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Society of Crystallographers in Australia

SCA

Newsletters

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FROM THE PRESIDENT

My term as President started in Thredbo while I was in the midst of trying to ensure the smooth running of Crystal XXI and after a pretty hectic month or so of the later stages of organising the meeting. Since then things seem to have quietened down somewhat and the task of being President does not seem quite so onerous. I will say a little more about the Thredbo meeting a little later but first let me say a few words about things that have progressed since Thredbo.

First, the postal vote on the proposal to change the name of the Society to the "Society of Crystallographers in Australia and New Zealand" has been carried out and the results were overwhelmingly in favour of making the change (50 for, 5 against). We will now take the necessary steps to do this, the ground work for which was undertaken by Max Taylor during his term as President.

It was decided in Thredbo to try to hold the next SCA (or SCANZ) meeting in Queensland sometime during the winter of 2001. This was to try to get back to a cycle in which local meetings are held more frequently than the 3 year cycle that seemed to have been dictated in recent years by the IUCr and AsCA meetings. Although some members of the Society are able to get to these overseas meetings, it is still a relatively small fraction of the total membership and I think that it is important that all local scientists with crystallographic interests have a frequent opportunity to get together. As a result, Jenny Martin was charged with the task of organising Crystal XXII and preliminary steps have already been taken.

A local organising committee has been established and has agreed that it will be possible to hold the Crystal XXII conference in Queensland in June or July 2001. The committee currently consists of Jenny Martin (UQ), Ian Gentle (UQ), Paul Bernhardt (UQ), Graham Smith (QUT), Ruth Drinkwater (UQ), Ray Bott (QUT) and John Drennan (UQ). The dates of the conference are yet to be finalised due to some confusion over AVCC weeks next year, but it is intended to hold it either just before or just after the IUPAC conference (which runs from July 1-6). The venue has not yet been finalised but the committee has narrowed it down to either Kingfisher Bay on Fraser Island or Couran Cove on South Stradbroke Island. Either of these sounds an attractive prospect as the Canberra winter approaches.

Returning to Thredbo, I would like first to reiterate my thanks to everyone who helped make this such a successful meeting. The feedback I have had has been all positive and this makes the work that the local committee put in, all worthwhile. I would like to say that I greatly appreciated being able to interact with our *1987 Lecturer*, Doug Dorset, and one of our other overseas visitors, Bill David, was able to find time to make visits to Sydney, Adelaide and Perth after the meeting. It was also very gratifying to witness the *Society* paying due honour to Hans Freeman during the Conference dinner. I think my own first memory of Hans was when he lead the meeting at which the SCA constitution was first established. We are all much indebted to him.

I would also like to say a special thank you to Alison Edwards, without whose tremendous help (and the experience she brought from being involved in the organisation of the Ballarat meeting) we would have been not nearly so organised and nothing would have run quite so smoothly (with the possible exception of the bus!). Alison herself has already paid tribute to all of the sponsers (February *Newsletter*), whose contributions greatly enhanced everyone's enjoyment of the meeting. From my own point of view I would like to say that I found the experience of being in charge of the conference organisation an interesting one, having previously only been involved in such things in very minor capacities. I have passed on some of the things we learnt and the difficulties we encountered to Jenny Martin and I wish her and her committee all success for Crystal XXII.

Richard Welberry

XTAL 3.7

As of March 2000, all XTAL source code, executables and documentation (for the latest version 3.7) are freely available from the website: http://www.xtal.uwa.edu.au. This includes all programs for the solution, refinement, display and publication of crystal structures. This version includes improved graphic software for PIG and ORTEP with interfaces to POVRAY and RASMOL. There were over 600 downloads from the XTAL website in the first month.

Syd Hall

CRYSTAL XXI

Student reports from Thredbo

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Organising a conference resembles nothing so much as the plight of the alchemist seeking the transmutation of lead into gold. Bringing such diverse fields as inorganic/mineral structures, small molecule and protein/biological work, soft-matter science and structure solution by powder diffraction all under the one umbrella of crystallography is a recipe for interesting times. Like grinding up soot, sulphur and nitre with a mortar and pestle and wondering what will happen when you throw in a match.

The thing that struck me the most about Crystal XXI, other than the idyllic locale, was the diversity of techniques and fields represented, all concerned with the resolution of structure, be they for cellulose orientation in wood, lead placement in synthetic apatites or rubredoxin isolated from *Clostridium Pasteurianum*. Something for everyone, even the most particular of crystallographers. And because the conference proceedings were all held in the one hall there was none of the usual getting lost in the crowd as

with larger meetings. If you wanted to have a chat with someone about their work after a talk you did not have to beat your way through the mob streaming out to the next session three rooms over.

From a powder crystallographer's perspective the first and second sessions of the first day and the last session of the last day were the most relevant. But who could not help but be interested in the story behind Peter Colman's work developing influenza drugs and the economic and political hurdles that were encountered along the way, not to mention the mixed, often conflicting media representation. It would have been funny if it were not such a poignant reflection of the level of journalistic expertise covering the sciences in the popular media.

Pleasing also, were the talks and demonstrations relating to the advances in hardware, designed to make the crystallographer's lot that little bit easier and more enjoyable. And while on the subject of hardware, could anything be more exciting than the plans for `Boomerang', the proposed Australian Synchrotron Light Source. Having been to Japan and the facilities at the ANBF, it seems clear to me that Australia could benefit greatly from a similar synchrotron source.

Might I take this opportunity to suggest that the No. 2 Sports Oval at the University of Sydney would be the perfect place for such an undertaking. Lots of space and friendly locals guaranteed.

All in all, a pleasant conference with a diverse range of topics, specialities and speakers. Thanks to the SCA for providing the travel scholarship and for the lovely choice of venue.

Rene Macquart

University of Sydney

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It is hard not to smile at the rather unforeseen circumstances that unfolded on a busy road on the outskirts of Canberra that hot February afternoon. As the bus stood still, no longer able to continue the journey it had started, the entertainment provided while waiting for a replacement means of transport was certainly not sparse. From the enthusiastic poetry recital by Ray Withers to the impromptu roadside mixer that followed, one could sense that something was going to be ‘different’ about this conference, and different it was! More than two months after Crystal XXI, fond memories still linger. I often find myself reminiscing back to the five days spent in the beautiful surroundings of Mt. Kosciusko, where new acquaintances were made, old friendships renewed and more importantly, where some great crystallography was shared by all.

Impressive was the vast array of crystallography that was presented, both through oral and poster presentations. There were some informative lectures closely related to my field of research on apatites, one of which was given by Andrew Christy on computer modelling of different apatites. Also interesting was Bill David’s talk on *Structure Solution by Powder Diffraction*, which illustrated various strategies used to solve different complex molecules using powder diffraction methods. As I am an X-ray synchrotron user at the Photon Factory in Japan, Richard Garrett’s presentation on the proposed ‘Boomerang’ Synchrotron Light Source stirred a lot of interest. Although it will not be ready before I finish my studies, I am sure the idea of not having to take ten-hour flights to Japan will certainly be appealing for future users. More importantly, it also opens up a vast array of possibilities for future work in crystallography using synchrotron radiation.

Crystal XXI was particularly memorable as it was the first time that I had to give an oral presentation at a conference. In this respect, it was also encouraging to hear the innovative work of other fellow students being presented. I am sure my thoughts are shared in that it proved to be an invaluable experience, where opportunities for discussion about research were given and ideas on future work suggested.

Putting crystallography aside, the opportunity to get to know other fellow students was fantastic. Although, initially, the thought of sharing an apartment with four others raised some concerns, it proved to be a great way of developing new friendships and gave the opportunity to discuss not only different aspects of crystallography, but also about future aspirations on a more casual level.

Finally, I would like to thank the SCA for providing financial assistance for the travel to Thredbo. I would also like to extend my congratulations to the organising committee for putting together a successful, well-organised and most enjoyable conference.

Jean Kim

University of Sydney

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The 21st meeting of The Society of Crystallographers of Australia recently held at Thredbo was my first experience of attending a conference where faces were not familiar. For me to have the chance to meet, socialise, confer and enjoy the company of such a diverse crowd, made the conference a success personally.

The Thredbo Resort is a fine venue, and the staff and service were first class. Everyone made the most of the opportunity to enjoy the beautiful countryside on Thursday afternoon. We were treated to a `flora walk' as my colleague and adviser Philip Reynolds is a wildflower buff. Phil described the surroundings on our trek up to the Kosciusko Lookout.

The content of the presentations over the days of the conference covered a wide area of interests with a little of something for all tastes from proteins to data collection. The overall standard was very high. I waited until Friday (am) to present my seminar, my first in open company, so I had much food-for-thought as I watched and listened.

My wife and I had watched David Suzuki's TV report on the controversy surrounding commercialising of the flu vaccine which Peter Colman and Graham Laver developed. I was fascinated to hear the description from the horse's mouth. I felt Peter gave a balanced and informative talk which highlighted some of the fundamental difficulties for scientists involved in direct commercialism. Given the current constraints we are all becoming increasingly subject to in our work this was a most informative session.

Andy Christy gave a fascinating description of modeling halite dislocations in apatites, a material that shows long range disorder. I found the techniques possibly useful in the future for analysis of my own materials.

Not only did Doug Dorset entertain us with his `House of the Dead' presentation, but over dinner, I was fortunate to enjoy his company and openness. This type of analysis lends itself to the soft matter mesoporous films which are the subject of my thesis. It showed that there is often hidden information that modern computing power can aid in analysis where previously it was not possible.

I travel to ISIS on a regular basis to perform neutron scattering experiments. Our group uses a modeling routine developed at ISIS which uses the algorithm which Bill David described in his presentations. The use of pictures to convey broader concepts was very professional. The routines and the ideas Bill talked about were enlightening.

I would like to thank the organising committee for allowing me to attend by trading a little labour. Also, I am grateful to the SCA for the Ted Maslen Scholarship without which I would have missed a truly pleasant

conference.

Jeremy Ruggles

Australian National University

SKETCHES OF CRYSTALLOGRAPHY LABORATORIES

Griffith University

Crystallography at Griffith was established in the School of Science at the beginnings of the University in 1975 with the purchase of a Phillips stationary tube X-ray generator, powder cameras and single crystal Weissenberg cameras. The unavailability of four-circle diffractometer facilities in Queensland at that time meant that for single crystal structure determinations, crystals were sent to the University of Western Australia Crystallography Centre for data collection and structure determination. The combination of single crystal X-ray structural data and solid state NMR spectroscopy using the facilities of the Griffith University Magnetic Resonance Centre (Bruker CXP-300, Varian Unity-400) yielded fruitful results over a period of many years, particularly in the area of structure and molecular properties of transition metal phosphine complexes.

In 1995 a successful Mechanism C Research Infrastructure Grant, together with funding support from Griffith University and the Queensland University of Technology resulted in the purchase of a Rigaku AFC7 Rotating anode X-ray diffractometer and the MSC teXsan software package for structure solution. This equipment has been in operation since that time, providing single crystal structure support for small molecule systems for the organic and inorganic chemistry groups at both institutions.

In 1990 an upgrade to the X-ray powder facility was funded by NERDDC, for *in situ* studies of hydrogen-absorbing metals under hydrogen gas pressure. A reconditioned Philips powder diffractometer with solid-state counter and computer control were added to the generator. This equipment still serves for in-house powder diffraction studies.

Since 1989, neutron powder diffraction has been used to study hydrogen- and nitrogen-absorbing metals *in situ* under deuterium and nitrogen pressure. The facilities regularly used are MRPD and HRPD at ANSTO in Sydney, POLARIS and HRPD at ISIS in the United Kingdom and HRPT at the Paul Scherrer Institute in Switzerland.

Since 1995, increasing use has been made of synchrotron X-rays, first at the Photon Factory in Japan (BigDiff, BL20B), and more recently at the Advanced Photon Source in the USA (SRI-CAT, 1-ID and ChemMatCARS, 15-BM) and the European Synchrotron Radiation Facility in France (Swiss-Norwegian Beamline, BM-1B). The work at these facilities centres on *in situ* studies of hydrogen- and nitrogen-absorbing alloys for hydrogen storage and permanent magnets. The technique now used is transmission-mode diffraction with samples up to 1 mm thick in a pressure cell sealed with Be windows. Energies above 30 keV are used exclusively.

Peter Healy

Evan Gray

FUTURE MEETINGS

CRYSTAL XXII

As mentioned in the *From the President* column in this *Newsletter*, the next meeting of the SCA, Crystal XXII, will probably be held in June or July, 2001. The dates of the conference are yet to be finalised, but it is intended to hold it either just before or just after the IUPAC conference (from July 1-6). The venue has been narrowed down to either Kingfisher Bay on Fraser Island or Couran Cove on South Stradbroke Island. Further information will be available in later issues of the *Newsletter*.

AsCA 2001

At a meeting of the AsCA council held during the IUCr Congress in Glasgow, it was agreed that the next AsCA meeting would be in Bangalore, India around 18-25 November 2001.

IUCr XIX

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

Science meets Parliament Day, 2000

The event will be held in Canberra on Tuesday October 31 and Wednesday November 1, and again provides an opportunity for scientists and technologists to personally put the case for science to their Members of Parliament. The Australian Institute for Physics is holding their Heads of Departments meeting in Canberra in the same week. Details about registration for the event will be available from the FASTS website at http://www.usyd. edu.au/su/fasts.

FOR THE WEB-BROWSERS

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

- There is now an Australian mirror of the International Union of Crystallography (IUCr) website available at http://www.au.iucr.org. The IUCr also provides software facilities for the checking of cif files if they are sent by e-mail to checkcif@iucr.org or, alternatively, through the web version at http://www.iucr.org/iucr-top/journals/acta/ services/checkcif.html.

NEW MEMBERS

The SCA welcomes the following new members for 2000.

Full members: Cameron Kepert and David Hibbs (School of Chemistry, Univ. of Sydney), Darren Goossens (Research School of Chemistry, ANU).

Student members: Douglas Smyth, David Clarke, and Clynton Stapleton (Department of Chemistry, University of Adelaide) and Suminar Pratapa (Department of Applied Physics, Curtin University).

CRYSTAL FRAGMENTS

- Bostjan Kobe (St. Vincent's Institute of Medical Research) has accepted an appointment of Associate

Professor in Structural Biology at the Department of Biochemistry at the University of Queensland, St. Lucia, Brisbane, where his group will be relocating in July 2000.

- Siegbert Schmid (ANU) is no longer working at the Research School of Chemistry. He joined the Wood Science group at the Department of Forestry, ANU in May 1999 to work on a project funded by the Norwegian company Jotun a.s., entitled "Novel Methods of Wood Protection".

- Nick O'Toole (UWA) has recently graduated PhD and has taken up a postdoctoral position in structural bioinformatics with Associate Professor Vakser at The Medical University of South Carolina.
