

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

In my last President's message I mentioned that I would be attending the IUCr Journals Commission meetings in Manchester prior to attending the Congress in Glasgow. These meetings of Editors, Co-Editors and Staff of the IUCr journals are always held in association with the triennial Congress, but are also scheduled at other IUCr sponsored meetings around the globe for any of the members who can get there. The Manchester meetings were well attended by Editors and especially by IUCr staff because of the venue's proximity to Chester. About 40 people were present at one time or another. The timing of the meeting coincided with the launch of the On-Line journals (free until the end of the year). Please have a look at <http://journals.iucr.org>.

The journals are under active scrutiny all the time to improve such things as publication times, standards, quality and saleability. **The latter is particularly important because 70% of the International Union's income derives from the sale of the journals.** If the journals do not produce the goods the Union will fail.

To keep subscription numbers up, the journals need more and high quality manuscripts for publication. I encourage SCA members to consider publishing more of their research in these foremost international journals. There are six journals to choose from, the four Acta Crystallographica sections plus the Journal of Applied Crystallography and the Journal of Synchrotron Radiation. In my view, it is usually best if small molecule structures are published along with the chemistry to which they are related in a chemistry journal, but if that is not possible, then Acta Crystallographica C is an excellent vehicle. Acta Crystallographica B (Structural Science) is a premier journal for publishing structural chemistry across the whole range, and considering the strength of structural science and materials science in Australia and New Zealand, the number of papers from this region seems too low.

Acta Crystallographica D (Biological Crystallography) is the top rating crystallographic journal for citations in macromolecular crystallography. There is currently a move to produce a purely electronic, cif-based, journal for rapid publication of small molecule structures.

Improved participation in the journals by SCA members is one thing, but it needs to translate into increased

numbers of journal subscriptions. Australian and New Zealand universities and research organisations are already good supporters in this respect, there being, for example, 13 and 3 subscriptions, respectively, to the full Acta set plus the Journal of Applied Crystallography, but there are few subscriptions to the Journal of Synchrotron Radiation. Never-the-less there are about fifty institutions in the two countries that are potential subscribers. Queensland seems to be an IUCr-journal-free zone, according to the information that I have, and the top half of the South Island is very light on as well.

On the 'Big Science' front, members may be interested to hear that a proposal to construct a third generation synchrotron in Australia has been prepared under the auspices of the Australian Synchrotron Research program and a request has been made to include this project in Federal Budget funding. (See report from the National Committee on page 2 of this *Newsletter*). AINSE received RIEF funds in the recent ARC round to continue the ISIS subscription for one year with indicative funding for a further two years.

At its meeting in Glasgow, the Council resolved to elect Emeritus Professor Hans Freeman to Honorary Life Membership of the SCA. Hans organised the first informal meeting of Australian Crystallographers in Sydney before the SCA was formed and has been an active participant since. Hans will be presented with the award at the conference dinner in Thredbo.

The professional way that Crystal XXI is being organised augers well for a great meeting, even if it contrasts somewhat with the image of the 'bush crystallographers'! See you there.

Max Taylor

SUBSCRIPTIONS

The Treasurer wishes to remind members that annual membership dues for 2000 are to be paid by December 31, 2000. A statement is included with this *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, 2000.

The NATIONAL COMMITTEE FOR CRYSTALLOGRAPHY

Glasgow, August 1999

Everyone who went to the Congress will certainly say what a good meeting it was both from organisation, scientific content and the weather. The Australian delegation, Mark Spackman, Mitchell Guss and John White attended all the meetings of the General Assembly and, as with a number of others at the meeting, were rather surprised when the decision that the 2005 assembly went to Florence rather than to Japan. The geographical distribution of venues for the General Assembly and Congress was utmost in our mind and subsequent to the Congress, the National Committee for Crystallography supported the Asian Crystallographic Association in writing a letter to the Executive of the IUCr pointing out the need for a major meeting in the Asia Pacific region. At the General Assembly, the membership of a number of commissions by Australians was maintained - Mark Spackman will lead the charge in the Momentum Distribution Commission, Stephen Wilkins will chair the Synchrotron Radiation Commission and others have retained their positions on other commissions. We congratulate those members.

There was once again a lot of discussion about the length of the meeting and its cost. The General Assembly resolved this time that the length of the 2005 meeting should be reduced to seven days maximum.

Synchrotron for Australia Proposal.

Crystallographers will be aware that the Australian Synchrotron Radiation Program (ASRP) has been supporting synchrotron access for Australians to Japan and most recently to the Advance Photon Source (APS) at the Argonne National Laboratory in Chicago. Facilities in Japan are now saturated, the facilities at Argonne look as if they are approaching saturation and so the ASRP Board has been considering throughout this year what steps to take for the future. The first of these is to consider the renewal of the ASRP Program itself for access to Japan and Chicago so that things continue for the next five years and the second is the consideration for a proposal for a synchrotron in Australia.

The ASRP Board established a Strategy Steering Committee with a national representation at its meeting in March 1999. This working party was chaired by John White and had representatives from the NH&MRC, the Australian Research Council, Western Australia, Victoria, Queensland, New South Wales, and South Australia. Professor Jim Piper (ARC) was the deputy chair of that Steering Committee. The Committee reviewed the documentation that Dr Boldeman had produced for an Australian Synchrotron proposal, let a contract to the Centre for International Economics to assess "the net benefits of a national synchrotron investment" and established an international technical reference committee on the reference design for an Australian synchrotron. This international reference committee is chaired by Professor Y. Petroff (ESRF), and has Professor Michael Hart (Brookhaven National Laboratory) and Professor Y. Matsushita (Photon Factory) as members.

At the ASRP Board meeting on Saturday 23 October, the recommendation from the Steering Committee to go ahead for an Australian synchrotron was accepted subject to various conditions suggested by the Steering Committee and after an assessment of the report of the technical reference group had been made. It is expected that a proposal will be submitted to government for preliminary consideration soon.

John White

CRYSTAL FRAGMENTS

- David Cockayne (Univ. Sydney) has accepted a position at Oxford University. He will take up the Professorship in the Physical Examination of Materials in the Department of Materials at the end of 1999. David holds a Personal Chair in Microscopy and Microanalysis at the University of Sydney. He has been the Director of the Electron Microscope Unit since 1974. In 1995, he was appointed as Director of the newly formed Australian Key Centre for Microscopy and Microanalysis. David's research interests include the development of electron optical techniques for revealing structure, defects in crystalline solids and electron scattering theory, and he has published over 150 papers in international journals. David has a keen interest in teaching and in research policy.
- Karen Edler (formerly at Cornell University and ANU) has taken up a three-year postdoctoral position with Dr Steve Roser at the University of Bath, UK working on X-ray and neutron reflectometry from surfactant-templated silica films.
- Tina Izard (formerly University of Leicester and Biomolecular Research Institute, Melbourne) has accepted a faculty position at St Jude's Children Research Hospital in Memphis, Tennessee.
- Mark Spackman (University of New England) has recently been promoted to Professor. Mark has also been head of department since January 1998.

NEW MEMBERS

The SCA welcomes the following new members for 1999/2000.

Full members: Dr Chris Chantler (Department of Physics, University of Melbourne) and Dr Janet Scott (Department of Chemistry, Monash University).

Student Members: Mr Jeremy Ruggles (Research School of Chemistry, ANU), Mrs Eman Mohamed (Physics Department, Murdoch University), Miss Michelle Dunstone and Ms Susanne Feil (St. Vincent's Institute of Medical Research), Mr Paul Jensen (Department of Chemistry, Monash University), Mr Brendan Mackey and Ms Connie Darmanin (Victorian College of Pharmacy).

Notes from

the SCA COUNCIL MEETING

Glasgow, August 1999

1. Appointment of Two AsCA Councillors

Although this is the responsibility of the SCA Council, a formal structure for the appointment of these has never been made. It was decided that the two Australian AsCA councillors should be appointed for a period of two AsCA meetings with alternate councillors being replaced every meeting.

2. Life Membership

The council decided to introduce an additional class of membership being "life membership". This class is open to members turning 60 and the one-off cost of this is three times the current subscription rate (ie \$60). This new class of membership is designed to enable members retiring from formal employment to remain in contact with the activities of the society.

3. Proposed Name Change

It has been suggested that the name of the Society be changed to reflect the involvement of New Zealand crystallographers in the Society. The proposed name is The Society of Crystallographers in Australia and New Zealand (SCANZ). The Council supports this move and it was decided to put the idea to the members at the next general meeting at Thredbo. Some advantages and disadvantages of the name change are highlighted below.

New Zealanders are a small but significant part of the Society - currently around 6% of the Society membership are New Zealanders. New Zealand has hosted a meeting of the Society and it is hoped that they would host future meetings of the Society. By formally recognising the importance of the New Zealand involvement in the Society, it is anticipated that the number of active New Zealand members would increase. Other societies including the Institute of Physics have altered their name to include

both nations.

A change in the name of the Society can have a number of effects. Two possible disadvantages for the present membership are that it would cost money (<\$500) to change the name and transfer funds to the new body. Secondly, the anticipated increase in student members from New Zealand would increase the pressure of the *1987 Fund* used to support student members' attendance at meetings. There are possible implications in respect to membership of the Asian Crystallographic Association.

The Council intends to further explore this and other potential disadvantages of the proposed name change in the lead up to the next SCA meeting. Any members who would like to comment on the proposed name change can do so by contacting the SCA Secretary, Brendan Kennedy, Department of Chemistry, University of Sydney, NSW 2006, or by e-mail to bkennedy@chem.usyd.edu.au.

Brendan Kennedy

STUDENT REPORTS FROM GLASGOW

(The following are reports from students who received Ted Maslen Travel Awards enabling them to attend the IUCr meeting in Glasgow in August, 1999).

1

With such a loud, impressive bang to the start of the XVIIIth IUCr Congress from the pipes, drums and brass of the Band of the 51st Highland Brigade, it was hard for the Congress to be anything but a great success.

As a first-timer to an international conference of such magnitude, I was bewildered to find myself in the company of not only the world's leading crystallographers, but also be amongst a sea of young, enthusiastic fellow scientists from all over the world, gathered in Glasgow, to present their work and to soak up the crystallography. And what a lot there was!

The enormity of the conference was highlighted as I found myself in the presence of such greats as Hugo Rietveld – a man, whose work has managed to be the cause of great hair loss and hair growth (all at the same time) throughout my studies. Besides the excitement of meeting such distinguished crystallographers, I attended some very informative keynote lectures and microsymbioses, which helped me gain greater insight into certain areas of my research. However, more significantly, the vast array of lectures that the conference provided also gave me the opportunity to see different aspects of science in a totally revolutionary light and to look beyond my world of apatite compounds. It was impressive to see such diversity and the very apparent degree of progress that has been made in the world of crystallography.

Despite being considerably outnumbered by protein crystallography and the likes, my poster ("Structural Studies of Synthetic Calcium and Lead Apatites") managed to provide temporary diversion and to attract a lot of interest along the way as well. There was enthusiasm shown not only by people from similar backgrounds, but more surprisingly, by people from institutions like NASA. It was most encouraging to hear so many positive comments and to even be given some thoughtful suggestions for future work.

Putting crystallography aside, a very precious and memorable experience would also be the many new friendships I developed over the course of the ten days. It was so much fun to discuss new and old research ideas with fellow students and to also learn the art of drinking whisky, the Scottish way.

Although the conference is well over now, the familiar sound of pipes and drums keep beating in my heart, and I have the SCA to thank for providing me the E.N. Maslen 1987 Travel Scholarship to enable me to attend such a magnificent affair.

Jean Kim

University of Sydney

2

In writing a report to the SCA on my experiences at the IUCr conference in Glasgow, it is difficult to know where to start. I could start with my first real memory of the city, and that is the destruction of the myth that the Scots speak a language closely resembling English. Understanding the locals was a real challenge. The conference itself was a huge affair, and although I knew that there would be in excess of 2500 delegates there, the scale of the event had to be seen to be believed. Mind you, the security presence was a little overdone. I am not sure it was really necessary to check that delegates had their identification to enter the poster hall.

My conference started with a day-long CCDC workshop. This was a useful session for me, being a fairly new user of the CSD, and it introduced me to some of the more obscure and advanced ways of using the Database. The opening ceremony was a seriously grand affair, including the obligatory bagpipe band. Many people who attended this conference will know that the World Bagpipe Championships were also on in Glasgow, and the pipers spent a lot of time practising outside my bedroom window.

Scientifically, the highlights of IUCr were many. The opportunity to interact with crystallographers, and especially students, from all over the world was extremely valuable. In Australia, and especially in Armidale, it is easy to feel isolated from the rest of the world. Jack Dunitz gave an excellent talk on polymorphism, suggesting that while this phenomenon was once considered an annoyance, polymorphism can now be both interesting and useful. Wilson De Camp from the US Food & Drug Administration gave us another view, where discovery of polymorphic forms of a potential drug with significantly different physical properties can cause a major setback to, or even completely derail, the development of the drug. His talk gave a fascinating insight into the approval process for potential new drug products. Jack Dunitz also contributed to the discussion from the audience in many of the microsymbiosia that I attended - his depth of knowledge across many areas of crystallography is truly amazing.

Another highlight was a talk by Ricardo Destro, whose interests are in the area of charge density studies. This was an excellent review of the contentious issue of the existence or otherwise of unusual bonds and molecular properties, the result being an intriguing chemical story rather than merely a summary of one group's recent work. Of course those talks mentioned above are only a selection of the many informative presentations, posters and discussions I witnessed at IUCr99, and in addition to those, the opportunity to present our group's work was especially valuable. The feedback and comments from the very busy poster session will be influencing my work significantly and I gratefully thank the SCA for the generous travel funding that enabled me to attend.

Joshua McKinnon

3

The Scots are renowned for their hospitality and warmth. This was a continuous highlight for me, right from the rousing and heart-stirring opening ceremony with its pipe bands, to the helpful people on the streets of Glasgow. This set a wonderful atmosphere for this international gathering, whose delegates were instantly recognisable from the bright green tartan bags issued at registration. Glasgow became peppered with them.

A big, yet pleasant surprise about the Congress was the diversity of themes that fell within the realms of crystallography. Having studied materials engineering prior to beginning a PhD in Physics, I really enjoyed the sessions on nanomaterials, as well as many others that were more related to electron and X-ray crystallography (the fields I am working in now).

The highlight of the nanomaterials oriented microsymbosia was unquestionably the lecture given by Professor K. Takayanagi on the "Structure and Quantized Conductance of Nanowires Studied by a Combined STM and Electron Microscope". I have never before heard so many gasps of amazement and pleasure from a critical group of scientists. Professor Takayanagi stole the show with his atomic resolution videos of gold nanowires being pulled out of a gold substrate using an STM tip inside the specially adapted high resolution TEM. It is rare to see such an elaborate experimental setup and its spectacular use. As the STM tip was pulled further away from the substrate and each clearly visible layer of gold atoms disappeared (accompanied by gasps from the audience) there was a step-wise decrease in the conductance all shown on video in real time and slow motion. Finally, there was just a single chain of gold atoms suspended between tip and substrate in the vacuum!

Coming from an inorganic background, it was absolutely fascinating to learn how instrumental crystallography is in determining the structures of viruses and other biological/organic molecules and structures. It was most eye-opening indeed to realise the enormous amounts of work being done with viruses and proteins, not only with X-ray crystallography, but also in novel ways with electron microscopy. Here, a keynote lecture springs to mind, given by Professor M. van Heel, "Cryo-Electron Microscopy of Single Particles: The Structure of the *E. Coli* Ribosome". In this work, they used specimens where the particles were randomly oriented, i.e. the exact opposite of crystallography. Many digitised images of the ribosome in its different orientations were collected without having to tilt the specimens. The images were used to build up a three dimensional image of the structure with a resolution of 13 Ångstroms. It became clear how enormous the computational effort was in doing this. It was also clear that this technique, whilst containing little crystallography, was trying to achieve the same aims as the more established crystallographic methods.

Most interesting as well as entertaining was the Monteath-Robertson Symposium which really described the history of crystallography, with special emphasis on Glasgow University. This was presented by some of J. Monteath Robertson's past students, which gave the symposium a wonderfully sentimental feel.

The atmosphere in the main exhibition centre during the poster sessions and commercial exhibits was vibrant and there was always so much to choose from, the presenters always being very engaging in discussion. There was never a lull in the action with the constant to and fro between interesting microsymbosia and poster sessions and exhibits.

The contacts and new friendships forged at this conference have opened many opportunities for collaboration as well as a sense of connection to the broader crystallographic community. Discussions I have had with so many different people at this Congress, have given me a new perspective of my own work along with many ideas that I seek to implement.

Many thanks to the SCA and IUCr for providing the vital funds for me to go and enjoy this enriching experience.

Philip Nakashima

University of Western Australia

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Glasgow was an wonderful choice of place to hold the IUCr XVIII Congress, and the timing was exceptional. The weather in August is as good as it gets for Scotland. It was really quite pleasant. The Edinburgh Festival was on at the time, and definitely a worthwhile stopover following the conference. Also, the sound of bagpipes could be heard throughout Glasgow during the week of the conference, as there was an International Bagpiping Conference held the week following the IUCr Congress. I was told that there were approximately 400 bagpiping groups practising all over Glasgow.

At the Congress I presented a poster entitled "*In situ* Neutron Diffraction Study of PZN-PT Piezoelectric Single Crystal Under an Applied Voltage", which seemed to be well received. I found this poster session rewarding as it provided an opportunity to speak with researchers in related fields of study. From the session I received many useful suggestions and comments for extension of my current work, and continuing these discussions via e-mail has been a valuable outcome for me.

Being in the audience of, and meeting researchers that I have admired for several years was an excellent experience. Amongst the more noteworthy for me were presentations given by E.K.H. Salje, Hugo Rietveld, Ray Withers, Jack Dunitz and E.J. Mittemeijer to name but a few. These presentations were all particularly relevant to my research. Other seminars presented on the examination of inorganic structures were thoroughly informative, and there was much to be learned from them.

On the whole, the Congress was very well organised, and appeared to flow without serious incident, which was amazing considering the large number of delegates, and the associated huge numbers of parallel seminar sessions, and even greater number of posters that were presented. I wish to express my appreciation for the financial assistance provided by the SCA to support my attendance at the IUCr XVIII Congress. It was indeed a worthwhile conference to attend for numerous reasons.

Jenny Forrester

University of Newcastle

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The congress organizers must have struck a deal with Mother Nature as the congress fell within the three-week British summer. The opening ceremony for the Congress was very grand and was held in an armadillo-shaped building (a copy of the Sydney Opera House).

It was great to put a face to the people that I had previously only read about during my research. I especially enjoyed Thomas Mak's talk on silver(I) complexes, which gave me many new ideas for my own copper(I) work.

Gervais Chapuis presented a great talk regarding crystallographic teaching on the Internet. The applications are platform independent, which means that students can learn on any modern computer at their leisure. Since the Conference, I have been in contact with Professor Chapuis regarding his presentation.

Jack Dunitz's Keynote Lecture on polymorphism caught my attention as it was very applicable to my research project. It was an eye-opener to see just how readily some common compounds showed polymorphism, with some easily observed and others not. I learned that as crystallisation is not controlled by thermodynamic factors, crystals obtained from solution may not be the most stable under the conditions used.

The vastness of the venue and the large number of presenters made choosing which of the six parallel talks to attend sometimes tricky, especially as many of the speakers were so passionate about their area of expertise. Wherever a gap in the sessions relevant to myself occurred, I would attend sessions unrelated to my area to soak up new ideas and interpretations. An example of this is the talk by Geoffrey Jameson. This described the problems and solutions of twinning in large protein molecules. Even though this topic was not related to my project, it was great to see different methods of solving various problems that arose.

Although only a small number of the poster presentations were relevant to my research, I feel I have returned to work with new ideas and a wider knowledge of crystallography. Another highlight was the commercial talks and displays that demonstrated the latest X-ray diffraction equipment.

I would like to take this opportunity to thank the SCA for the generous funding which allowed me to attend this superb gathering. Attending the conference allowed me to meet many interesting colleagues from around the world. I hope that these funds continue to be available for students wishing to attend meetings in the future.

Neil Somers

University of Western Australia

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As I was sitting in the Clyde Auditorium during the opening ceremony I was awe-struck by the number of people there and I was really proud to be a part of this huge group of scientists gathered in the name of crystallography. It was an awesome experience to be amongst, sometimes even speaking to, so many people that I had previously only heard of.

But, possibly more importantly than this for me, I had the chance to listen to and learn from these eminent people. The Glasgow meeting was an opportunity to learn about new (and old) techniques and their application to the work that I hope to do, in the field of powder diffraction. It was an opportunity to also see the vastness of crystallography, to discover that it is not just about solving single crystal structures, and also to realise the breadth of application of crystallography to 'the real world'.

Also, while in Glasgow I attended the Powder Diffraction Workshop, on the first day of the conference. The workshop awakened me to some of the options available for solving structures *ab initio* from powder diffraction data. Although we did not get any hands-on experience with the methods that were discussed, which was a disappointment to me, it was never-the-less an instructive experience.

Following the conference, I attended the Computing School, held on the beautiful grounds of the Wellcome Trust Genome Campus, in Hinxton, (outside Cambridge). Although the Computing School focused primarily on macromolecular crystallography, (outside my current field of expertise) it reinforced some of the ideas that I had been introduced to at the conference and it gave me a chance to begin to wind down after the hectic conference schedule.

I have come away from the meeting with a sense of purpose and an eager anticipation of my attempts to

apply some of the techniques that I have learnt about.

I would like to thank the SCA for the financial assistance that they provided, not only did this assistance allow me to attend the conference, but it also gave me the opportunity to take my first trip overseas.

Kia Wallwork

Flinders University

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My experiences in Glasgow got off to a good start when British Airways managed to lose my baggage. Free from the physical constraints of an over-packed backpack, I was able to wander around the city and find my accommodation, safe in the knowledge my luggage would be couriered to me at a convenient time. That backpack got a good deal more over-packed when I collected the tastefully decorated conference satchel. The sheer weight of the abstracts booklet immediately alerted me to the range and quantity of science presented at the Conference. It was something I was expecting, but was still eye-opening as the meeting proceeded. The last conference I attended (in 1997) was a small specialist meeting, at which in an informal setting, I was able to meet and talk with many of the leaders in my relatively small field of electron density analysis. That was very beneficial, and so too was the IUCr Congress, but in a different way. By being exposed to the full breadth of crystallographic research I was able to identify, and learn a little about, the particularly active or interesting fields in the science, which is important as I finish my PhD studies and look to the future. My own field was well represented, with two sessions of talks, on chemical insights from charge density analyses and developments in the use of synchrotron radiation for the acquisition of charge densities, containing several interesting presentations. I heartily thank the SCA for their generous provision of funds (which is fittingly named in honour of my late supervisor Ted Maslen) to assist in my attendance at Glasgow.

Nicholas O'Toole

University of Western Australia

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The opening ceremony for the IUCr Congress was extremely well organised and included, as I had expected, a lot of bagpipe playing. In fact the bagpipes could be heard most of the week since Glasgow was not only holding the XVIII IUCr Congress, but also the World Bagpipe Playing Championships. Glasgow proved to be a city full of life with enough bars, restaurants and shops to satisfy any visitor, whilst the Glaswegians themselves are very hospitable.

The actual venue for the conference was huge and the schedule very full. There were six sessions taking place in different lecture theatres at any one time with two plenary sessions, first and last thing. There was a huge hall full of exhibitors, posters and delegates, all carrying green tartan bags. I never imagined that my day could be so packed, learning about old and new techniques and structures, whilst socialising with people I had heard of but not yet had the chance to meet.

As a new student to the field of crystallography, I learnt much from the many speakers and presenters who in turn helped me see the direction in which my own work is heading. I very much enjoyed the CCP4 Introductory Workshop for protein crystallography which I attended and found it to be very informative. As a protein crystallographer, I particularly enjoyed the session on New Frontiers in Macromolecular Crystallisation.

The presentation of my poster was more daunting than I had imagined it would be but I am grateful I had the experience to present one as a student. In fact the whole visit was an extremely valuable experience both scientifically and socially. I am extremely grateful to the SCA for the generous funding which enabled me to attend. I have returned with a greater enthusiasm for my work and for the field of crystallography as a whole.

Elisabeth Fletcher

Victorian College of Pharmacy

SKETCHES OF CRYSTALLOGRAPHY LABORATORIES

Biomolecular Research Institute

Protein structure analysis at Parkville dates back to the 1950s, with Bruce Fraser and Tom MacRae using X-rays and, later, Peter Tulloch using electron diffraction to study natural fibers. However, the laboratory took a substantial new direction in 1978 when Peter Colman joined what was then the CSIRO Division of Protein Chemistry to set up protein crystallography. Peter brought with him some of the first crystals of influenza neuraminidase and, with the help of Bert van Donkelaar, began trying to determine the structure of this protein. Jose Varghese joined the laboratory in 1981 as a postdoctoral fellow and, by 1983, the structure of neuraminidase had been solved. This was a landmark in protein structure determination as it was large for its day and it was the first protein structure to be solved by averaging density from different crystal forms. Furthermore, the structure was solved without the use of computer graphics and most of the computation was performed remotely in Canberra.

In 1983 the possibility of using the neuraminidase structure to develop antiviral compounds was suggested and, after Glaxo showed only tentative interest, Biota Holdings was floated in 1985 to support the development of neuraminidase inhibitors in conjunction with the Victorian College of Pharmacy. From the structures of the protein with transition state analogues, a number of neuraminidase inhibitors were synthesised. Glaxo developed one of these compounds as the drug, Relenza, which has gone on sale this year. Other structure work in the 80's included electron and X-ray crystallography of neuraminidase-Fab complexes by Peter Tulloch and Bill Tulip, respectively, single crystal studies of a plant virus and structure determination of a seed storage protein by Mike Lawrence who joined the group in 1988.

In 1990, following a recommendation from a working party of the Victorian State Government, the Biomolecular Research Institute was formed with Peter Colman as Director. With structural biology at its core, BRI incorporated a novel idea of combining virology, biochemistry and organic chemistry, in addition to providing an integrated approach to structure-based drug design. The structure group diversified, drawing some staff from CSIRO and hiring others, such as Brian Smith, Vidana Epa (theoretical chemistry and modelling) and Tom Garrett (X-ray crystallography). BRI also added an NMR group.

The focus of the work is on proteins of medical interest and X-ray structures have been determined to understand infection by viral and bacterial pathogens as well as diseases such as diabetes, cancer, auto-immunity and allergies. Other areas of interest are growth factors, antibodies (including engineered smaller, single-chain forms), carbohydrate processing enzymes and engineering protein thermostability. Having an emphasis both on basic research and on its application, a number of projects have now been taken through to the stage of drug design and synthesis. A thermostable enzyme has also been produced for the brewing industry.

The X-ray instrumentation consists of Elliot, Siemens and Rigaku rotating anode generators and four image

plate detectors. In addition, Jose and Bert have been helping develop capillary optics with David Balaic and Zwi Barnea from Melbourne University. These optics are particularly suitable for small crystals (<100micron) where increases in diffraction intensities by over a factor of 20 have been observed. As well as those mentioned above, the crystallography group consists of Mei Lou, Pat Pilling (crystallisation); Jenny Carmichael, Lin Chen, Ross DeGori, Robyn Malby (crystallography); Lyn Lawrence (electron microscopy) and Rob Downes (instrumentation). Adrian Batchelor has a joint appointment with the Walter and Eliza Hall Institute to work on structural aspects of malarial proteins. Recent past PhD students include Joao Barbosa, Tina Izard, Airlie McCoy and Kelly Maxwell.

Last year, and with great sadness, we mourned the loss of Peter Tulloch.

Tom Garrett

CRYSTAL XXI

The twenty-first meeting of the Society of Crystallographers in Australia will be held at the Thredbo Alpine Hotel Conference Centre, Thredbo Alpine Village, NSW from February 1-4, 2000. The deadline for the submission of Abstracts, Registration and Accommodation bookings was November 5, 1999.

The *1987 Lecture* will be given by Dr Douglas L. Dorset (Electron Microscopy/Diffraction), Principal Research Scientist at the Hauptman-Woodward Medical Research Institute, Buffalo.

Other invited lecturers are: Ian Grey (CSIRO Div. Minerals), Colin Raston (Monash University), Bill David (UK) Peter Colman (BRI) and Stephen Hyde (ANU).

Accommodation has been reserved in the Thredbo Alpine Hotel and the Thredbo Alpine Apartments, which should be able to cater for the majority of attendees. Both of these are directly adjacent to the Conference Centre, but there is a large range of other accommodation available in the village within easy walking distance. It is hoped that most people will choose one of the two options provided on the Registration Form, as this will keep the cost of the hire of the conference facilities to a minimum.

The Registration, Accompanying Person and Payment Forms and the Call for Abstracts document may be downloaded from the website. Thredbo is about 2.5 hours drive from Canberra. Bus transport from Canberra on the afternoon of 1st Feb will be provided and similarly return after the conference on the morning of Saturday 5th Feb.

Further information can be obtained from the conference website at [http:// rsc.anu.edu.au/~welberry /crystal21/](http://rsc.anu.edu.au/~welberry/crystal21/).

Call for applications for the E.N. (Ted) Maslen 1987 Studentships and Scholarships

CRYSTAL XXI

Thredbo, NSW, February 1-4, 2000

The Council of the Society of Crystallographers in Australia is calling for applications from postgraduate students of crystallography for the E.N. (Ted) Maslen 1987 Studentships and Scholarships to fund attendance at the twenty-first meeting of the Society of Crystallographers in Australia to be held at Thredbo Village, New South Wales from February 1-4, 2000.

Details of the conference are available on the Internet at: <http://rsc.anu.edu/~welberry/crystal21/>.

SCA 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 SCA Council regards these awards as an important means of introducing young crystallographers to the national and 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 1987 Scholarship should forward to the Secretary, Dr Brendan Kennedy, School of Chemistry, University of Sydney, NSW 2006 the following:

.A abstract of the presentation sent, or to be sent, to the Organising Committee.

.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 SCA.

The deadline for applications is December 7, 1999.

FUTURE MEETINGS

11RACIC

The 11th Royal Australian Chemical Institute Convention will be held at the Australian National University in Canberra between February 6-11, 2000, following Crystal XXI. Held every 4 years, the conference is a major activity of the Royal Australian Chemical Institute. Chemists worldwide are invited to participate in this major scientific gathering of national and international authorities in all areas of Chemistry. Further information can be obtained from the conference website at <http://www.11racic.conf.au>.

The Lorne 2000 Conference

The 25th Annual Lorne Conference on Protein Structure and Function will be held at Erskine House, Lorne from February 6-10, 2000. The conference website is <http://grimwade.bichem.unimelb.edu.au/lorne.htm>.

IUCr XIX

The 19th Congress and General Assembly of the IUCr will be held in Jerusalem, Israel, August 6-15, 2002. The Congress Web page is located at: <http://www.kenes.com/iucr/>.

The next issue of the *Newsletter* will be in February, 2000. Contributions should be e-mailed to the Editor by January 31. The website of the Society of Crystallographers in Australia is located at <http://www.sca.asn.au>.

