled for 1-2 pm on Thursday, 15th October. At this meeting the position of Vice-President and two positions on the Nominations Standing Committee will fall vacant. The Nominations Standing Committee have nominated the following people:

- Vice President: Dr T. Richard Welberry (Australian National University, A.C.T.).
- Member of the Nomination Committee for three terms: Dr Andrew W. Stevenson (CSIRO, Vic.).
- Member of the Nominations Committee for two terms: Dr Christopher J. Howard (ANSTO, NSW).

Additional nominations for these positions are now invited. Additional nominations should be submitted to the Secretary (at the address below) over the signatures of two members and prior to June 13th.

Trevor Hambley

AsCA

**October 13-15, 1998
Bangi, Malaysia**

Call for applications for the 'E.N. (Ted) Maslen 1987 Studentships and Scholarships' The Council of the Society of Crystallographers in Australia is calling for applications from postgraduate students of crystallography for the 'E.N. (Ted) Maslen 1987 Studentships and Scholarships' to fund attendance at the Third Meeting of the Asian Crystallographic Association to be held in Bangi in the state of Selangor, Malaysia, from October 13-15, 1998. Details of the Congress are available on the WWW at the address: <http://telperion.otago.ac.nz:800/rweavers/ASCA/asca98.htm>. SCA student members from both Australia

and New Zealand are invited to apply for the Scholarships, which will make a substantial contribution to the international travelling costs. Selections will be based upon merit, geographic distribution and previous and/or future opportunities of the candidates. As the SCA Council regards these awards as an important means of introducing young crystallographers to the international scientific community, students awarded Scholarships will be expected to make a presentation of their work at the meeting.

The method of application is straightforward, but a strict deadline will apply. Method of Application Postgraduate students applying for a '1987 Scholarship' should forward to the Secretary the following:

- An abstract of the presentation sent, or to be sent, to the Congress Secretariat.
- A covering letter from the applicant's supervisor providing a brief reference and verifying that the applicant is a bona fide student at the time of the meeting.
- An indication of what other funding may be available from the applicant's own institution.
- An indication as to whether the applicant has previously received funding from the SCA.

Applications must reach the following address by June 15, 1998: A/Prof. Trevor Hambley, SCA Secretary, School of Chemistry, University of Sydney, NSW 2006.

Alternatively, applications may be sent by FAX to 02-9351-3329.

NEW MACROMOLECULAR X-RAY LABORATORY

A new macromolecular X-ray laboratory is being setup at Monash University following the appointment of Dr Ossama El-Kabbani. Several crystallographic projects of pharmaceutical interest funded by research grants from NHMRC, ARC, Monash University and industry will be investigated. Projects include enzymes involved in the metabolism of carbohydrates, neurotransmitters and hormones. The new laboratory is located in the Department of Medicinal Chemistry at the Victorian College of Pharmacy (Parkville Campus). Data collection equipment will include a Rigaku RU-300 rotating anode generator with a MAR-345 image plate detector system, focussing mirror system, Oxford cryogenic low temperature system and an SGI O2 workstation. It is expected that the new X-ray laboratory will be operational in August 1998.

Ossama El-

Kabbani

FUTURE MEETINGS

Small Angle Scattering and Reflectometry Meeting

There are tentative plans for a hands-on workshop on reflectometry and SAXS at the Research School of Chemistry at ANU sometime in the spring. This will provide those interested in microstructures of all types

with the basic knowledge required to perform these types of experiments. Those interested are asked to contact Philip Reynolds (phil@rsc.anu.edu.au).

AsCA'98

The third Meeting of the Asian Crystallographic Association is to be held in Bangi in the state of Selangor, Malaysia, from 13-15th October, 1998. The Second Circular has been posted to those who requested it and is available on the AsCA'98 Homepage at: <http://telperion.otago.ac.nz:800/rweavers/ASCA/asca98.htm>. An edited version has been distributed with this Newsletter together with the Abstract Submission and the Registration and Accommodation Forms. A call from the Secretary of the SCA for applications for travel awards is on Page 3 of this Newsletter.

XVIII IUCR Congress Glasgow,

Scotland, August 4-13, 1999.

The venue for the XVIII IUCR Congress is the Scottish Exhibition and Conferences Centre (SECC) in the centre of Glasgow. The Congress Web page is located at: <http://www.chem.gla.ac.uk/iucr99/>.

The next issue of the Newsletter will be in August. Contributions should be e-mailed to the Editor by July 20.

FOR THE WEB BROWSERS

Some useful addresses:

- Society of Crystallographers in Australia (SCA): <http://www.sca.asn.au/>.
- ICSD - Inorganic Crystal Structure Database: http://www.fiz-karlsruhe.de/fiz/products/icsd_.html.
- ICSD - Users' Group: <http://www.rhrz.uni-bonn.de/~unc442/icsd.html>.
- PDB - Protein Data Bank at Brookhaven: <http://www.pdb.bnl.gov/>. (
- Studsvik Disordered Structures Database: <http://www.studsvik.uu.se/sdsd/Sdsdhome.htm>.
- CSD - Cambridge Structural Database information: <http://www.ccdc.cam.ac.uk>.
- CSD documentation: <http://wawona.ethz.ch/D-CHEM/CSD/docmain.html>.
- CIF - Crystallographic Information Files: <http://www.iucr.ac.uk/iucr-top/cif/index.html>.

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