Society of Crystallographers in Australia and New Zealand
SCANZ

Newsletters

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

FROM THE PRESIDENT

Another year already, and this is now my fifth contribution to the SCANZ *Newsletters*. These columns are an excellent opportunity to say a little about what is going on in the Society, and especially recent events in crystallography. In case you were not aware, 2003 is rather a special year in the history of crystallography as it was in the April 25 1953 issue of Nature, that Watson and Crick published their famous paper on the structure of DNA (it is actually available free on the web as both HTML and also a pdf page-image of the original article: www.nature.com/genomics/human/watson-crick/).

Many celebrations and events are being planned worldwide to celebrate this important work (if you don't believe me, type 'watson crick 50th dna' into Google, and see what you end up with!). Our New Zealand colleagues are even making the most of the fact that Maurice Wilkins was born there, although he returned to the UK with his parents at the age of 6, and never returned (see www.rsnz.govt.nz/news/releases/wilkins_dna.php). But as crystallographers, you owe it to yourself to go back to volume 171 of Nature, and not to rely too much on the hype surrounding this anniversary. In particular, read the Watson & Crick paper (pages 737-738), and take special notice of the first sentence: "We wish to suggest a structure for the salt of deoxyribose nucleic acid (D.N.A.). This structure has novel features which are of considerable biological interest". Further into the brief article you will find: "So far as we can tell, it is roughly compatible with the experimental data, but it must be regarded as unproved until it has been checked against more exact results. Some of these are given in the following communications. We were not aware of the details of the results presented there when we devised our structure, which rests mainly though not entirely on published experimental data and stereochemical arguments."

So, you will see that the famous paper on the structure of DNA, the one that introduced the elegant double helix, is really presenting little more than a hypothetical structure. No crystallographic information is presented and no crystallography experiment was reported by Watson & Crick. So why is crystallography so inextricably connected with the discovery of the structure of DNA? The answer can be found in the "following communications" referred to by Watson & Crick. Their article is followed immediately by a paper on the "Molecular structure of deoxypentose nucleic acids" by Wilkins, Stokes & Wilson, and that in turn is followed by a paper on "Molecular configuration in sodium thymonucleate" by Franklin & Gosling. Although not obvious from the titles, it is these two papers that present the crystallographic evidence, not just for a helical structure, but for the actual dimensions - radius and repeat unit - that were reported by Watson & Crick. I leave it to you to decide whether the Watson & Crick structure could have been devised while being "not aware of the details" of the crystallographic results.

In line with similar meetings worldwide, the scientific program for AsCA/Crystal23 includes a session entitled "Nucleic acids and their protein complexes (50 years since the double helix)". There is a considerable amount of work being done behind the scenes on the Broome 2003 conferences, and elsewhere in this *Newsletter* you will find some details of this, as well as reminders of deadlines for registration, submission of abstracts, and applications for financial support. The scientific programs are falling into place nicely, and these meetings promise a feast of excellent science, and a great line-up of invited speakers, all in the unique and exotic environment of Broome. And don't forget that it is not just a single conference - AsCA/Crystal23 is being followed by a Biological Workshop in parallel with the Sagamore XIV meeting on Charge, Spin & Momentum Densities. Check out the Broome 2003 website (www.broome2003.uwa.edu.au) for updates on the scientific programs for these meetings. You just might be surprised at what is in store!

Finally, a few words about SCANZ. There will be a SCANZ Business Meeting in Broome, and that is an excellent opportunity for members to put forward and discuss a range of issues that might have cropped up since the last meeting (which was at Couran Cove in 2001). But time at these meetings is always limited, so considerable effort must be expended beforehand. Now is the time to initiate discussions with the SCANZ Executive, or to canvass the membership about issues that might be of direct concern to you, and more than likely to others as well. Do you have any issues that concern you? Do you know much about the financial state of the Society? Apart from scholarships to support student attendance at meetings, what else might SCANZ and so-called "1987" funds be spent on to benefit crystallography - and crystallographers - in Australia and New Zealand? Some members have raised the possibility of funding named prizes to honour some of our distinguished members of long-standing. Do you have an opinion on that? It's time to become more proactive about your membership of this Society and, in doing so, have some say in its future direction.

E-mail Brendan Kennedy or me if you wish to place an item on the agenda in Broome, and if it requires feedback or input from the membership we will initiate that.

Mark Spackman

University of New England

BROOME 2003

The three international crystallography meetings in Broome are coming up fast and have a raft of high-quality national and international speakers. Details of the AsCA' 03 / Crystal 23, the Structural Biology Workshop and the Sagamore XIV Conference are on the website **www.broome2003.uwa.edu.au**.

To participate in this meeting it is essential that you **make your accommodation and travel bookings NOW**. The demand on accommodation in Broome this year is much higher because Australians are taking their winter break at local resorts, rather than at Bali. A number of hotels/appartments are already completely booked for August, and the Cable Beach Club has a waiting list on the rooms reserved for conference goers. In keeping with the conference reservation agreement, 50% of the unbooked rooms will be released soon. Please make your accommodation arrangements today – and do your travel bookings at the same time!

TravelWorld is the designated travel agency and they have made block bookings of seats over this period. Contact Ruth Carlton Ph: 1800-065-152 or 61-7- 3844 - 4999, Fax: 07-3846-5988, or by e-mail: rcarlton@travelconnect.com.au. Give the password "Crystal-23" and you will get conference rates.

Participants should register via the website. **The abstract submissions deadline, and late registration fee date, is March 15th**. **The application deadline for "young scientist" scholarships is now March 1st.** Details of the abstract submission process and scholarships are on the website. The lecture venues at Broome have a maximum capacity of 300 and registrations will be limited to this number.

Syd Hall

IAN DANCE SYMPOSIUM

The distinguished career of Ian Dance officially came to an end at the end of 2001 when Ian retired and was appointed as Emeritus Professor. Since then, Ian has actively continued his research, mainly from the comfort of home, but with occasional visits to the Campus at UNSW. To honour Ian's career, a one-day symposium was organised on 2nd December 2002 at the University of New South Wales.

Ian was born in Maitland and educated in Sydney. At the University of Sydney, his B.Sc (Hons) and M.Sc. research were inspired by Prof. Hans Freeman. His Ph.D. (1966) was with Prof. Jack Lewis at the University of Manchester. He then moved to the USA for postdoctoral research with Prof. Richard Holm at the University of Wisconsin and the Massachusetts Institute of Technology, followed by a faculty position back at Wisconsin. In 1975 he moved to the School of Chemistry at the University of New South Wales, and was appointed Professor of Inorganic Chemistry in 1986. He was elected a Fellow of the Australian Academy of Science in 1997. He served as Chairman of the Inorganic Division of the RACI (1985-98) and was awarded the Institute's Inorganic Medal, the Burrows Award in 1996. He has been a member of the Chemistry panel of the ARC. He was the Royal Society of Chemistry Lecturer of Australia and New Zealand, the Stranks Memorial Lecturer at the University of Melbourne, the Albright and Wilson Lecturer at Warwick University, the 3M Lecturer at the University of Western Ontario, and lectured the Troisieme Cycle in Switzerland.

Guests from all over Australia assembled to hear speakers from as far as a field as Townsville and Auckland. The theme of the day was, not surprisingly, Inorganic Chemistry, with contributions highlighting work in both the solid and gas phases.

Chairman for the morning session was Hans Freeman, with the following program: Richard Keene (JCU), *Stereochemical consequences of intervalence transfer in dinuclear ruthenium and osmium complexes*. Graham Bowmaker (Auckland), *Spectroscopy and structure of copper(I) cyanide and copper(I) thiourea complexes*. Richard Robson (U.Melb.), *Oxy-anions old and new and some derived coordination networks*.

After lunch, Len Lindoy took over the chair for the following presentations: Marcia Scudder and Keith Fisher (UNSW), *I Dance with ions in two phases*. Alan Canty (U.Tas.), *Exploring potential roles for high oxidation state palladium in catalysis*. Roger Bishop (UNSW), *Between a rock and a hard place: The attractions of crystal engineering*. Colin Raston (UWA), *Controlling the van der Waals interplay of fullerenes*.

Ian then presented the 2002 Dwyer Memorial Lecture to the UNSW Chemical Society. The title of his talk was "Inorganic Choreography: The Chemical Mechanism of Nitrogenase and Hydrogenase".

The day was concluded when about 40 people attended a sumptuous dinner in Ian's honour.

Marcia Scudder

SMALL MOLECULES AT THE BOOMERANG WORKSHOP

A workshop for potential users of the Australian Synchrotron was held at the University of Melbourne School of Law from 29-31 January 2003. The workshop was part of the process of developing the first group of Australian Synchrotron beamlines to meet the needs of Australian science and industry. It brought together researchers who using synchrotrons now and also those who could use the Australian Synchrotron in the future. International experts in synchrotron design, operation and experimentation helped enhance Australian understanding of what we can expect from the Australian Synchrotron and its beamlines.

Small molecule single crystal diffraction (SMX) made its first appearance at the workshop proceedings on the morning of the first day when Richard Garret mentioned the ASRP's SCrAPS program in an overview of Australian Synchrotron research. Later in the afternoon Syd Hall gave a photon fast introduction to the usefulness of synchrotron light for small molecule single crystal studies, being restricted to a maximum presentation time of 5 minutes. The new version of the Australian Synchrotron, Boomerang20, is to be bigger, brighter and better and the beamline presenters clearly had to be correspondingly faster.

In the afternoon of the second day of the workshop, participants dispersed into beamline specific discussion groups (breakout groups) to discuss and prepare detailed summaries of the needs and costs for their proposed beamlines. The small molecule demand for beam time is unlikely to require a dedicated end station in the foreseeable future. Consequently the small molecule group, represented and led by Syd Hall, have primarily pursued a share in one of the two beamlines being proposed for protein crystallography (PX). Small molecule crystallography and protein crystallography have significant areas of technical and scientific overlap; more so than with any other beamline group. Accordingly, the small molecule group primarily participated in the protein breakout session. The discussion session canvassed a number of technical, managerial and financial matters, and concluded that there were good reasons and no significant obstacles in having SMX share the proposed PX micro-crystallography undulator beamline.

The SMX group was fortunate to have Simon Teat present at the workshop. Simon is a Senior Station Scientist at the Daresbury Laboratory Synchrotron in the United Kingdom. Simon is the manager of station 9.8, which is currently the only dedicated small molecule single crystal crystallography station at any synchrotron. Over the past year Simon and David Cookson, Deputy Project Manager and beamline scientist at ChemMatCARS, have provided significant and valuable information for the case for a SMX facility at the Australian Synchrotron. As a visiting researcher he has an ongoing involvement in the commissioning of the small molecule beamline at the ALS. At the protein crystallography discussion group Simon gave an impromptu overview of the benefits of synchrotron light for small molecule crystallography, and answered questions arising from that overview. He then contributed to the technical, beamline cost assessment and synchrotron management discussions of the protein group. Simon also participated in the powder diffraction discussion group, where he gave a prepared presentation on current trends in small molecule single crystal synchrotron crystallography.

The relevance of single crystal studies to powder diffraction was highlighted with an example of an incommensurate structure requiring single crystal synchrotron data for its structural resolution. In addition to providing structures and charge density distributions from weakly diffracting crystals, wavelength tuneable synchrotron light offers the possibility of utilising anomalous dispersion effects in single crystal diffraction, to reliably determine mixed metal site and multiple oxidation state occupancies. Simon's presentation to the powder group was followed by a brief assessment of the likely demand for SMX studies at Boomerang, from the perspective of my involvement in the SCrAPS program, and then Stuart Batten (Monash) further outlined areas of overlap between powder and single crystal interests.

From the small molecule perspective, the organisers should be congratulated for bringing potential users and experts together to more clearly define Boomerangs future
shape.

Peter Turner

ASRP RESEARCH FELLOWSHIPS

The Federal Minister for Science, Peter McGauran, recently announced six recipients of the Australian Synchrotron Research Program (ASRP) Research Fellowships, of whom three are members of SCANZ. These are:

• Barbara Etschmann, CSIRO (formerly at the South Australian Museum). Her project is: *Nuclear microprobe and synchrotron-based spectroscopy of inorganic materials and solutions, opening new opportunities in fields such as hydrothermal ore processing and mineral exploration*.

• Joshua McKinnon, University of New England. *Optimising data collection strategies to refine synchrotron-based charge density analysis techniques*.

• Kia Wallwork, ANSTO (formerly at Flinders University). *Investigation of pressure-induced phase transitions using powder X-ray and neutron diffraction techniques, including the study of oxides such as zeolites.*

CRYSTAL FRAGMENTS

Richard Welberry (ANU) is now the Australian co-editor for J. Appl. Crystallogr. having taken over from Chris Howard in October.

THE NATIONAL COMMITTEE

With the obvious go-ahead of the national synchrotron the comments on national priorities made by the National Committee at its Geneva meeting in August are very relevant. These were:

At its meeting on the 8th August in Geneva for the XIX General Assembly and Congress of the International Union of Crystallography and by a consultation through e-mail with those members not at Geneva, the National Committee suggests that a policy for funding access to and development of major research facilities should be a National Priority. The sessions at Geneva have amply illustrated this.

In particular;

(1) Access by Australians to major neutron and synchrotron radiation facilities overseas has kept key aspects of Australian structural biology, chemical physics and materials science at the cutting edge of international activity both through the experiments done and the exchange of ideas and collaborations. Maintaining this is a high priority.

(2) Australia has a wonderful opportunity to be leader in all manner of structural research by virtue of the two new leading-edge facilities presently under construction, namely the synchrotron at Monash and the research reactor at Lucas Heights.

(3). Governance and instrument development are matters underneath these major considerations, policy for which should be developed with the experience of related international centres in mind.

At the National Committee meeting in Melbourne on the 29th January these points were affirmed again in the context of the committee's discussion of recent developments for the synchrotron. The Committee warmly congratulates those responsible for ensuring that the capital cost of the synchrotron and building will be met.

John White

FUTURE CONFERENCES

IUCr XX

The twentieth Congress and General Assembly of the International Union of Crystallography will be held in Florence, Italy from 23-31, August 2005 at the Congress Centre. The committee chairpersons are Carlo Mealli (Scientific Program) and Paolo Dapporto (Local Organising Committee). The Congress Centre is located in the very heart of the city, within walking distance of the main tourist attractions and most of the hotels. Further information, including an Interest Form, can be found at the Congress website: http://www.iucr2005.it.

SUBSCRIPTIONS

The Treasurer wishes to remind members that annual membership dues for 2003 are to be paid by December 31, 2003. A statement was included in the October 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, 2003. 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).

Paul Carr

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Australia and New Zealand

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IUCr XXI

The twenty-first Congress and General Assembly of the International Union of Crystallography will be held in Osaka, Japan in 2008.

AsCA'04

The next full meeting of AsCA will be held in Hong Kong in late July 2004, at a date yet to be fixed. Professor Ian Williams will Chair the Organising Committee.

Three international crystallography meetings will be held in Broome next year. They are the combined AsCA' 03 / Crystal-23 meeting that runs from Aug 10 to 13, a Structural Biology Workshop from Aug 13 to 15 and the Sagamore XIV Conference from Aug 13 to 18. See full details at www.broome2003.uwa.edu.au. Significant international participation is anticipated at these meetings and SCANZ members are advised to make accommodation and travel arrangements as early as possible. TravelWorld is the conference travel agency and they have made block bookings of seats to and from Broome over this period. Reservations can now be made by contacting Ruth Carlton Ph: 1800-065-152 or 61-7- 3844 - 4999, Fax: 07-3846-5988, or by e-mail: rcarlton@travelconnect.com.au.

Say that the travel is to " Crystal-23" and you will be given conference rates. TravelWorld is setting up a special website for travel to the Broome meetings, and the conference website will link to this. Note also that pre- and post-conference 4-wheel drive tours of the Kimberley region have been arranged and these are described on the conference website.

Participants can register via the website. The registration fee includes the cost of social evenings, coffees and lunches for full and student registrants. The abstract submissions deadline, and late registration fee date, is fixed at March 15th. The application deadline for " young scientist" scholarships is February 15th. Details of the abstract submission process and scholarships are on the website.

Because the lecture venue has a maximum capacity of 300 registrations will be limited to this number. The recent Bali tragedy has greatly increased the pressure on Broome accommodation for next year, and the Cable Beach Club will be releasing half of the reserved accommodation for these meetings on February 10th. Because of this and the registration limit of 300, participants must register and book their accommodation, and make travel arrangements, as soon as possible.

Syd Hall

Financial Assistance

There are three sources of financial support for young scientists as follows:

Australian and New Zealand (Members of SCANZ)

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 the combined AsCA'03/Crystal-23 conference to be held in Broome Australia, from 10-13 August, 2003.

Details of the meetings are available on the WWW at the address: http://www.broome2003.uwa.edu.au

SCANZ student members from both Australia and New Zealand are invited to apply for the Scholarships, which will make a substantial contribution to the travelling 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.

* 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 SCANZ.

Applications must reach the following address by March 1 2003

Dr Brendan Kennedy

SCANZ Secretary

School of Chemistry, F11

University of Sydney

NSW 2006

Alternatively, applications may be sent by FAX 02-9351-3329.

Other Nationalities (Participants from Australia, New Zealand and Japan are not encouraged to apply for the IUCr bursaries)

Financial support for a limited number of young scientists (graduate students or post doctoral fellows with less than three years postdoctoral experience) are available from funds provided by IUCr. These awards will contribute towards travel and subsistence costs of attending any or all of the three meetings held in Broome. Applications for support from the IUCr funds should be sent to XXXX before XXXX. There is no application form but each application must be accompanied by:

A brief curriculum vitae

1. 2. List of publications
2. 3. Abstract for presentation at one of the three meetings
3. 4. Estimated cost of excursion economy airfare
4. 5. Letter of recommendation from the applicant's supervisor, in the case of students.

Successful applicants will be notified by XXX

Science meets Parliament Day 2002

November 12-13

This year's the Science Meets Parliament Day will be held on November 12-13. This is an opportunity to meet Federal Parliamentarians in their Canberra office and talk to them about the national investment in science and research. There will be opportunities for networking and discussion, with guest speakers Sir Robert May, Dr Brendan Nelson, Peter McGauran, Simon Crean, Dr Keith Williams, CEO of Proteomics Ltd at the National Press Club; and Bob Herbert, CEO of Australian Industry Group at the optional dinner.

Science meets Parliament Day brings together scientists from research organisations, universities and industry from over Australia. It is an opportunity to discuss issues with a cross-section of Australian science.

More information including registration is available on the FASTS websit: http://www.fasts.org.

The next issue of the *Newsletter* will be in August 2001. Contributions should be e-mailed to the Editor by 10th August.

Check AscA website about conference news and then email sec

SKETCHES OF CRYSTALLOGRAPHY LABORATORIES

Griffith University

FOR THE WEB-BROWSERS

- The website of the Society of Crystallographers in Australia is located at http://www.sca.asn.au.

Australian Chairs of IUCr Commissions:

Mitchell Guss: Biological Macromolecules

Mark Spackman: Charge, Spin & Momentum Densities

Steve Wilkins: Synchrotron Radiation

XVIII IUCR Congress

Profit and account from CRYSTAL21

Ian Gente new member

Peter Colman gone to Eliza Hal

Next CRYSTAL meeting

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websites for Journals see link from cww website

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recipients of arc and nhmrc funds

CRYSTAL FRAGMENTS

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sketch from dance, melbourne