

## Society of Crystallographers in Australia



# SCA

### Newsletters

## No 30, December 1995

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

### FROM THE PRESIDENT

AsCA '95, the second meeting of the Asian Crystallographic Association, was held at Chulalongkorn University, Bangkok from 22-24 November 1995. Students who attended the meeting with financial support from SCA have been invited to write reports on this meeting to appear in the next issues of the *Newsletter*. It seemed to me that the meeting was well organised (any problems that did arise must have been quietly and effectively resolved) and successful. Ward Robinson, Phathana Phavanantha, Y. Ohashi and the other members of the various conference committees, are to be congratulated on their efforts. There seems little doubt that a third meeting will be held in 1998, at a venue yet to be decided. By my reckoning, there were something like twenty-seven Australians in attendance, and twenty-four Australian presentations, a pleasing representation given that the meeting was held only seven months after Crystal XIX. New Zealand was also well represented.

While others of us were in Bangkok, we asked Ray Withers to represent the SCA at the Annual Council Meeting of the Federation of Australian Scientific and Technological Societies (FASTS) which was held at the ANU on November 23rd. Ray's report appears elsewhere in this *Newsletter*. Having read the FASTS policy document produced in July, I recognised some elements of the FASTS policy appearing in the Prime Minister's Innovation Statement. Perhaps FASTS is beginning to influence government (or vice versa?).

The detail of the Innovation Statement conveyed exciting news for crystallographers. The proposal to obtain access to the Advanced Photon Source (Argonne National Laboratory), described at some length in the January 1995 *Newsletter*, has been approved for funding. The funding also provides for the continuation and further development of the Australian National Beamline Facility at the Photon Factory, Tsukuba, Japan. (See John White's report in this Newsletter.) John White, John Boldeman, Peter Colman and Richard Garrett will be starting detailed discussions with the Advanced Photon Source in mid-January - we wish them success in this important mission.

Finally, some information on future meetings. The International Schools and Conference on X-ray Analytical Methods organised by the Australian X-ray Analytical Association, to be held in Sydney, 18-25 January 1996, will certainly interest many of our members. And the IUCr XVII Congress and General Assembly is to be held August 8-17, 1996, in Seattle, Washington. As usual, there will be several satellite meetings and workshops associated with the Congress. Full details are available in the Second Circular, which has now been circulated, or on the WWW (address as in 'call for applications'). Student members of the SCA who wish to attend the IUCr Congress are invited to apply for financial support from SCA, in the manner detailed in the separate announcement ('call for applications'). Young scientists seeking financial assistance who do not meet the SCA guidelines are advised to apply for travel grants direct from the Congress organisers.

As I finish writing this contribution, I am looking forward to the Christmas festivities. By the time you read it, however, the festive season will be over. I hope you enjoyed it, and I wish you all an interesting and successful 1996.

*Chris Howard*

## Sketches of Crystallography Laboratories

### Monash University

The X-ray crystallography laboratory at Monash University is part of the Chemistry Department and began with the appointment of Bryan Gatehouse to the department in January 1965. An 'apprenticeship' with the late A.D. (Dave) Wadsley in the early 1960's resulted in the structure of the high-temperature form of niobium pentoxide being determined and a gift of a PW1008 generator, a Weissenberg goniometer, and a Debye-Scherrer camera, being made by CSIRO. This equipment became the beginnings of crystallography in the Chemistry Department.

At the time, the late 1960's and early 1970's, the main crystallographic work was that on mixed-metal oxides such as alkali metal molybdates, tungstates, niobates and tantalates. A number of structures determined in the latter two groups were using crystals supplied by Dr. R. S. (Bob) Roth from his group at the then, National Bureau of Standards (now N.I.S.T.) in the U.S.A.. Bob has visited and worked in our laboratory on a number of occasions.

The pace increased with the provision of two more PW1008's and Weissenberg goniometers together with the light boxes necessary for the measurement of intensities. Computing in the early 1960's was done on SILLIAC in *continued on next page*

Sydney, subsequently at Fishermen's Bend on the Elliott 803 and then on a CDC 3200 in the Computer Centre at Monash University.

With the extension of the buildings of the Chemistry Department in the early 1970's, \$63,000.00 was made available for the purchase of a single crystal diffractometer. The Philips PW1100 was selected even though we had to wait upwards of two years for the production model to arrive. This machine has served us well and although at the time of writing we are having trouble with one of the discrete components on a board in the interface, I am confident that it will run for some years to come. It must be admitted that the drive program is still on paper tape!

In May 1989 the second diffractometer, a Nicolet, arrived in response to the demand for more and more structures; data collection can be carried out from room temperature down to -100 C. The crystallography 'service' is run by Dr. Gary Fallon. Gary nurses the diffractometers, looks after the software, rejects crystals firmly when necessary and provides the necessary information for publication of the results. The major program used for many years has been that by George Sheldrick; SHELX, of various years.

By far the majority of structures determined in the laboratory at Monash University are of the coordination or organometallic type reflecting the interests of staff mainly in the inorganic area. Over the years many organic and mixed metal oxides structures have also been determined, again reflecting the interests of other staff members.

With the appointment recently of Professors Raston and Bond, added impetus has been given to the upgrading of our facilities. Colin Raston enabled the provision of a Silicon Graphics computer together with the TeXsan software and it is likely that the rate at which we are able to collect data will undergo a transformation in the not too distant future.

Structure determination is alive and well at Monash University but with the passing of time crystallography is slipping away from us.

*Bryan Gatehouse*

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## Prime Minister's Innovation Statement.

### Major National Research Facilities Program

The Prime Minister's Innovation Statement has funded a Major National Research Facility for synchrotron radiation research available to the whole of Australia's research community. National Committee for Crystallography took the lead in 1994 to examine Australia's needs and options in this area and reported to the Academy of Science in December. For this project, National Committee had been enlarged to a working group with representative crystallographers from a number of universities nominated by their vice-chancellors, CSIRO and ANSTO as well as Australian Spectroscopy and Surface

Science groups. This group became a Steering Group for the proposal which was submitted in February 1995 through ANSTO. (John Boldeman and Richard Garrett deserve our thanks for finishing a fine document and for the follow through.) The proposal has now been funded at a level of \$12.2M over five years.

Key aspects of the program are:

- Maintenance of the strong links created with the Photon Factory, Tsukuba, Japan through developments at the now very successful Australian National Synchrotron Beamline there and possibly other beamlines.
- Access to the 1,000 million dollar Advanced Photon Source (APS) at the Argonne National Laboratory, Chicago, USA. This ranks with the ESRF (Grenoble) as the world's prime sources of the high intensity, pulsed X-rays needed by Australian biologists, chemists, crystallographers, materials scientists and physicists. The intense X-rays provided by this facility will allow a major component of Australian science to stay at the forefront of international competitiveness.
- A Fellowship Program to which members of the Steering Group, the Australian National University and the Universities of Melbourne, Monash, New South Wales (ADFA), Queensland, Sydney and Western Australia, as well as ANSTO and the CSIRO, have promised cash contributions amounting to more than a million dollars. This program will ensure that a new generation of scientists skilled in synchrotron radiation X-ray methods will enter the Australian scientific community.
- A detailed study of the technical possibilities and scientific/technological needs for a future Australian based synchrotron.

At a meeting in the Australian Academy of Science on 7 December 1995 representatives\* of all of these universities and ANSTO and CSIRO responded to the Prime Minister's announcement with decisions on the next steps for negotiation and formation of a business plan.

John Boldeman, Peter Colman, Richard Garrett and John White will go to the Advanced Photon Source in Chicago, mid January 1996, to discuss with them and the CARS consortium the details of Australian involvement there. Also a letter is to be sent to the Director of the Photon Factory (current chairman of the Australian-Japanese Steering Committee for the Australian National Beamline) expressing our pleasure that the present work and future development at the Photon Factory have been funded.

*John White*

\* The representatives were Dr John Boldeman, Dr Richard Garrett (ANSTO), Dr Peter Colman, Dr Steven Wilkins (CSIRO), Professor Hans Freeman (Sydney University), Dr Ian Gentle (University of Queensland), Professor Dudley Creagh (University of New South Wales, ADFA), Professor Syd Hall (University of Western Australia), Professor Keith Nugent (University of Melbourne), Professor Robert Leckey (La Trobe University), Professor John White (Australian National University, Chairman). Monash University was represented by Professor Nugent and Dr Wilkins. Dr Mitch Guss (Sydney University) was unable to attend.

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## **Report on FASTS Council Meeting**

A FASTS (Federation of Australian Scientific and Technological Societies) Council meeting was recently held at the ANU in Canberra on November 23. Due to the pleading of Chris Howard, and as the only token crystallographer not in Bangkok on the chosen day, yours truly got to attend as the SCA representative. This is my report of what went on.

For those who don't know, FASTS is a lobby group comprising numerous Scientific and Technological Societies (including RACI, AIP, ANZSCB, SCA, etc) organised into 9 sections (Biological, Earth, Mathematical, Chemical, Marine, Medical, Physical, Plants & Ecology, Associate members) which lobbies politicians, business etc. on behalf of ~40,000 working scientists across Australia. It has an elected President (as from November 24 Joe Baker, ACT Commissioner for the Environment), Secretary, Treasurer, an 80% full-time Executive Director (Toss Gascoigne, Executive Director, FASTS, PO Box 218, Deakin West, ACT, 2601; Ph: 06-282 2026; Fax: 06-282 2953; E-mail: [fasts@anu.edu.au](mailto:fasts@anu.edu.au)), a new office in Deakin, Canberra and a World Wide Web site (<http://bimbo.pharmacol.su.oz.au/fast>)

/fasthome.html) which is currently in the process of being linked to its member societies' pages.

What does it do? Over the past 12 months FASTS has produced a well-received policy document *A Science Policy for Australia in the 21st Century* launched at Parliament House in July, made submissions on science and technology policy to numerous parliamentary committees e.g. to the House of Representatives Standing Committee on Industry, Science and Technology Inquiry into Innovation Policies, the NSW Review of Profiles and Outcomes, to PMSEC regarding medical research funding, to DEET regarding ARC, to DIST regarding the upcoming Innovation statement and the Effective Patent Life for Pharmaceuticals etc.

On behalf of FASTS the President has participated in ASTEC's Future Needs study as a member of the Reference Group, spoken at the CSIRO's Post-Budget Forum in Canberra and at the RACI's Public Relations Forum in Adelaide, been a member of the round table chaired by Senator Cook on innovation in the pharmaceutical industry and in Senator Cook's teleconference on S&T inputs into the APEC Forum. Toss Gascoigne has addressed scientists in Brisbane and Perth on the importance of scientists communicating their work to the public. Significant radio and print media coverage on a wide range of science and technology-related issues has also been obtained over the past twelve months. (Several journalists were present at the November 23 meeting to report on the comments of Senator Cook and Robert Hill). Further details are available in the President's report to the Council meeting.

What were some of the issues discussed at the November Council meeting? What FASTS did well during the year and where it should do better (interacting with member societies', interactions with consumer and related organisations, making the case for basic research, lobbying State and Territory Governments rather than the Federal Government), how to build up the FASTS member base, how can FASTS have a more substantive route into Government, possible changes to the policy document and what questions should be asked of Senator Cook and Robert Hill (the Opposition spokesman on Education and Science) who each addressed the meeting for about 20 minutes and answered questions for around 30 minutes. Originally the Government's Innovations Statement was to be the basis of the questions asked of the politicians. The delay in releasing the policy however, meant the questions had to be of a rather more general nature. Questions asked of both politicians included what was the future of ASTEC, the Office of the Chief Scientist and the Australia Prize, how can FASTS contribute to the development of policy on S&T, what is the strategic plan of the Government when it comes to S&T, what are the implications of regional development for science policy?

What were the answers? To be honest - I can't remember too well!! Impressions? Both politicians made the point that Australia has a very strong fundamental science base. We evidently rank 4th out of 25 OECD countries as regards public spending on R&D as a function of GDP. Our public sector spending on ARC and NH&MRC are at record highs e.g. NH&MRC funding increased 11% from \$129.7 million in 1995 to \$144 million in 1996. On the other hand, private sector spending on R&D is abysmal. We rank about 18th out of the 25 OECD countries. It does not take a genius to see where Government priorities are going to lie almost irrespective of who gets in at the next election. To paraphrase Senator Cook "we are good at creating new knowledge but not at creating new products or at commercialising ideas".

There was talk of international consortia to share expensive infrastructure, of increased dialogue between the financial and scientific communities, of PMSEC/ASTEC orchestrating a national debate on what Australia's national science priorities should be, of building programs which might more successfully encourage private sector R&D, etc. At this point your eyes are probably starting to glaze over like mine were so I had better stop here.

All in all, the day was a useful learning experience about an important scientific lobby group that we would do well as practising scientists to learn more about and to support.

Ray Withers

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## Ballot

Results of the postal ballot to change the constitution regarding the appointment of the SCA Newsletter Editor as described in the previous *Newsletter* are as follows: Thirty three ballots were received with 31 being in favour of the change and 2 against.

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## Report from the National Committee for Crystallography

The National Committee for Crystallography met on Wednesday 22 November 1995 in the context of the Asian Crystallographic Association meeting in Bangkok. Apart from formal business, a number of matters were discussed which might be of interest to all members of the Society.

In connection with the General Assembly of the International Union in Seattle, August 1996, there was some discussion of the role played by the various commissions and it was felt that there was tendency with the growing number of commissions for the focus of the Union to become too diffuse. There was some support for a request to the executive to re-examine the role of the commissions. Also the new tendency in this year's program introduced by a working party under David Cox and Jim Jorgensen, for more science-oriented microsymbosia e.g. on hot topics in materials science, to replace more technique-oriented microsymbosia, was supported.

Reports were taken from various members of the National Committee who had been concerned with different aspects of the Major National Research Facilities proposal for Synchrotron Radiation research. The result of the competition had not been announced at that time, but it was resolved that there should be a meeting of the proponents as soon after the announcement as possible whether the result was positive or not.

There was some discussion about the next steps to be taken with respect to neutron facilities in Australia, in particular the need for a cold source HIFAR as an immediate method of addressing the problem of Australia falling behind the rest of the world in this area from the point of view of home-based facilities. The crystallographic development in Asia was also discussed, in particular the possibility of a future venue for the Asian Crystallographic Association meeting in Indonesia. Chris Howard was asked to follow this up and Professor O'Connor said he would use his contact as well.

*John White*

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## **IUCr XVII Congress and General Assembly**

**August 8-17, 1996, Seattle, Washington, USA**

### **Call for applications for '1987 Scholarships'**

The Council of the Society of Crystallographers in Australia is calling for applications from postgraduate students of crystallography for '1987 Scholarships' to fund attendance at the Seventeenth International Congress of Crystallography to be held in Seattle, USA, from 8-17 August 1996.

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, as the deadline for submission of abstracts to the IUCr Congress Secretariat is February 15, 1996, and for registration, June 1 1996. Full details of the Congress are available on the WWW at the address: <http://nexus.hwi.buffalo.edu/ACA/IUCr/index.html>.

#### **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.

Applications must reach the following address by February 15, 1996: Dr Mark A. Spackman, SCA Secretary, Department of Chemistry, University of New England, Armidale, NSW 2351

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