

Society of Crystallographers in Australia



SCA

Newsletters

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

FROM THE PRESIDENT

I am writing this column on Wednesday November 12. This is important because despite being only six weeks until Christmas, I, like many others around the country, am still awaiting the results of grant applications to the National Health and Medical Research Council and the Australian Research Council. This is a national disgrace. Many young capable scientists, postdoctoral Fellows funded by these granting agencies, on fixed term appointments which expire at the end of the year depend on the results of these applications to plan their careers. As researchers based in universities or research institutes, we are expected to be more professional and manage our research in a business-like manner. The real needs of our research community have been paid scant attention by those who administer our competitive grants. Any increase in the ARC base as a result of possible recommendations by the West Committee to return all institutional research block funding to the competitive system should be treated with great caution given the present state of the administration.

On a brighter note it was pleasing to see that the Nobel prizes awarded this year in both Medicine and Chemistry were for work associated with protein structure although neither of the recipients was a protein crystallographer. The medicine prize, awarded to Stanley Prusiner for his discovery of Prions, proteinaceous infectious particles, and the supposed disease-causing agents of Scrapie, CJD and Mad Cow Disease among others, has thrown down the challenge to structural biologists to establish a plausible mechanism for the transmission of these diseases. John Walker and Paul Boyer were awarded the Chemistry prize for their work on the structure and mechanism of the proton-translocating ATP synthase, the enzyme which uses external energy to produce ATP (adenosine triphosphate), the chemical energy currency of all living systems. Their hypotheses that had resulted from over 20 years of exacting biochemistry were ultimately confirmed by the crystal structure of the enzyme solved by Andrew Leslie and John Walker and their colleagues in Cambridge in 1994.

The award of the Nobel prize for Chemistry illustrates how even protein crystallography is now a servant of biology and not an end in itself. In the early 1970's every new protein structure was a significant event as was each small molecule structure in the 1950's. These days hundreds of structures are solved each year and it is the significance of the chemistry, physics or biology that really matters. This has consequences for our *Society*. Chemical crystallographers, who were a significant part of the membership 20 years ago, now find their first allegiances elsewhere. Crystallography Societies and crystallographic meetings overseas have

prospered with the enormous growth in research on the structures of macromolecules and with advances in materials science. What is the future in Australia? We should be thinking about how these changes will need to be addressed to build on the past successes of the SCA.

Mitchell Guss

AsCA'98

Plans for the forthcoming AsCA'98 meeting in Malaysia (13-15 October 1998) are proceeding very well. The First Circular has been printed and sent to the various National representatives for distribution and will also be printed in the Journal of the Crystallographic Society of Japan. A copy of this circular, together with a form to register interest in the conference and a request for a copy of the Second Circular are also available on the AsCA'98 Homepage on the internet: <http://gandalf.otago.ac.nz:800/rweavers/ASCA/asca98.htm> which can also be reached by a link from the SCA Homepage: <http://www.sca.asn.au>.

Plans for a wide ranging scientific program are also well in hand and the meeting will feature a half day IUCr50 Symposium to celebrate the 50th Anniversary of the IUCr.

I have also heard from Professor Sen Gupta that he is organising an International School on Powder Diffraction (ISPD-98) in Calcutta, India from 7-10 October, 1998. Since this is just before AsCA'98 it is hoped that many participants from Asian countries may like to attend both meetings. Further details will be available shortly.

Jim Simpson

THE NATIONAL COMMITTEE FOR CRYSTALLOGRAPHY

The National Committee for Crystallography met on 4 September 1997 at the Academy of Science. This report covers some of the matters discussed in the Agenda and the National Committee would be grateful for comments on these items from the SCA membership.

International Union of Crystallography

The Committee agreed that names canvassed at the April 1997 meeting for nomination to Commissions would be forwarded to the IUCr.

Professor White reported that the Neutron Scattering Commission at the closed meeting in Toronto (August 1997) had agreed to sponsor a second round of the powder diffraction project done ten years ago at PETTEN. Dr Jorgensen had agreed to coordinate the project and to edit the book. The Commission asked that the Powder Diffraction Commission be consulted about their collaboration. Professor O'Connor and Dr Howard agreed to participate.

Dr Howard advised that he is in his last term as Co-Editor of the Journal of Applied Crystallography and as member of the Commission of Journals and may choose to retire at the end of his term. Other IUCr business flagged included the issue of the cost of journals and developments in electronic publishing.

It was noted that the World Intellectual Property Organisation (WIPO) is meeting in Geneva in late September and is in the process of developing a treaty on databases which could have a profound effect on the free exchange of data. The National Academy of Sciences prepared a publication in April 1997, called Bits of Power, and an extract of this relating to Crystallography will be forwarded separately.

Congress 1999

There was a wide-ranging discussion on the structure of the Assembly and Congress and the Scientific Program. The following comments were made during the discussion for the Chairman to relay to the Conference organisers.

Macromolecular crystallography takes up a very large portion of the total Program and Professor White asked if people had suggestions about ways to solve this, to forward these to him.

There was some discussion on whether the success of satellite meetings has weakened the Congress. It was suggested that the view that the macromolecular field dominates the Congress may be partly accounted for by the fact that it has no satellite meeting. One of the problems is the size and the long duration of the Congress. There is value as the world crystallography community attends but, given the number of satellite meetings, there is a lot of repetition as papers are repeated at both forums. Dr Howard commented that he does not believe the success of the satellite meetings has 'weakened' the Congress, especially if participant numbers are anything to go by.

Microsymposia

Professor White asked if the Committee members had any suggestions for the Microsymposia, he could take to the Program Committee. There was general endorsement of the suggestions put forward by Cox and Jorgensen that the program should have a series of scientific themes and not be too technique orientated.

Congress 2005

There was some discussion about whether Australia should put in a bid to host the 2005 Congress, noting that it would be 20 years since the Congress has been held in Australia. After discussion, it was agreed to explore with the Society of Crystallographers in Australia (SCA) if there is enthusiasm to hold either a regional meeting or the 2005 Congress in Australia. Dr Guss has subsequently reported that he has found little enthusiasm for a bid for this Congress.

Recent Developments in Synchrotron Radiation Research in Australia

The Chairman sought the Committee's comments on developments regarding access to Synchrotron Beam Radiation, following the Academy's 1994 paper on the subject and developments since.

Photon Factory

It was reported that there were an increasing number of Australians and groups using the Beamline at Tsukuba, although there were some structural matters that needed to be attended to with the establishment of the Australian Synchrotron Radiation Program (ASRP). These include arrangements for representation on the Australian-Japan Steering Committee.

Access to the Advanced Photon Source (APS) at the Argonne National Laboratory

This is proceeding smoothly, but no results will be available for another year. As Australia is already two years into the program, good results are needed to ensure future funding. At the APS, all experimental beamline facilities are being funded and constructed by Collaborative Access Teams (CATS). Australia is a member of the CARS Consortium (University of Chicago and others) and the SRI CAT of the APS. The Australian Synchrotron Radiation Program (ASRP) is now incorporated and has a Policy and Review Board under which an Executive Committee and four specialist committees operate. The committee structure is serviced by ANSTO.

National Facility for Synchrotron Radiation (Australia-based)

The Committee considered the merits of undertaking a study and if the Academy should lobby for a synchrotron radiation facility in Australia.

Professor O'Connor commented that the management of a neutron scattering program is a fundamental problem and there is a need for a study which involves both neutron scattering and an Australian synchrotron. There is a synergy between the two techniques and there needs to be an overriding management of the two activities. The concept of a national facility was proposed. The success of the Australian Synchrotron Radiation Program was mentioned and this model should be paralleled in neutron scattering.

Recent Developments in Neutron Scattering Research in Australia

A most timely discussion on the facilities for neutron scattering in Australia was held. The Federal Government had announced its plans to build a replacement reactor for the HIFAR reactor at Lucas Heights only a few days before.

Professor White referred to the submission the Academy had prepared to the 1993 Review conducted by McKinnon. One of the strengths had been that it was a non-partisan document. The Academy's recommendations to the McKinnon Review had stressed issues such as safety, the need for a new reactor to be of scientific value to the whole region, and that one of the tests of quality is competition for access and complementarity to existing resources in the region.

The report to the Executive and Council of AINSE, by Dr Laurence, was largely endorsed. This paper was attached with the business papers. In particular, Dr Laurence's comments that a reactor neutron source is complementary to, rather than superseded by, access to good synchrotron radiation sources or spallation neutron sources and that a new Australian facility should be designed to fulfil a regional role building on Australia's strengths in instrumentation and experience in operating such a research facility. It was agreed that access to the overseas sources continued to be a high priority in widening of Australia's science and technology base as well as preparing for the new facilities. It was agreed to stress Dr Laurence's point that 'the relationship between AINSE and ANSTO is highly relevant - the missions of both bodies are in general agreement, but differ significantly; they exist in a necessary but difficult alliance, and the aims of the universities, represented by AINSE, do not always match the very different corporate requirements of ANSTO. Neutron science continues to be an important part of AINSE activities, reflecting the interest by university research groups, but just as ANSTO changes the relative importance of its major activities, so does AINSE.'

Other points in Dr Laurence's paper which were given strong endorsement were that 'a new neutron science facility should be seen as part of Australia's regional involvement. Linked to the cold source, our instrumental excellence will be a real resource for the region and Australia could assist in the development of neutron

instrumentation throughout the area. However, there are important time constraints and the opportunity to develop as a specialist regional centre will not persist.' Committee members agreed that an Academy study should stress the importance of the cold source.

International S&T Collaboration Program

It was noted that the funding provided by DIST for access to the Major Research Facilities Program, managed by ANSTO, has increased from \$150,000 to \$326,000, with \$20,000 deducted for ANSTO management. There is a Review of this Program under way and it was suggested that the Academy write to Mr Bob Pegler, who is managing the Review, advising that the Access Program is very valuable in terms of performance for unit dollar. Data from the reports provided with the agenda papers substantiated this. For example, a table prepared by Dr Margaret Elcombe, and attached with the Laurence paper, illustrates the way that having access to overseas facilities has had a big impact on increasing the number of neutron scattering publications from Australian researchers.

Other Business

Professor White sought the Committee's comments on producing a publication similar to the National Committee for Astronomy. Members saw benefit in such a publication. It was suggested that a title like Structure of Matter may have more meaning to people than "crystallography". It was agreed that there are some good examples which would sell the interests of crystallographers, such as the work of Peter Colman on the influenza virus, work on surfactants, and the Buckminster Fullerenes

After discussion, it was agreed that a small group, comprising Dr Chris Howard, Dr Steven Wilkins, Dr Ian Grey and Professor Brian O'Connor, would form a working group to develop the concept further and to seek funding.

Professor White sought comment from Committee members on Australia's participation in IUCr Commissions. He advised it is now time to put forward nominations.

John White

SUBSCRIPTIONS

The Treasurer wishes to remind members that annual membership subscriptions for 1998 are now payable. A statement was included with the previous Newsletter.

The amounts are \$25 for a full member and \$7 for a student member, with these discounted to \$20 and \$5 respectively if payment is made by April 1, 1998.

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SKETCHES OF CRYSTALLOGRAPHY LABORATORIES

James Cook University

In the late 1960's Les Power was appointed to the Department of Chemistry and crystallography had its roots at James Cook University in the purchase of a Philips 1010 generator with Powder Cameras. These were used by both the Chemistry and Geology Departments until 1970 when a Weissenberg camera and a Joyce Loebel densitometer were acquired for use in general crystallography.

With the appointment of Chris Cuff in 1971, links were made with the minerals industry following a purchase of a X-ray powder diffractometer. Early Ph.D. graduates from the joint programs were Ken Turner and John King. Between 1972 and 1982 diffraction studies were undertaken on many minerals by, among others, Ken Turner, Ian MacKinnon, and John Parise.

In 1975 a Siemens Elmiscop 102 TEM and an Analytical Etec SEM were purchased and lattice imaging work commenced. Single-phase transformation work was initiated in 1976 with the acquisition of a high pressure anvil cell. Les Power, the father of crystallography at James Cook University was killed tragically in a plane crash in 1977.

In 1982 a second X-ray powder diffractometer was purchased and initial visits by Sharon Ness (ex-Flinders) commenced. During 1982-86 John Thompson (Geology/

Chemistry) began studies on Rietveld powder refinements and their correlation with magic angle spinning NMR spectroscopy. In 1987 the Cuff/Ness collaboration on carbonate minerals began with the then recently acquired Jeol 2000 FX Analytical TEM. A Jeol 840 microprobe was purchased in 1988. 1989/90 marked the beginnings of the Instrumentation Centre/Advanced Analytical Centre. A Siemens 303 X-ray Fluorescence Spectrophotometer was also purchased during this period with collaborations with Judge Bevan beginning in 1991. A Siemens D 5000 X-ray powder diffractometer was purchased in 1993, and in 1994 an initial suggestion to form a Siemens Applications Laboratory was put

forward by Sietronics Australia Pty. Ltd.

Sharon Ness was appointed Director of the Advanced Analytical Centre in 1995/96 and soon thereafter the Siemens Applications Laboratory opened within the confines of the Centre. A Jeol SEM and an X-ray Fluorescence Spectrophotometer were purchased for the Cairns arm of the Advanced Analytical Centre. A Siemens D 5005 X-ray powder diffractometer and an Enraf-Nonius CAD4 single crystal diffractometer (acquired from the University of Auckland) were purchased in this period.

With the appointment of Peter Junk in early 1997, X-ray diffraction studies on small molecules using the CAD4 diffractometer began in earnest. The structures now being studied range from small organic and organometallic compounds through coordination complexes up to relatively large supramolecular compounds. The XTAL suite of programs is used for structure solution and refinement.

In 1997 the Advanced Analytical Centre became the first laboratory in Australia to acquire a Siemens General Area Detector Diffraction System (GADDs) for micro X-ray work. The Centre performs many functions including collaborative and service research work for many departments within the University, such as Earth Sciences, Chemistry, Chemical Engineering, Archaeology, Biochemistry and the Australian Centre for Tropical Freshwater Research. Most of this work involves the identification of phases and quantification of samples using X-ray diffraction, TEM, and X-ray Fluorescence. A considerable amount of service work is performed for external industries, mainly in the identification of samples such as oils, liquids, minerals and plant materials. While the work for external areas can be rather diverse, particularly that for the forensic sciences, the bulk of the work arises from the mining industry

Society of Crystallographers in Australia

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