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Society of Crystallographers in Australia and New Zealand SCANZ

Newsletters

No 48, February 01

The SCANZ homepage is located at http://www.sca.asn.au

FROM THE PRESIDENT

Since the last Newsletter we have sadly received news of the death of Arnold Beevers at the age of 92. Many older members of SCANZ will be familiar with his contributions to the crystallography field, most notably the famous Beevers-Lipson strips which assisted the computation of structure factors in the days before computers came to crystallography. More recently he was well known for developing the Beevers Miniature Models, of which

most, if not all, crystallography laboratories possess examples. Although I have been aware of him and his achievements ever since my student days I only ever met him once, on his visit to Australia in the early eighties, and I was struck then by his friendliness, good humour and enthusiasm. Over the years, his contributions to science, to the communication of science, and simply to the good humour of scientist and non-scientist alike have been enormous. He will be sadly missed.

On a quite different front there appears to be increasing concern about the continuing regional tensions in Israel and how they will affect the 2002 IUCr Congress. Even though colleagues from Israel assure me the impact of the trouble is minimal, the situation cannot, unless there is substantial improvement soon, but have an adverse affect on attendance figures and ultimately the success of the meeting. Word has been received that the IUCr Executive was to discuss this problem sometime in February, but at the time of writing no further word has been received on the outcome of this.

At the end of January I attended the meeting of the National Committee of Crystallography on which John White has reported in this issue of the Newsletter. One outcome of the wide-ranging discussions was that it was deemed that it would be useful to take stock of the state of crystallographic research in Australia. I undertook to make a first step by consulting the membership of SCANZ and I plan to put together a (short) questionnaire which I will circulate to the membership within the next month or two. The aim is to find out who is doing what kind of work with what facilities etc. and how this impinges on the new research reactor, the proposed synchrotron, the Australian Synchrotron Research Program and the Government's Innovation Statement, etc. I hope I can rely on everyone to take a few moments to give us this information.

Crystal XXII is fast approaching and details of registration are now available on the website (see Jenny Martin's report). I would encourage everyone to support this meeting and make the hard work that I know Jenny and her team have been putting into the organisation all worthwhile. Register early if you possibly can

as it takes a lot of burden off the organisers if everyone doesn't leave it until the last possible moment.

Richard Welberry

CRYSTAL FRAGMENTS

Alison Green has been appointed Editor of the Australian Journal of Chemistry. After spending her honours year with Richard Robson and Bernard Hoskins at Melbourne University doing supramolecular chemistry and crystallography, she undertook her PhD with Jonathan White. After graduating, she spent a year and a half in Marburg, Germany as a Humboldt Fellow with Professor Gernot Boche and two years at Wiley-VCH working, initially as a trainee Editor, and then as Associate Editor on the journal Advanced Materials.

Barbara Etschmann (formerly at UWA, and Tokyo Institute of Technology, Yokohama) has taken up an appointment at the South Australian Museum, Adelaide.

Stephen Holt (ANU) has taken up a position at the Rutherford Appleton Laboratory in the United Kingdom.

Colin Raston (Monash) has been appointed Professor of Inorganic Chemistry at the University of Leeds.

SUBSCRIPTIONS

The Treasurer wishes to remind members that annual membership dues for 2001 are to be paid by December 31, 2001. A statement was included with the November issue of the Newsletter. The amount payable is \$130 for a corporate member, \$25 for a full member and \$7 for a student member, with these discounted to \$100, \$20 and \$5 respectively if payment is made by April 1, 2001. Members who are over 60 years of age at the time subscriptions are due can elect to become Life Members of the Society by paying a one-off amount of five times the current (discounted) subscription rate (i.e. \$100).

NATIONAL COMMITTEE FOR CRYSTALLOGRAPHY

The National Committee for Crystallography at its meeting on 31 January 2001 was glad to hear from Stephen Wilkins that the project for a glossy brochure – the material largely exists already – would be converted to a website to which members of the crystallographic community can contribute and that Dr Sherry Mayo will be in charge of this. The main item of business concerned a review of crystallography in Australia, especially in the context of the recent Federation Statement by the Prime Minister. The National Committee discussed the possible ways in which the newly announced major national research facilities program might be implemented and, in particular, its relationship to a proposal for the renewal of the Australian Synchrotron Research Program (ASRP) as well as the proposal for a synchrotron in Australia.

In a statement from the Australian Academy of Science the importance of curiosity-based research was emphasised, the Prime Minister's statement being the first steps in Australia catching up with its competitors in North America, Japan and Europe in scientific infrastructure and industrial investment.

The formation of an Asian-Pacific Neutron Scattering Association was also discussed. Extensive discussions

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held at meetings in Japan in November 2000 look as if they will have an outcome in the formation of an Asian-Oceanian Neutron Scattering Association in conjunction with the Asian Crystallographic Association meeting in Bangalore in November 2001. Very encouraging news for those interested in the use of neutron scattering in our region is the recent funding of the joint JAERI (Japanese Atomic Energy Research Institute) – KEK (Tsukuba) project for a high intensity spallation neutron source costing more than \$US1 billion.

The National Committee noted the number of Australians participating in IUCr Commissions and other offices and will be making nominations for the Executive in May this year. The National Committee also strongly endorsed Professor Mark Spackman's proposals for a Sagamore Conference between 17 and 22 August 2003 in Australia.

John White

ChemMatCARS UPDATE

The Australian Synchrotron Research Program is an Institutional member of ChemMatCARS, which operates Sector 15 at the Advanced Photon Source, the 7 GeV third generation synchrotron light source at Argonne National Laboratory in the USA. Australian users, via the ASRP, will have access to around 20% of the beamtime at ChemMatCARS starting this year.

ChemMatCARS operates one insertion device beamline with three experimental stations. A bending magnet beamline is planned for the second phase of the facility.

The current capabilities are:

*Surface X-ray Scattering and diffraction,

*Small and ultra-small angle X-ray scattering,

*High-resolution crystallography, including "micro" crystal, time-resolved and multi-wavelength capabilities.

David Cookson, the resident ASRP scientist, and the rest of the ChemMatCARS team are nearing the end of the beamline construction phase, and are to be congratulated on producing a world class facility, both in terms of scientific capability and their emphasis on user support. The SAXS and crystallography facilities are largely complete, and accepting users as part of the commissioning process. The current status of the three experimental stations is:

Crystallography

A Bruker kappa diffractometer, incorporating a CCD detector, was commissioned in late 2000. Good data has been obtained from crystals with dimensions in the 10-20 micron range. Dr James Hester, from the ASRP staff in Japan, was the first Australian to use the diffractometer (in November of last year) and reports: "The Bruker area detector system on the ChemMatCARS beamline provided data with which a number of structures were solved for tiny single crystals (maximum dimension < 50 microns). No data had been obtainable with a laboratory system. Crystal twinning, when present, posed no significant problem, and data collection times were of the order of five hours for a highly redundant data set. While some doubts remain as to the possibility of doing electron density studies with the current configuration, it is eminently suitable for structural studies of small crystals."

SAXS

The first SAXS patterns from rat-tail collagen have been obtained, using a 100 ?m pinhole, a sample to detector distance of 1.8 metres, an image plate detector and 120- second exposures. Further optimisation should reduce the required time to below 10 seconds. While the minimum Q range achieved with the beam stop used in this trial was about 0.01 Å-1, it is anticipated that using the full flight tube will allow a minimum Q of about 0.003 Å-1.

Surface Scattering/Diffraction

The liquid surface reflectometer is largely complete. It is anticipated that it will be commissioned in February-March 2001.

Further Information and Proposal Submission

Proposals are currently being accepted for crystallography and SAXS at ChemMatCARS. Prospective users should contact the author in the first instance (see e-mail address below). Further details on the status and performance of the ChemMatCARS beamline and experimental stations can be found on the ASRP and ChemMatCARS websites at http://www.ansto.gov.au/natfac/asrp.html (ASRP) and http://cars9.uchicago.edu/chemmat/chemhome.html (ChemMatCARS). The proposal package can be mdownloaded from the ASRP site.

Richard Garrett

CRYSTAL XXII

Crystal XXII is the twenty-second conference of the Society of Crystallographers in Australia and New Zealand and will be held from 7-10 July 2001, directly after the Brisbane IUPAC conference. The conference seeks to bring together all with an interest in crystallography and related fields from Australia, New Zealand and beyond. The venue is Couran Cove, an eco- tourism resort on South Stradbroke Island, just a short distance from Brisbane and the Gold Coast.

Registration forms are now available on the Crystal XXII website <u>http://www.chemistry.uq.edu.au/crystal22</u>. Registration forms and abstracts are due on 27 April 2001. A variety of accommodation styles are available at Couran Cove. Floor plans of the various types of rooms, suites and cabins can be found on the Crystal XXII website and more information about the facilities at the Couran Cove Resort can be found on the website <u>http://www.couran-cove.com.au/</u>.

Program Information

The conference will begin with registration in the late afternoon of Saturday 7 July followed by a welcome barbecue that evening. Sunday 8 July and Monday 9 July will have a full program of presentations including a poster session. A conference dinner is planned for Monday evening. Tuesday 10 July will have a half-day program of presentations and the conference will wrap up with a farewell lunch that day. The plenary speaker is Professor Sung Hou K im from Berkeley University, California and keynote speakers are Jacqui Gulbis (Walter and Eliza Hall Institute of Medical Research), Trevor Hambley (U. Syd), Pat Kelly (U. Qld), Mark von Itzstein (Griffith U.) and Richard Welberry (ANU).

Transfer Information

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If travelling by plane to Brisbane, you will need to travel from the airport to Runaway Bay, about 40 minutes south. CoachTrans runs a regular coach service from both domestic and international terminals at Brisbane Airport to Runaway Bay. You can purchase your tickets with CoachTrans upon arrival at Brisbane Airport, asking to be dropped off at the Couran Cove Check-In desk at Runaway Bay. When you arrive at Runaway Bay you will need to check in your luggage at the Couran Cove desk and board the catamaran for transfer to Couran Cove.

A special price for the catamaran return trip has been negotiated for the Conference and this can be booked on the Registration Form.

If you have any further questions, contact the local organising committee by e-mail at crystal22@chemistry. uq.edu.au.

Young post-graduate and post-doctoral SCANZ members (other than student members) are invited to apply for financial support to attend the Crystal XXII meeting under the "Young Scientist" support initiative. Each application will be considered on its merits.

Jenny Martin

COUNCIL ELECTIONS AND BUSINESS MEETING

Members are advised that a Business Meeting of SCANZ will be held during Crystal XXII at the Couran Cove Resort from 7-10 July.

This meeting brings with it the end of the current terms of office of Dr Max Taylor (Past President), Dr Richard Welberry (President), and Dr Brian Skelton (Treasurer). To fill the vacancies thus created, the Nominations Committee, in accordance with Article IV and Rules III and IV of the SCANZ Constitution, has nominated Dr Jenny Martin (Univ. of Queensland) for Vice-President, Dr Paul Carr (ANU) for Treasurer, and Dr Brian Skelton (Univ. of Western Australia) for Council.

Thus, taking account of the pre-determined positions, officers standing for re-election and new nominations, the proposed composition of Council and Standing Committees for the term beginning in July 2001 is:

President: M.A. Spackman (University of New England, NSW)*

Vice-President: Jenny Martin (Univ. of Queensland)+

Secretary: B.J. Kennedy (Univ. of Sydney, NSW)*

Treasurer: P.D. Carr (Australian National University, ACT)+

Council

- S.W. Wilkins (CSIRO Materials Science, Vic)*
- G.B Jameson (Massey University, NZ)*
- B.W. Skelton (Univ. of Western Australia, WA)+
- ANCCr Representative: J.W. White (Australian National Univ., ACT)* ex officio

Past-President: T.R. Welberry (Australian National Univ., ACT)*

Nominations Standing Committee

S.R. Hall (Univ. of Western Australia, WA)*

C.J. Howard (ANSTO, NSW)*

A.W. Stevenson (CSIRO Materials Science, Vic)*

*pre-determined position,

+new nomination

Dr Brian Skelton will also continue as Newsletter Editor.

The invitation is now extended for any member to submit additional nominations for any of the positions for which vacancies will occur, i.e. for all but pre-determined positions.

Nominations must be submitted to the Secretary, over the signatures of two members, by June 1 2001. If none are received, the candidates nominated by the Nominations Committee will be deemed to have been elected and will take office at the Business Meeting in July 2001.

Brendan Kennedy

MASLEN SCHOLARSHIPS

The Council of the Society of Crystallographers in Australia and New Zealand is calling for applications from postgraduate students of crystallography for the 'E.N. (Ted) Maslen 1987 Studentships and Scholarships' to fund attendance at Crystal XXII to be held at Couran Cove Resort from 7-10 July 2001.

Details of the Conference are available in this Newsletter and on the conference website at: <u>http://www.chemistry.uq.edu.au/crystal22.</u>

SCANZ student members from both Australia and New Zealand are invited to apply for the Scholarships, which will make a substantial contribution to the travel costs. Selections will be based upon merit, geographic distribution and previous and/or future opportunities of the candidates. As the SCANZ 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 'Maslen 1987 Scholarship' should forward to the Secretary the following:

*An abstract of the presentation sent, or to be sent,

*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,

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*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 SCANZ.

Applications must reach the following address by 1 May 2001:

Dr Brendan Kennedy,

SCANZ Secretary,

School of Chemistry, F11

University of Sydney

NSW 2006

Alternatively, applications may be sent by FAX (+61)-02- 9351-3329.

AsCA'01

AsCA'01 is the fourth meeting of The Asian Crystallographic Association (AsCA) and will be held at the Indian Institute of Science, Bangalore, India, during November 18-21, 2001.

The First Announcement is included in the posting of this Newsletter. Some information was also included in the November 2000 issue. The second announcement will include more information about the scientific and social programs, submission of abstracts and hotel accommodation etc. Further information, including a reply form, is available at the Conference Website: http://www.iisc.ernet.in/~asca401.

An international symposium on Crystallography and Bioinformatics in Structural Biology is planned for 22-25 November 2001 at the Indian Institute of Science, Bangalore, India to follow the AsCA'01 meeting.

Registration will be US\$100 for full participants, US\$70 for students and US\$50 for accompanying persons. Accommodation will be arranged in hotels of categories ranging in price per day from US\$15 to US\$150. Social Programs for registered delegates and accompanying persons will be organised. The second announcement will include more information about the scientific and social programs, submission of abstracts, hotel accommodation etc. and will be available on the website http://www.iisc.ernet.in/~asca401/satellite.