



Society of Crystallographers in Australia and New Zealand SCANZ

Newsletters

No 47, November 00

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

FROM THE PRESIDENT

In the previous *Newsletter*, I referred to an article published in the *St George & Sutherland Shire Leader* attributing to the Chief Executive of ANSTO (Professor Helen M. Garnett), a statement that ANSTO expects to save \$200 million per year on the cost of Australian scientists using neutron scattering facilities overseas following the establishment of the replacement research reactor. As a result of my comments I received a letter from Professor Garnett who, while welcoming SCANZ's interest in and support for the replacement reactor, wishes to set the record straight on this issue. Apparently she made no such statement. Her reference to \$200 million was in the context of the potential benefits to Australian industry from the replacement reactor – a figure derived from a consultancy study undertaken by Access Economics for ANSTO in 1997.



While on the subject of the replacement reactor, since the last *Newsletter*, a Senate Inquiry has been set up to look at the process by which the contract was awarded. As a result of some prompting by FASTS, I was invited to make a submission to the Senate Inquiry on behalf of the Society. This I did after consulting with other members of the SCANZ Council. Although the terms of reference mostly covered areas involved with the process of awarding the contract, the first was 'the need for a replacement reactor', and in my submission I deemed it only appropriate to comment on this item. Since this document is no longer in the public domain, I am not at liberty to publish the details. Suffice it to say that I reported that members of the Society were strongly in favour of the replacement reactor irrespective of whether they were themselves involved in neutron scattering. I understand that details of the Inquiry will eventually be published on the Web.

Following the submission, I was invited to give evidence before the Senate Committee on 27th October. (Brendan Kennedy similarly gave evidence on behalf of ANBUG on the 26th). Since I have little first-hand experience of neutron scattering I thought it would be a good idea to take along Darren Goossens (my Post-Doctoral Fellow, less than a year out of his PhD in neutron scattering). Darren is not only articulate and well versed in neutron matters but also is part of the youth of SCANZ for whom the new reactor represents the future. The experience giving evidence was an interesting one. We were allocated 30 minutes, which allowed for us to make an opening statement followed by the opportunity to answer questions from the Senators. The proceedings were running late so that our arrival coincided with the beginning of the submission given by the Institute of Engineers. It was a public hearing so we were at liberty to hear others'

evidence. This was useful since it gave us an indication of the types of questions we might be asked and was also reassuring because the arguments the Engineers were putting were much the same as ours. Less reassuring were the names of other groups giving evidence on the same day, e.g. the 'Medical Association for Prevention of War'.

Early this month there was a 'Science meets Parliament Day' We were asked by FASTS to send a representative to this and Alison Edwards agreed to go on our behalf. Alison's report on this meeting appears on page 4 of this issue of the *Newsletter*.

Jenny Martin and her committee organising Crystal XXII have been working hard on our behalf, with the First Circular being included in the posting of this *Newsletter*. Jenny has had to grapple with the intricacies of GST and ABN's, things that were mercifully absent when I was involved with Crystal XXI. As a result of this, it has been decided that SCANZ needs to have its own Australian Business Number (ABN) and Brian Skelton is organising this at the moment.

Richard Welberry

SUBSCRIPTIONS

The Treasurer wishes to remind members that annual membership dues for 2001 are to be paid by December 31, 2001. A statement is included with this *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).

SAGAMORE XIII

The Sagamore meetings focus on aspects of charge, spin and momentum distributions, their determination from a wide variety of experimental techniques, and their detailed analysis and comparison with theory, and have a considerable history, recently documented by Malcolm Cooper (see http://alpha.uwb.edu.pl/sagamore/page_history.html). In particular they are traditionally located in "an isolated place near water or otherwise beautiful place, where the participants would have the possibility to enjoy sports and outdoor activities" (Pekka Suortti).

Perhaps the most important, and probably unique, feature of the Sagamore meetings is that they provide an opportunity for so many scientists from quite disparate disciplines to meet scientifically and socially, and this in turn must lead to closer collaboration and a better mutual understanding and appreciation of one-another's science.

Hotel Anders provided some excellent outdoor facilities beside the lake, but one had to judiciously choose

which lectures not to attend in order to take advantage. The meeting attracted just over 100 participants, with nearly half of those in attendance from either France or Poland. Ludwik Dobrzynski and his Local Committee did a truly superb job of organising the meeting, impressing all with their warm hospitality and the ease with which they assisted with all manner of requests, not to mention their dancing and piano playing skill. As expected, the oral and poster presentations contained more physics than chemistry, but that did not distract from some wonderfully lively discussions, even if there was always the perception that most present worked and thought in either direct space or momentum space, and had some difficulty traversing the landscape in between.

Many presentations dealt with the use of synchrotron radiation in various forms, and this was reflected in the large number of participants from ESRF and Japan. However, there was a disappointing turnout from the charge density, neutron and electron diffraction communities, and the discussions could have benefited from a few more theoreticians. A number of talks described quite substantial and dramatic improvements in methods and measurements (shorter times and increased accuracy and precision), and it was clear that maximum entropy methods are being employed to great effect in all aspects of charge, spin and momentum density research.

Particular highlights included talks by Heinz Graafsma (ESRF) on electron densities from synchrotron sources, Francis Tasset (ILL) on spherical neutron polarimetry (which promises to enable solution of magnetic structures that were previously intractable), Wolfgang Jauch (Hahn-Meitner Institute), on the benefits of gamma radiation (in particular he presented evidence that the long-standing discrepancy between X-ray and neutron ADPs is due to the use of graphite-monochromated Mo radiation, and also detailed studies on extinction which strongly corroborated the standard Becker-Coppens model), Dylan Jayatilaka (UWA) on the extraction of density matrices from X-ray diffraction data, Abhay Shukla (ESRF) on Compton scattering (which was claimed to be more sensitive to intermolecular interactions than conventional charge density studies), and Keijo Hämäläinen on high-resolution Compton scattering.

As is often the case for meetings like this, there was a surprisingly high attendance by Australian scientists in various guises, and Australians contributed four of the 36 oral presentations: Erich Weigold and Maarten Vos from the RSPSE at ANU (Maarten spoke on results obtained with the new (e,2e) spectrometer constructed at ANU), Victor Streltsov and Dylan Jayatilaka from UWA (Victor spoke on the use of complementary synchrotron and electron diffraction data in a charge density study of Al_2O_3 , work done with Philip Nakashima and Andy Johnson at UWA), Barbara Etschmann from Tokyo Institute of Technology (who presented a poster describing a synchrotron charge density study of the high-Tc material $\text{La}_{1.88}\text{Sr}_{0.12}\text{CuO}_4$, work done with Nobuo Ishizawa), and Mark Spackman from the University of New England (who presented results from a recent CCD charge density study on benzene, a collaboration with Judith Howard's group in Durham).

Even with such a large number of oral presentations over the five days, the meeting was not devoid of social diversions. One of the sponsors was the Dojlidy Brewery, and beer was provided free of charge on most evenings. A bonfire night served to break the ice the following evening at the Warminska Inn, with a superb show of regional singing and dancing by the WARMIA ensemble was enthusiastically enjoyed by all, especially those who "sampled" vodka with their meal, and the morning excursion to nearby Olsztyn and Ostroda, including visits to castles with a show of old knights' fights (somewhat too realistic for some!) was a welcome opportunity for most to see something of the countryside.

As an interesting footnote, the IUCr Commission on Charge, Spin and Momentum Densities was formed in 1975 as an outcome of the Sagamore meetings, and to this day the CSMD Commission is actively involved in the planning and execution of these conferences. An offer to host the next Sagamore meeting in Australia was

endorsed at an open meeting of the Commission, so those with an interest in charge, spin and momentum distributions should pencil in Sagamore XIV for mid-August 2003, hopefully on an island off the southern Queensland coast.

Mark Spackman

University of New England

FUTURE MEETINGS

AsCA'01

Asian Crystallographic Association

18-21 November 2001

Indian Institute of Science

Bangalore, India.

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 scientific program includes plenary lectures, symposia and poster presentations. A number of satellite symposia and workshops will also be organised, either before or after AsCA'01. It may be possible to provide partial financial support to selected young crystallographers to enable them to attend the Conference.

The venue of the meeting, the Indian Institute of Science (IISc), founded in 1909, is one of the oldest modern research centres in Asia. Bangalore weather is good throughout the year and is very pleasant during November.

Symposium topics

A1 Foundation, theory and history of crystallography

A2 Instrumentation and Techniques

A3 Crystallography in physics

A4 Crystallography in chemistry

A5 Crystallography in materials science

A6 Crystallography in biology, medicine and Pharmacology

A7 Powder methods

A8 Aperiodic structures

A9 Charge density studies

A10 Crystallographic education

Registration

1. Full Participants (Before Jun 30, 2001) \$US150, (After June 30,2001) \$US180
2. Student Participants (Before Jun 30, 2001) \$US100, (After June 30,2001) \$US120
3. Accompanying persons (Before Jun 30, 2001) \$US40, (After June 30,2001) \$US 50

Registration will cover conference material, local transport, coffee, snacks and lunch served during the meeting.

Organising Committees

The International Organising Committee is chaired by Zihe Rao (China), and the International Programme Committee by C.J. Howard (Australia). The National Organising Committee consists of M. Vijayan (Chair, Bangalore), Krishan Lal (Co-Chair, Delhi), M.R.N. Murthy (Secretary, Bangalore) and T.N. Guru Row (Treasurer, Bangalore).

Other Information

Accommodation will be arranged in hotels of categories ranging in price per day from \$US15 to \$US150. 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 and hotel accommodation etc. Further information, including a reply form, will be available soon at the Conference Website: <http://www.iisc.ernet.in/~asca401>.

All correspondence should be addressed to Prof. M.R.M.Murthy, Secretary of AsCA'01, e-mail: murthy@mbu.iisc.ernet.in.

CRYSTAL XXII

Crystal XXII, the twenty second conference of the Society of Crystallographers in Australia and New Zealand, will be held in Queensland in 2001. Dates for the conference are Saturday 7 July to Tuesday 10 July, 2001, and follows the IUPAC conference in Brisbane. The venue for Crystal XXII is Couran Cove, an eco-tourism resort located on South Stradbroke Island, close to both Brisbane and Gold Coast (Coolangatta) airports. The First Circular has been distributed with this *Newsletter*. Further information will be available in the next issue of the SCANZ *Newsletter*, due out in February, and on the Conference Website: <http://www.chemistry.uq.edu.au/crystal22>.

Jenny Martin

IUCr XIX

The 19th Congress and General Assembly of the IUCr will be held in Jerusalem, Israel, August 6-15, 2002. A Preliminary Registration form can be found on the Congress Web page at <http://www.kenes.com/iucr/>.

MASLEN SCHOLARSHIPS

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

Applications will be required early 2001 and will require the following information:

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 Society.

Further information will be available in the next *SCANZ Newsletter* in February 2001.

Brendan Kennedy

Secretary, SCANZ

SCIENCE MEETS PARLIAMENT DAY

On November 1st it was my privilege to be the SCANZ delegate to the Science Meets Parliament Day. This is the second time that FASTS - the Federation of Australian Scientific and Technological Societies - has run

this event and it appears to be gaining strength with around 160 scientists attending.

The day before the event, we gathered at the National Press Club to hear Dr Neal Lane, science adviser to President Clinton, enumerate the profound effects of scientific advance on the U.S. economy. He presented a compelling case for the funding of basic research from the public purse based strongly on the demonstrable public benefits arising from such research. He made a case that even the most hard-nosed economic rationalist would not be able to beat. It was heartening to hear of his success in working with the U.S. President to propose an increase in the Science Research budget of some 17% to Congress and ultimately achieving a 14% rise in this budget. I am sure all of us present hoped that our Prime Minister and his advisers paid close attention to what Dr Lane had to discuss with them in their subsequent meetings.

Perhaps one of the most notable aspects of this talk was the quality of his presentation. It is clear that as a scientist he has been doing an outstanding job of promoting science to politicians by presenting the case for science in terms that politicians understand. The text of Dr Lane's speech is available at <http://www.usyd.edu.au/su/fasts/2000/Lane.html>.

Once this presentation was over, we were treated to a crash course in how to lobby politicians. FASTS had organised a series of speakers to fill us in on what would and would not work in our discussions and also outlined a series of priorities, which were to form the basis of the discussions with politicians the following day. The dominant theme was to emphasize the need to view science as an INVESTMENT. These lobbying lessons were a worthwhile exercise, as I believe that most of the scientists present had little if any idea of how to go about effective lobbying. I hope that SCANZ will continue to participate in this endeavour in future as this aspect of the meeting on its own could have profound benefits for science - particularly if the opportunity to participate can be shared widely in the membership.

The preparation day concluded with a cocktail reception in the Mural Hall at Parliament House. This concluded at around 8pm, and I think most of us retired to locations where we could assimilate the large quantity of material that we had been provided with to help prepare for our meetings.

The day designated Science Meets Parliament Day dawned bright and sunny and after receiving our accreditations, we were permitted unescorted access to most areas of Parliament House. Perhaps the biggest challenge was finding the way to our meetings on time. After an initial phasing problem, a rotation through π was required, this being not too much of a problem for those of us prepared to read signs! Most scientists had at least two meetings with Parliamentarians, generally along with one or two colleagues.

I was assigned to meetings with Sid Sidebottom (ALP Tas.) and Senator Lyn Allison (Dem. Vic.). Both were clearly pro science research and our interaction with them was very positive. I will endeavour to follow these meetings up in some of the ways suggested over the next few weeks.

I would like to thank SCANZ for providing me with the opportunity to participate in this event and I hope that the Society will continue to participate in future years.

Alison Edwards

ANU