

## Society of Crystallographers in Australia



# SCA

### Newsletters

## No 41, April 99

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

### FROM THE PRESIDENT

It is an honour to write to you as President of the SCA. It is a long time since, as a graduate student, I was present at the first "bush crystallographers" gathering at the University of Sydney and was somewhat awed to find myself in the company of the leading crystallographers in Australia. In that time the Society has grown to be a valuable contributor to scientific life in Australia and New Zealand.

In the last *Newsletter*, Mitchell Guss, my predecessor and wise counselor, surveyed the state of crystallography in Australia and elsewhere very effectively, and mused about the continued viability of a society of specialist crystallographers. As he noted, we may be victims of our own success because crystallography has become an integral part of so many disciplines. But this, in my view, is also a source of strength because crystallographers are at home talking to and working with scientists in many interdisciplinary areas.

This is the year of the major triennial crystallographers jamboree, that is, the International Union of Crystallography Congress and General Assembly (the 18th such meeting). By all accounts it is going to be a wonderful exhibition of the crystallographers art. We have all seen via the internet how the abstracts continue to pour in. If you can afford the time and the money I urge you to attend. It is great to have 10 days to immerse yourself in so many aspects of the science. It will be an expensive meeting and I have complained to the organisers on behalf of Society members about having to send a minor fortune to the University of Strathclyde for accommodation so far in advance, but it seems that this is beyond the organisers control. Accommodation is at a premium at Strathclyde and we are in competition with a piping conference being held there.

I have attended several of these meetings during my career and have always found them rewarding. I was booked to attend the 6th Congress in Rome but didn't finish my thesis in time so the first one that I attended was the 9th in Amsterdam. It was memorable to be able to discuss research face to face with people that previously I had only known by name. The social side was great too. I have vivid memories of the Australian contingent on the stage of the Concert-gebouw at the end of the Philips party gathered around the piano singing "Waltzing Matilda".

As a Society, we are very fortunate to have the E. N. (Ted) Maslen Travel Award Fund to provide funds to help students attend conferences. Eight of our student members from across the country, working in diverse areas of crystallography, have received awards so that they can attend the Glasgow meetings where they will present their own work and soak up the crystallography.

For those who like smaller meetings, the next gathering of the bush crystallographers (aka SCA) at CRYSTAL XXI to be held at Thredbo early next year will be a must. Richard Welberry and his committee will no doubt arrange an excellent program. (See page 4 of this *Newsletter* for further details).

For those members who are interested in the history of crystallography or who would like a nostalgic trip into the past, I notice that the newsletter of the British Crystallographic Association has published an article entitled, "The Mechanism of Beavers-Lipson Strips" (also available at <http://gordon.cryst.bbk.ac.uk/BCA/CNews/Dec98/>). The American Crystallographic Association has reproduced this in their recent newsletter along with an article on Patterson-Tunnell strips. If anyone would like to enlighten our younger members on some other aspect of historical interest, please write to Brian Skelton.

I hear that now the EIS statement has been accepted for the new reactor at Lucas Heights, the matter is now before the Public Works Committee with the prospect of tender activity by July - more good news for the scientific community in Australia.

Best wishes for the year ahead and for those of you in academia; I hope that you can find time for research in the few spare hours not occupied by teaching and administration.

*Max Taylor*

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## **The National Committee for Crystallography**

The National Committee for Crystallography continues to be a focus for action on the Australian and international crystallographic scenes. The nominated members of the National Committee for 1999 are: Dr Evan Gray (Griffith University), Professor Brian O'Connor (Curtin University), Professor John White (Australian National University), Dr Ian Grey (CSIRO), Dr Mark Spackman (University of New England), Dr Stephen Wilkins (CSIRO), Dr Mitchell Guss (University of Sydney) and Dr Peter Colman (Centre for Molecular Structure, CSIRO). A number of the members of the committee are involved in preparations for the forthcoming IUCr General Assembly and Congress in Glasgow and Mark Spackman and John White are members of the program committees.

The Committee and its members have been strongly involved in formulating advice on the Australian synchrotron radiation projects as well as the developments in connection with the proposed new research reactor at Lucas Heights to replace HIFAR.

Last year the Australian Synchrotron Radiation Program, formed by a consortium of universities, CSIRO and ANSTO, moved into its study for an Australian based synchrotron. At the most recent meeting of the National Committee, the draft proposal for the device provisionally named "Boomerang" was discussed and found to be promising for future Australian needs. Much work remains to be done and in the meantime, the access by Australian crystallographers to synchrotron radiation is increasing strongly through the programs of the Australian national beamline at the Photon Factory in Japan and through the newly established routes at the Advanced Photon Source, Argonne National Laboratory, Chicago. The most recent news from Japan is that a second beamline to provide soft X-rays for surface science will be established and that James Hester

from Western Australia now joins Garry Foran on the Australian Staff there. David Cookson, having moved from the Photon Factory to the ChemMatCARS beamline under construction at the Advanced Photon Source, is making a strong contribution there as are Anton Stampf (at the SRICAT beamlines) and Harry Tong (at the BioCARS beamlines).

Australians have been using the BioCARS beamlines in "friendly" mode since July 1998 and some structures have been solved. John White and Hans Freeman participated in a recent meeting of the CARS (Consortium for Advanced Radiation Sources of the University of Chicago) Board of Governors (April 1999) and worked through a number of the teething problems for Australian access at the BioCARS beamline with members of the CARS staff. A shortage of beamline staff appears to be an international problem developing at synchrotrons and a key matter for discussion was how to devise future strategies to maximise the convenience and scientific return from experiments as CARS gets into full gear during 1999 and 2000.

The Australian Synchrotron Research Program has set up a strategy working group to advise the Program and Review Board about a coordinated strategy for Australian overseas access to synchrotrons and the eventual construction of an Australian facility. This working group will contain members of the National Committee as well as Board members and participants from Australian industry.

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 UK. 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. 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. 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 gave evidence to the Senate Committee of Inquiry in May 1998 and will appear before the Public Works Committee in May 1999. The National Committee and the working party of the Australian Academy of Science have made a submission to the Senate Inquiry and copies of this should be available on the Academy Web page.

## **International Development**

A major development in neutron science has been foreshadowed in Japan. Professor John White (as Chairman of the National Committee) and Dr Claudio Tuniz (ANSTO) were invited to the Japanese Atomic Energy Institute (JAERI) Workshop and Advisory Committee in March 1998 and John White will return for presentation of the project in April 1999. This is a project to produce an accelerator which would deliver up to five megawatts of energy to a target from a proton accelerator working at about 1 GeV. The project might lead to the possibility foreshadowed by the Japanese colleagues, of "spallation burning" of transuranic waste in the first thirty to forty years of the next century.

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.

*John White*

## NEW XTAL 3.6 VERSION

Syd Hall and Douglas du Boulay at the University of WA and Roeli Olthof at Utrecht University have announced the release of a new version of the Xtal Crystallographic System. Unlike previous distributions, this release will be entirely via the [Xtal home page](#).

Xtal3.6 has a number of new additions to its 50-calculation repertoire. They include

- a new automatic structure solution package CRISP, employing random phase direct methods, FFT coupled with least squares atom refinement
- a new SFLS refinement package with riding constraints
- a new reciprocal-space visualisation program GIP
- a new crystal/diffractometer visualisation tool PREABS
- an improved structure manipulation tool PIG with auto hydrogen atom generation and ORTEP output
- a new colour-fill version of CONTRS and PLOTX
- scripts for attaching Xtal to Netscape for CIF data
- a web based manual which may be accessed from the Xtal homepage or downloaded for local installation.

The web approach to distribution, along with supply of executables for specific workstations (most models) rather than source files, has reduced development and distribution costs and hence the charges. In recognition of the reduced administration costs, the fees for Australian users will be A\$300 for new Xtal users and A\$150 for existing users. Other details are available on the web site.

*Syd Hall*

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## DIFFRACTOMETER UPGRADES

### **St Vincent's Institute of Medical Research**

As a part of the re-establishment of the Protein Crystallography Unit at St. Vincent's Institute of Medical Research, we purchased a MAR Research Imaging Plate detector in 1992. This detector has been pivotal for the determination of more than a dozen new protein structures over the last few years. Despite this success, some of our projects have suffered because of limitations with the current system. The availability of larger plates and easy-to-use high performance mirrors have lead us to consider the purchase of a second detector. With the generous support of the U.K. Wellcome Trust and the BHP Community Trust, we have recently purchased a large plate (345mm diameter) MAR Research scanner together with X-ray mirrors and an Oxford cryo-cooling system. We have also chosen to upgrade our existing detector with a second set of mirrors. The upgraded data collection facility will help us cope with pressing demands on the existing detector and to pursue projects which have not been previously possible because of weakly diffracting crystals and/or crystals with long cell edges.

## Maslen Travel awards

The following students have received Edward Maslen Travel awards to assist in the costs of attending the IUCr meeting in Glasgow: Kia Wallwork, (Department of Chemistry, Flinders University), Jean Kim (School of Chemistry, Sydney), Elisabeth Fletcher (Victorian College of Pharmacy), Neil Somers (Department of Chemistry, UWA), Joshua McKinnon (School of Physical Sciences and Engineering Chemistry, University of New England), Nicholas O'Toole (Crystallography Centre, UWA), Jennifer Forrester (Department of Mechanical Engineering, University of Newcastle), and Philip Nakashima (Department of Physics, UWA).

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## CRYSTAL FRAGMENTS

- Husin Sitepu (Curtin University) has graduated PhD and has taken up a position as Postdoctoral Fellow at the NIST and the State University of New York.
  - Tony Brown (ANU) has taken up a position with the public service in Canberra.
  - Alison Edwards (formerly Chemistry Department, Melbourne University) moved to ANU in January. Her position is a three year Research Fellowship working in the area of diffuse scattering from disordered systems with Richard Welberry.
  - Allan White (UWA) has recently been promoted to Professor.
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## NEW MEMBERS

The SCA welcomes the following new members for 1998/1999.

Full members:

Dr Philip Davies (Flinders University), Dr Bret Church (Garvan Institute of Medical Research, NSW), Prof. Jim Simpson (Otago University, New Zealand), Dr Ken Haller (Suranaree University of Technology, Thailand), Dr Jan Wikaira (University of Canterbury, New Zealand), Dr Mathew Wilce (University of WA), Dr Bostjan Kobe and Dr Jaime Rossjohn (St Vincent's Institute of Medical Research), and Dr Chaveng Pakawatchai (Prince Songkla University, Thailand).

Student Members:

Mr Husin Sitepu (Curtin University), Ms Helen Webb (Monash University), Mr Brett Pool (University of Melbourne), Ms Kelly Maxwell and Ms Jennifer Carmichael (Biomolecular Research Institute), Ms Kia Wallwork (Flinders University), Mr Joshua McKinnon (University of New England), Mr Philip Nakashima (University of WA), Ms Jennifer Forrester (University of Newcastle), and Ms Elisabeth Fletcher (Victorian College of Pharmacy).

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## FUTURE CONFERENCES

### CRYSTAL XXI

#### First Announcement

The Twenty First meeting of the Society of Crystallographers in Australia will be held at the Thredbo Alpine Hotel Conference Centre, Thredbo Alpine Village, NSW from February 1-4, 2000. The Organising Committee consists of Richard Welberry, David Ollis, Ray Withers, David Rae, Elliott Gilbert and Alison Edwards.

The important dates are:

September 1999: Call for Abstracts and Registration and November 5<sup>th</sup> 1999: Deadline for the Submission of Abstracts and Registration.

#### Accommodation

Accommodation in Thredbo varies in both price and standard with a wide range of options. At this time, the organisers propose to handle bookings at the Thredbo Alpine Hotel (3 star) at \$52 per person per night (double occupancy) or \$92 per person per night (single occupancy), inclusive of breakfast. There will be a second option of 4 star 3 bedroom self-catering apartments at a room only rate of \$35 per person per night where up to five can be accommodated in separate beds. These prices are subject to confirmation when prices for 2000 are finalized but are not expected to vary significantly. We hope that most people will choose one of these two options as this will tend to lower the price.

Suggestions for sponsors for CRYSTAL XXI are welcome and should be sent Alison Edwards. Further information will be included in the [conference website](#) and in the next issues of the *Newsletter*.

*Alison Edwards*

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## 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/>.

Note that the deadline for reduced rate registration and for accommodation bookings is June 1, 1999.

Forms for registration and accommodation bookings were included in the 2<sup>nd</sup> Circular which was distributed with the previous *Newsletter*. Copies can also be downloaded from the Congress web page and mailed or

faxed to the organisers.

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## SUBSCRIPTIONS

The Treasurer wishes to remind members that subscriptions for 1999 are due. The amounts payable were quoted on the blue statement forms distributed with the November 1998 *Newsletter*. The year up to which you have payed is recorded on the top right hand corner of the mailing label for this *Newsletter*. Annual Subscriptions are \$25 for full members and \$7 for student members. Payment should be sent to the Dr Brian Skelton, Treasurer SCA, Department of Chemistry, University of Western Australia, Nedlands, WA 6907.

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## Society of Crystallographers in Australia

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