Society of Crystallographers in Australia and New Zealand

SCANZ

(formerly: Society of Crystallographers in Australia (SCA))

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

January 2009 Newsletter

From the President *(Steve Wilkins, CSIRO)*

The society of crystallographers is a wonderful international fellowship and conglomerate of a diverse range of scientific disciplines. At the Osaka IUCr Congress last August, the IUCr achieved its 60th anniversary of the first IUCr Congress and General Assembly that was held at Harvard. It also marked the 60th anniversary of the birth of *Acta Crystallographica*, which was one of the main reasons for the formation of the IUCr. The founding editor of Acta and a protagonist in the formation of the IUCr was Paul Peter Ewald, notable also for his pioneering of the dynamical theory of X-ray diffraction (and the eponymous sphere used in depicting Bragg scattering geometry in reciprocal space).

Around 40 Australians attended the Congress in Osaka. Such Congresses are a chance to look both backwards and forwards. They are also a great opportunity to catch up with old colleagues and to make new contacts. Among the 60th Anniversary commemorative events were many lectures on the past, notable among which was an overview talk by Ted Baker and from the journals side by Andre Authier, and also a substantial exhibition of historical photos organized by Bill Duax with major input from the SCANZ side by Syd Hall.

One of the amazing aspects of IUCr Congresses as well as regional crystallographic conferences such as CRYSTAL and AsCA meetings is that they bring together a diverse range of scientific disciplines. I would venture to suggest, that these days very few people are crystallographers first and some other discipline second. Nowadays they seem to be structural biologists or oxide chemists or materials scientists or… first and crystallographers second. They may have different types of samples and types of applications, but there is a considerable commonality of interest in methods, results, sources, detectors and approaches to data analysis. This unity in diversity is one of the enduring and regenerative strengths of the crystallographic community.

As we approach the holding of our own biennial CRYSTAL conference (formerly the "Bush Crystallographer's Meeting"), I encourage you to attend and also to especially encourage any young scientists in your area who are embarking on a PhD involving crystallography, to also attend.
The details are:

CRYSTAL 26
14-17 April 2009
Novotel Barossa Valley Resort, Rowlands Flat, Barossa Valley, SA
http://xrsi.cmit.csiro.au/SCANZ26/

Information on how to apply for Studentships is also contained. In case of any queries, contact

Crystal26@csiro.au

Finally, the passing of Hans Freeman on the 9th November last is noted with much sadness. Hans was a pioneer of structural biology in Australia and a colleague and mentor to many. He was the First President of SCANZ (then SCA), even though he initially argued against formalization of the "Bush Crystallographers" into the SCA, but changed his view once Australia secured the rights to hold the 1987 IUCr Congress in Perth and formalization became desirable. This Perth meeting was a great success in no small part due to Hans very able chairing of the Program Committee. Hans also played an important role in various aspects of the establishment and operation of a synchrotron capability for Australia.

Obituary – Hans C. Freeman (1929–2008) (*by Mitchell Guss, USyd*)

Australia's scientific community lost a leading figure when Hans Freeman, Emeritus Professor at the University of Sydney, his alma mater, died on November 9, 2008. Hans was a pioneer first of chemical and later of biological crystallography in Australia. He was the first president of the Society for Crystallographers in Australia (later to become the SCANZ). He served for many years as the Chair of the National Committee for Crystallography of the Australian Academy of Science. His former students and post-doctoral Fellows hold positions in many leading laboratories in Australia and overseas.

He will be remembered as much for his influence on science policy as for his research and as a great teacher and mentor. Hans was born in Breslau, Germany and migrated to Australia at the age of nine in 1938. Hans completed his schooling at Sydney Boys High and then proceeded to Sydney University where he graduated with first class Honours and the University Medal in Chemistry. His Honours and Masters research were conducted in the laboratory of Professor Raymond LeFevre on the dipole moments of organic compounds. The award of a Rotary Foundation Fellowship permitted Hans to spend a year at the California Institute of Technology. It was there under the guidance of Eddy Hughes that Hans was seduced by the beauty of molecular structure and the tools of crystallography.

Hans completed the structure of biuret hydrate for his PhD which was awarded by the University of Sydney in 1957. This led naturally to a study of the copper complex of biuret that gives its name to a method for determining protein concentration. A *Nature* paper describing this structure was published in 1959. During the course of this early structural work Hans acquired an interest in the methods of crystallography and the supporting technology. He published two papers in the *Australian Journal of Chemistry* in 1957 and 1958 describing the use of Australia's second digital computer, SILIAC, for crystallographic calculations. At the same time he published papers on "A Polynomial Approximation to the Atomic Scattering Factor" and on "Scattering from an Infinite Elliptical Cylinder" both in *Acta Crystallographica*. During most of the 1960s the crystallographic laboratory at the University of Sydney determined the structures of a large number of metal complexes of amino acids and peptides. This work resulted in the publication of two large reviews that remained the definitive works in the field for many years, establishing Hans as a leading figure in the field of bioinorganic chemistry.

In 1970 Hans took the next logical step, and, with the support of the University of Sydney, formed what was to become the first protein crystallography group in Australia. Others in the crystallographic community feared, with some justification, that macromolecular research would drain funding from other aspects of the field. The success of macromolecular crystallography in Australia supports Hans' vision and may justify the fears of the critics. Hans' initial aim for protein crystallography was focussed on a single target – the 'blue' copper protein plastocyanin. Inorganic chemists were fascinated by its intense blue colour and unusual redox chemistry but had failed to create a small molecule mimic. In the days before recombinant protein expression, the group in Sydney purified plastocyanin from thirteen different plants before suitable crystals were finally obtained from extracts of poplar leaves pruned from trees on the university campus. The highly cited work that described the structure was a significant achievement in the field of bioinorganic chemistry and is widely quoted in many texts to this day.

Hans was a regular and enthusiastic participant at casual meetings of the so-called 'Bush Crystallographers' in Australia held every couple of years. These meetings were characterised by a total lack of formality. Hans chaired the organising committee for the meeting of the Bush Crystallographers held at the Hawkesbury Agricultural College in 1976. It was at this meeting that a formal proposal to create a society for crystallography in Australia was put forward. Hans was a vocal opponent of the idea favouring a continuation of the informal meetings. But once it became obvious that a society would be formed, Hans produced a fully-fledged constitution out of his pocket (actually a slightly altered version of the American Crystallographic Association articles) and then graciously agreed to be the first president of the SCA. The constitution written for a much larger association created practically as many committees as there were crystallographers in Australia making the SCA the most over-organised group despite its humble and informal origins. The constitution was subsequently modified to remove the unnecessary levels of governance.

One early outcome resulting from the creation of the SCA was the award of the IUCr Congress and General Assembly to Perth in 1987. Hans was the programme Chair for the meeting and he ensured that there was a focus on outstanding science. The exceptional local organisation, led by Ted Maslen and Syd Hall, together with the strong programme resulted in a financial as well as scientific success. A lasting legacy of this meeting is the ability to fund the Maslen travelling scholarships for Australian and New Zealand students and to bring a distinguished lecturer to each of the local meetings of the society.

In total, Hans authored over 160 research papers, and received practically every honour available to a chemist in Australia including the Burrows and Leighton medals of the Royal Australian Chemical Institute and the Craig medal for chemistry from the Australian Academy of Science. He was elected as a Fellow of the Academy in 1984 and was recognised by the Australian Government for contributions to chemistry by being made a Member of the Order of Australia in 2005.

Once elected to the Academy, Hans used the opportunity to make a significant and lasting contribution to Australian science when he co-authored a report entitled "Small Country, Big Science". The report highlighted the need for access to major research facilities not available in Australia at the time, including high intensity neutron and synchrotron X-ray sources. As a result, the Australian government made travel funds available for qualified Australian scientists to access overseas facilities. Indirectly this led to the establishment of the Australian Synchrotron Research Programme (ASRP) of which Hans was a board member until its incorporation into the Australian Synchrotron in 2008. Access to synchrotron sources, first at the Photon Factory in Tsukuba, and later at the Advanced Photon Source, Argonne was a major boost to crystallography in Australia.

Hans listed his non-scientific interests as opera and travel and he indulged these whenever he had the chance. Hans Freeman leaves behind a legacy of significant research, institutional innovations and generations of students imbued with a love of science. He is survived by his wife, Edith, of more than forty years, his loving children, Maeva and Philip, and his sister, Eva.

1987 Maslen Scholarship Recipient Reports

Nyssa Drinkwater *(Institute for Molecular Bioscience, UQ)*

Erice 2008, From molecules to medicine: integrating crystallography in drug design, May 29- June 8, 2008

As we drive from Palermo (the main airport of Sicily, Italy), the crystal blue water of the Mediterranean behind us, we approach a looming mountain with a small town visible on top – our destination for the 40th crystallographic meeting of Erice. This year the annual crystallographic course held a focus on drug design, and the who's who of crystallography and drug design have assembled to participate in this unique meeting. The opening address was given by the director of the school Sir Tom Blundell from Cambridge University, which set the tone for a stimulating and productive nine days.

My first and foremost opinion on this meeting is that there is none other quite like it. The Erice meeting is a school, with the primary focus remaining on students and young scientists. As such, students made up the majority of the participants, and were all given the opportunity to present their research at poster sessions. The program however was designed to suit everyone. Lectures were held in the morning, workshops in the afternoon, and evenings were spent in a casual interactive atmosphere around tables at local restaurants or at parties at a central venue. The result was an ideal mixture of conference, meeting, and school, with a level of interaction between participants of all levels of experience as well as between industry and academia, unlike no conference I have attended.

Speakers were carefully selected to cover a wide variety of topics and issues relevant to drug discovery. These ranged from historical topics (Trevor Petcher spoke on Crystallography and drug design: where from?) to the most up-to-the-minute international research (Bill Weiss of Stanford University on the structure of the beta-adrenergic receptor). Speakers covered traditional crystallography approached with new directions (Terese Begfors from the University of Uppsala on the crystallisation strategy at the RAPID center), as well as using crystallographic information in combination with bioinformatic tools (John Irwin from UCSF speaking on virtual screening).

Workshops were run by the experts in hands-on and demonstrative environments. Again the depth of the field was demonstrated by the choice of workshops ranging from crystallization to database resources (CCDC, EBI and PDB) and computational tools (CCP4, DOCK and GRID).

After an inspiring meeting, the participants parted ways, and there wasn't one person I spoke to who didn't vow to keep in touch and to attend an Erice course again soon. I sincerely thank the conference organisers and directors for putting together an amazing meeting and for inviting me to attend. I also thank SCANZ for supporting my attendance with the Maslen award.

Anthony Chesman *(School of Chemistry, Monash University)*

IUCr 2008 Osaka, 23-31 August, 2008

Being awarded a Maslen scholarship allowed me to attend the XXI Congress of the International Union of Crystallography Congress and General Assembly held in Osaka, Japan. This conference provided the opportunity to see a diverse range of lectures covering a wide spectrum of crystallographic topics, from the floating zone method of crystal growth to improving the efficiency of protein crystallisation and everything in between. It also exposed me to size of the international crystallographic community, a fact that can be lost on a student in Australia.

Personal highlights of the conference included Masahiro Irie's excellent lecture on photochroism with reversible colour and shape changes and Sumio Iijima's work on carbon nanotubes. With six concurrent lecture streams there was always something to see and the bento boxes at the luncheon seminars were a tasty diversion. The poster presentations contained some great displays, particularly interesting was current work to send proteins to the International Space Station for crystallisation under zero gravity conditions.

After hours I walked around streets of Osaka to find a new place to eat or to simply try to find my hotel again. The kind people of Osaka happily tolerated another disorientated conference attendee pointing wildly at menus and despite the frequent communication breakdowns would always point me in the right direction when I was lost. I recommend any student interested in pursuing further study in crystallography apply for a generous Maslen scholarship if wishing to attend an international conference. It is a great chance to experience a new culture while learning of the great advances being made across all areas of crystallography.

Forthcoming Major Meetings

April 14-17, 2009 CRYSTAL XXVI –Biennial meeting of the Society of crystallographers in Australia and New Zealand.
July 25-30, 2009 ACA 2009 – XXI Toronto, ONT, Canada. www.amercrystalassn.org
August 9-14, 2009 ECM 25 – Istanbul, Turkey. www.ecm25.org/

Australasian Crystallography School – Chardonnay Style– July 6-12, 2008

(by Jamie Rossjohn, Monash, on behalf of the co-chairs Matt Wilce & Stuart Batten))

X-ray crystallography (both Chemical and Biological) has impacted profoundly on basic and fundamental science and has been central to many important Australasian-centric discoveries spanning a number of decades. Thus, more laboratories are interweaving crystallography into their armoury of techniques to address their particular chemical or biological question. Given this crystallographic explosion, and the improved and more rapid methodologies available to determine crystal structures, there has been a long-standing concern that researchers involved in this technique do not have sufficient theoretical or practical knowledge in the technique itself. Hence, largely due to the pioneering efforts of A/Prof. Matthew Wilce and Dr. Stuart Batten (Monash University), the inaugural Australasian Crystallography School was held from 6th-12th July 2008 at the Yarra Valley Conference Centre, near Melbourne. The conference centre, its staff and dining was excellent and made for a very relaxing atmosphere whilst the participants grappled with the fundamentals of crystallography during a very busy week.

The School combined the interests and expertise of small molecule crystallography and protein crystallography, and was attended by 42 researchers (PhD students or post-doctoral researchers) with representations from Victoria, New South Wales, South Australia, Queensland and New Zealand. The lecturers and tutors came from all over Australia, and we were particularly grateful to those who travelled interstate to participate, namely Dr. Paul Carr (ANU), Dr. Darren Goossens (ANU), Dr. Janet Newman (CSIRO), Dr. Tom Caradoc-Davies (Australian Synchrotron), Dr. Peter Turner (University of Sydney), Dr. Paul Jensen (University of Sydney), Dr. Julian Adams (Australian Synchrotron), Dr. Jason Schmidberger (Monash University), Dr. Marcia Scudder (University of N.S.W.), Nathan Cowieson (Monash University), Fasseli Coulibaly (Monash University). Moreover, the international profile of the Crystallography School was enhanced by the invaluable addition of four eminent crystallographers who have significant involvements in overseas crystallography schools, namely: Prof. Peter Main (York University, UK), Prof. David Watkin (University of Oxford, UK), Prof. Murray Stewart (Cambridge University, UK) and Prof. Garry Taylor (University of St. Andrews, UK).

The school provided a refreshing mix of the theoretical and practical aspects of crystallography, with the former being held in the morning and hands-on tutorials in the afternoon/early evening where each student was provided with their own workstation. The initial aspect of the course focussed on common (chemical and biological) sessions on basic aspects of crystallography, including Fourier syntheses, reciprocal space, Bragg's law, symmetry, and twinning. In the later part of the week the program was divided into two parallel streams, one for protein crystallographers (29 students), and one for small molecule crystallographers (13 students). These parallel sessions concentrated on aspects of specific interest for each stream. In addition, the course also incorporated a remote access session to the Australian Synchrotron, in which a crystal was mounted in

the X-ray beam and data collected without leaving the Yarra Valley). Moreover, we also learned about the research interest of the participants courtesy of rapid-fire short presentations each evening which were sporadically interrupted by hearing of the exploits of Matt's previous incarnations.

Judging by the feedback from both the students and the tutors the school was an outstanding success and the obvious question arises when will the next one be held? The organisers would like to thank the generous sponsors (Monash Centre for Synchrotron Science, the CCDC MMSN, SCANZ, AINSE, Monash University, Bruker, Meeco Holdings, Oxford Diffraction, the Australian Synchrotron, and Faculty of Medicine, Monash University) that enabled the course to be held with minimal costs to the students.
Moreover, we are very grateful of the tutors, the local and international lecturers who put in considerable time and effort into developing and delivering the course, and also to the students for their enthusiastic participation.

Medals Update

As detailed in the previous newsletter, SCANZ is seeking to institute two new medals to be presented by the Society at our CRYSTAL meetings. These will be an open award and a mid-career award. The proposed guidelines were published in the previous issue of the Newsletter and comment invited then; further comment is still welcome. A related issue to be addressed is that we would like to name each of them after an eminent scientist (or scientists) with links to the areas covered by the Society, preferably with an Australian or New Zealand connection (Dummy names are given below). Thus we are seeking suggestions and supporting comments from members. Please send your comments to me (Stuart Batten; stuart.batten@sci.monash.edu.au) by the end of March so that they may be considered by Council. It is intended that the guidelines will be put to the general meeting at Crystal 26 for formal approval and, if approved, then the medal names agreed on by the Council will be announced.

The Don Bradman Medal

for distinguished contributions to science involving X-ray, neutron or electron diffraction and/or imaging

1. The Medal shall be awarded to a financial member of the Society who, in the opinion of the SCANZ executive or duly appointed representatives, has contributed most towards the development of a branch of science associated with X-ray, neutron or electron diffraction and/or imaging.

2. The award is based on consideration of the candidate's published scientific work, together with other evidence of his or her standing in the international community. A major portion of the relevant scientific work must have been carried out in Australia and/or New Zealand while the candidate was a member of the Society.

3. The medal shall be awarded to coincide with SCANZ conferences, and the successful candidate will be required to deliver a lecture at the appropriate conference.

4. The award will consist of a medallion, free registration at the SCANZ conference at which they will receive the award, a return economy airfare from the awardee's home city and $750 towards accommodation expenses (if the awardee is not a resident of the city in which the meeting is held). This will be provided by SCANZ in conjunction with the conference organisers.

5. The nominee must have been a member of SCANZ for the previous 10 years.

6. Nominations (including self-nominations) should contain the following information: a brief curriculum vitae; a list of publications; reprints of no more than 10 of the most significant of these publications; and any supporting information that could be helpful to the Selection Committee. Nominees should also arrange for two independent testimonials to be forwarded to the SCANZ Secretary.

7. Nominations should be forwarded to the SCANZ Secretary by the advertised deadline.

The Ricky Ponting Medal

for distinguished contributions to science involving X-ray, neutron or electron diffraction and/or imaging by a researcher under 40 years of age

1. The Medal shall be awarded to a financial member of the Society who, in the opinion of the SCANZ executive or duly appointed representatives, has contributed most towards the development of a branch of science associated with X-ray, neutron

or electron diffraction and/or imaging. This person shall be under the age of 40 at the time of close of applications, except in the case of significant interruptions to their research careers.

2. The award is based on consideration of the candidate's published scientific work, together with other evidence of his or her standing in the international community. A major portion of the relevant scientific work must have been carried out while the candidate was a member of the Society. Due consideration will be given to nominees with interrupted careers.

3. The medal shall be awarded to coincide with SCANZ conferences, and the successful candidate will be required to deliver a lecture at the appropriate conference.

4. The award will consist of a medallion, free registration at the SCANZ conference at which they will receive the award, a return economy airfare from the awardee's home city and $750 towards accommodation expenses (if the awardee is not a resident of the city in which the meeting is held). This will be provided by SCANZ in conjunction with the conference organisers.

5. The nominee must have been a member of SCANZ for the previous 5 years.

6. Nominations (including self-nominations) should contain the following information: a brief curriculum vitae; a list of publications; reprints of no more than 10 of the most significant of these publications; and any supporting information that could be helpful to the Selection Committee. Nominees should also arrange for two independent testimonials to be forwarded to the SCANZ Secretary.

7. Nominations should be forwarded to the SCANZ Secretary by the advertised deadline.

From the Newsletter Editor *(Paul Jensen, USyd)*

Finally…. another SCANZ newsletter! Not as much info as last time, but hopefully something to bring you up to date on some recent and future SCANZ news. Included with this mail out are the IUCR newsletters that have arrived since our last newsletter and also issue 14#1, which is the special on Crystallography in Australia and New Zealand. These newsletters are also available in electronic format from the IUCR website (www.iucr.org). SCANZ membership subscriptions can be paid by contacting our treasurer Bostjan Kobe (b.kobe@uq.edu.au). Most likely you will receive a reminder email shortly if you haven't already. Please also pass on details to anyone you think will be interested in becoming a SCANZ member (a copy of the membership form is included). Details of our upcoming biennial meeting, CRYSTAL 26, and registration form are also included with this newsletter, along with an application form for the 1987 Maslen scholarship, which is available to student members attending the meeting. Thanks to those who made newsletter contributions this time around. Future items for inclusion can be emailed to me at p.jensen@chem.usyd.edu.au.

Society of Crystallographers in Australia and New Zealand

SCANZ

(formerly: Society of Crystallographers in Australia (SCA))

APPLICATION FOR SCANZ MEMBERSHIP

Please fill in and mail with cheque to:

SCANZ Treasurer:
Bostjan Kobe (University of Queensland, Qld),

Tel: (07) 3365-2132
Fax: (07) 3365-4699
E-mail: b.kobe@uq.edu.au
Postal Address: School of Molecular and Microbial Science, University of Queensland, Cooper Road, Brisbane, Qld, 4072 Australia.

Name:
(Please print and include formal title e.g. Ms, Mr, Dr, Prof. etc)

_____ _____ _____
Title Surname First name and initial

Mailing address: (business address preferred)

_____

_____

_____

_____

E-mail address:

_____

Membership category:

Regular ($25)___ Student ($7)___ Corporate ($130)___

These amounts are reduced to $20, $5 and $100, respectively, if paid by April 1. Membership is on a calendar year basis. Applications received after June 30 will apply for the following year unless otherwise requested.
Therefore, to join the Society the appropriate fees are $20, $5 or $100, respectively.

Sponsors

Two current members of the Society must sponsor the application. Please write to the Secretary if you do not know any sponsors.

SCANZ Secretary:
Stuart Batten (Monash Univ. Victoria),
Tel: +61 (3) 9905-4606 Fax: +61 (3) 9905-4597
E-mail: Stuart.Batten@monash.edu.au
Postal Address: Monash University, Clayton, VIC 3800, Australia

	Sponsor 1	Sponsor 2
Name (please print)	_____	_____
Signature	_____	_____

Student certification

If requesting student membership, please complete the following and have it certified by a Faculty member of your institution.

The applicant is known to me and is a bone fide student at:

_____

_____

For the current academic year _____

Faculty member _____ _____
Name Signature

Special interests

Please indicate your major fields of interest. Students should indicate the degree or diploma sought and the name of their research supervisor if appropriate.

_____

_____

_____

_____

Payment

I enclose $_____ for membership for the year _____

Signature_____ Date_____

Application for 1987 Maslen Scholarship - CRYSTAL 26 Meeting

Name:

Address:

E-mail: **SCANZ Member:** Yes/No

Degree in progress or thesis submitted (with date):

Supervisor(s):

Is supervisor a SCANZ Member (if unsure please indicate):

Date Commenced Post Graduate Studies:

Presently full-time or part-time student:

Anticipated Completion Date:

Area of Research:

Abstract Title:

Previous SCANZ Support (please list any support previously received from SCANZ):

Previous SCANZ/AsCA/IUCr Meetings attended:

I have attached with this application a copy of the abstract of the paper that I will present at CRYSTAL 26 together with a brief CV (2 pages or less).

I certify that the above information is correct

Signature: **Date:**

Please forward applications marked "Maslen Scholarships" to:

Dr Stuart Batten
Hon Secretary of SCANZ
e-mail: Stuart.Batten@sci.monash.edu.au

OR

Fax: 03-9905 4597

by midnight on 5 February 2009

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