SOCIETY OF CRYSTALLOGRAPHERS IN AUSTRALIA INC.

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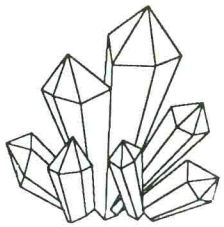

From the President

This year has held mixed blessings for scientists in Australia. It started with submissions to the Research Reactor Review, and the subsequent meeting with the McKinnon Committee to explain the position of the SCA expressed in the submission the executive made on your behalf. The findings of this enquiry were not entirely to the liking of the Minister, and also not entirely to the liking of many crystallographers.

In brief: the RRR found the existing Lucas Heights operation and reactor to be safe and capable of operation for perhaps twenty years. It failed to find proved the claim that a new research reactor should be built. Rather it put off the decision for five years. In the meantime Ansto is supposed to receive additional funding to upgrade the HIFAR neutron scattering facilities.

This sounds as though great progress was made, and we can now relax. Nothing could be further from the truth. The Sutherland County Council, the prime adversary of Ansto at the RRR, has had the Local Government Association accept a resolution that "no new nuclear reactor would be build on land over which the LGA has control". This has the effect of severely limiting the number of possible sites for construction of a new reactor. And current action in the USA with respect to the reprocessing of the nuclear fuel rods currently at Lucas Heights gives the Green Lobby plenty of ammunition for a motion to close down, or scale back, the use of HIFAR.

In a separate move the Minister tried to incorporate Ansto within CSIRO against considerable opposition from scientific and technological societies throughout the country. This move was eventually defeated in Cabinet. To increase the CSIRO control of Ansto the Minister sacked the Ansto board. The new members of the board do not seem to me to be competent to manage a facility with interests as diverse and complex as those which exist at Ansto, and I see no member as having any expertise in nuclear science. An indication of the highly politicized nature of the new board is the retention in the board of the Executive Officer of the NSW Labour Council, the only member of the previous board to be re-instated. The whole procedure does not give one confidence in the survival of a neutron scattering facility in Australia!!

But we must keep trying. Our next move is to write a submission to the Australian Academy of Science to support moves to have the HIFAR facility to be modified to include a cold source, thereby increasing the range of neutron scattering experiments which can be undertaken.

There have been some successes.

On 15 October 1993 the Minister for Science and Small Business opened the Australian National Beamline Facility at the synchrotron radiation source, the Photon Factory, at Tsukuba in Japan. This was the culmination of initiatives which Stephen Wilkins and I took in 1986, and which, with the help of a number of people over the years, we managed to have funded in 1990. The consortium which provided the funding (ARC, CSIRO, Ansto, DITAC, ADFA and ANU) must now feel that their contributions to the project ($ 3.3 M) were well spent, and Australian scientists now have access to high quality beamline on which is mounted a novel and very versatile diffractometer system. The beamline and diffractometer system were brought into operation within budget and on schedule. Experiments performed so far include X-ray powder diffraction, protein crystallography, diffraction at high pressures, topography, tomography, and XAFS.

We have just received the consortium partners' contributions for operation for 1994. This includes funding from DITRD for travel to the PF to use the facilities available there.

Discussions with other science and technological societies, catalyzed by FASTS, appear to have halted the implementation of the new unified science curriculum. This may seem to most members to be a retrograde step but I assure you the proposed curriculum had so little science in it that it made nonscience of the whole proposal. Again the halt is only temporary and it is essential that we all involve ourselves in this particular aspect of community affairs. Australia's scientific and technological future is really at stake

Continued on page 2

Editorial

This issue of the SCA newsletter brings a new format and a new Editor. It must be something of a relief to many of you to know that your society is still in existence! There is more good news.

The SCA newsletter will from now on appear quarterly and will be distributed with the IUCr newsletter. Arrangements have been made to have the IUCr newsletters air-freighted in bulk to the secretary for distribution to SCA members whose addresses are within Australia. This will mean that members will get their copy of the IUCr newsletter much sooner. In future, IUCr newsletters will not be sent to crystallographers in Australia who are not financial members of the SCA, unless they make private arrangements. We also plan to send copies of the newsletters to vice-chancellors, relevant government ministers and departments etc.

One consequence of this arrangement is that the SCA newsletter will usually be much smaller than in the past because it will only contain extra Australian news. Another is that, although the SCA newsletter will appear four times per year, the time of issue cannot be guaranteed by the Editor. This will be determined by the time of arrival of the IUCr one. As the publication of this issue was expected about a month ago the Christmas Greetings from Dudley are somewhat belated, but they have been left in as he would no doubt wish you all to know that he was thinking of you.

This issue contains reports by five of the six recipients of '1987 Scholarships' who attended the Beijing Meeting. Other news of the meeting is in the IUCr newsletter. We congratulate Ted Baker who was elected to the Executive Committee of the IUCr and Ward Robinson who is the new President of AsCA.

A very interesting article by Sandy Mathieson is also included. The Editor would welcome other submissions of this type and also items of news or personalia for publication in future newsletters. If at all possible please submit this material by e-mail in ASCII format. *MRT*

Council Notes

The Council has confered via AARNet during the year. Matters discussed include:

Crystal XVIII, 5-8 April 1994

Council has allocated $3500 from the '1987' fund and $1500 from SCA funds to support the appointment of Professor John Helliwell as a '1987 Fellow', and to provide '1987 Studentships' to assist students to attend the meeting to be held at Medlow Bath.

Cambridge Structural Database

David Winkler has decided not to continue as manager of the Australian affiliated centre of CSD beyond the date of the Medlow Bath meeting. Council was pleased to hear from Chris Howard that ANSTO will take over the role of affiliated centre and thus ensure that the database is available to users in Australia. The crystallographic community in Australia recognises the enormous importance of the work that has been done by David over several years.

IUCr Newsletter

Council decided that the SCA would take over the role over distributing these newsletters to the membership. To reduce mailing costs they will not be sent to members with overseas addresses unless requested.

President's message continued from page 1

here. If we do not succeed in having sensible national curricula adopted in mathematics and science there is a real possibility that our children may become the uneducated poor white trash of Asia.

Speaking of Asia: Ward Robinson and Syd Hall are investigating venues for the next Asian Crystallographic Association Meeting. The proposed site is in Malaysia. I would value suggestions by members of a theme for this meeting. If you have suggestions please send them to our Secretary, Max Taylor.

This column reads like doom and gloom, and well it might. Australia is very definitely at the crossroads, and if we do not become efficient at producing value-added goods very soon we will slide as a nation to the status of a Third World Power. One reason for our dismal performance is the fact that almost in Government and in the bureaucracy appears to understand science and technology. And few private firms and and banks are prepared to provide risk capital for the creation of innovative technologies and products.

Much can be sheeted home to the fact that scientists are regarded by people as oddballs, brilliant but a little mental. Politicians, since they react only to societal attitudes, do not take us seriously. We must reverse that image!

It is essential that each of us tries to make contact with real people at the social, school and even party political level.

Make New Year's Resolutions: tell a new person about your work, or the work of your institution each week. Harass a politician whenever you feel something unscientific is being done by government. Be active...

It will be hard, require effort...but our children will thank us for the effort we make!!

Have a Joyful Christmas, and keep to those New Year Resolutions!!

DCC

Revisiting Darwin (C.G.) then on to Tsukuba

by A. McL. Mathieson

Although my basic degree was in chemistry and my research experience before joining C. S. I. R. in 1947 had been chemical crystallography, the stimulating atmosphere of the Chemical Physics Section resulting from the mixture of physicists, chemists and mathematicians, together with the ambitious expectations of Lloyd Rees, encouraged one to explore more closely the beginnings of one's subject, in this case, X-ray diffraction. For some reason, I latched onto C. G. Darwin's papers, especially the third one.

Darwin's was one of the earliest attempts to provide a theoretical basis for the intensity distributions observed when diffraction from single crystals occurred. His first two papers[1,2] were in 1914. I still have the photo-copies of these made for me in 1949 (no xerox machines then so even copies were rather valuable) and on occasions over the years, I have dipped into them—not for the mathematics with which I have never been comfortable but rather for the natural philosophy insights. Both papers were, in a sense incomplete in that they referred to the two extreme cases—coherent diffraction corresponding to the later so-called dynamical case—and incoherent diffraction corresponding to the so-called kinematical case. No reasonable explanation for the actual sorts of intensities observed in practice was proferred in those papers. It needed quantitative experimentation to provide numerical material and thereby stimulus for a further development of the theory. The results presented by W. L. Bragg, James and Bosanquet[3] in 1921 did just that. In order to establish the electron distribution in crystals of NaCl and hence the ionic state of Na and Cl a rather important and critical result at that time—they sought to establish accurate structure factors for NaCl. To this end, they measured the diffracted intensity from an extended-face crystal (Bragg-type reflection). They realized that this measurement was influenced by multiple-scattering (the effect which is now referred to as extinction) which required the standard formula for the integrated intensity, namely $Q/2\mu$, to be modified by replacing the normal absorption coefficient μ by μ' which included the effect of diffraction scattering. The question was—could one make an experimental estimate of μ'. They tackled this problem in a roundabout way by preparing a series of crystal plates of NaCl of diminishing thickness, t. With each plate, they measured the intensity diffracted through the plate (Laue-type reflection). By plotting these measured intensities versus t, the slope gave a measure of μ'. So, combining the results from **two different types of measurement**, they were able to establish numerical data **corrected for extinction by an experimental procedure** without having recourse to theoretical models of extinction—the bane (and temptation) of crystallographers. Darwin was aware of this work. It was now some 7 years since his original theorizing. These results of Bragg, James and Bosanquet allowed him to have another crack at the problem of diffraction from "real" crystals. We should note his cautionary statement in this paper[4]—"The imperfections of crystals may take either of two forms, warping or cracking. Either the atoms may be arranged on surfaces that are not quite flat or else they may be arranged in blocks, each block a perfect crystal, but adjacent blocks not accurately fitted together. An examination of rocksalt suggests that the first is probably more the nature of its imperfections but the second is much more tractable to mathematics and so has been adopted here."

So his choice of model was determined essentially by the then tractable mathematics which could deal with a distribution of crystallites. It is from this early decision of Darwin's that we as crystallographers have continued to use the term "mosaic" distribution (the actual word "mosaic" was due to Ewald). (Recently, there has been a different theoretical approach by Kulda more in line with the alternative that Darwin recognized as more realistic.)

In this 1922 paper[4] he developed the theoretical treatment which has been basic for most subsequent discusssion and calculations relating to imperfect crystals. He established the differential equations —the so-called Darwin Energy Transfer equations— and worked through a number of cases. Also, he considered a number of approximations. It is a paper still worth reading and pondering on. What is passing strange is that, despite this lead, crystallographers did not envince any great desire to carry out further exploratory experiments involving accurate measurements to test critically Darwin's theoretical offering. Perhaps they were concerned that experiments might give disturbing results not compatible with theory. One might even get the impression that fiddling with theory was easier that doing experiments.

In 1925, there was a small high-level meeting in Germany concerning the intensity of X-ray reflections to try and answer the question—"Is intensity proportional to to F or F^2?" In fact, no great clarification resulted and each protagonist group largely went on its own way. W. L. Bragg, Darwin and James[5] recorded their contribution regarding imperfect crystals to this meeting. Then photographic recording

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Darwin to Tsukuba continued from page 3
with its potential for measuring hundreds of reflections took over from diffractometry and the explosive activity of structure analysis began. So quantitative measurement of diffracted intensity and the insight which can arise from the derivation and close scrutiny of accurate data were largely put away. With the return of diffractometers in the 1950's onwards, there was a resurgence of concern with measurement procedures but essentially the approaches taken were again constrained to aspects of diffracted intensity and there was no indication of a wider appreciation of other components of diffraction experiments.

Recently, on re-reading Darwin's third paper[4] I was interested in one particular point. Although Darwin was aware of W. H. Bragg's careful observation in 1914[6] that the transmitted beam dips in intensity when a diffraction point is traversed, nevertheless he only ever dealt with the intensity of the diffracted beam, despite the fact that his equations involved both transmitted and reflected beams. There were, of course, good reasons for this restriction, at least experimentally. The transmitted beam in those days was often "messy", i.e. it consisted of a range of wavelengths whereas the diffracted beam was rendered relatively monochromatic by the very process of diffraction. Why not measure both beams? Obviously if one could simultaneously measure the reflected and transmitted beam profiles point by point, one would have a much more powerful hold on the situation. For meaningful measurement of the transmitted beam, the incident beam would have to be highly monochromatic. The situation would be even more clearly defined if the radiation could be highly-polarized. It then struck me that, in 1973–4, Larry Calvert, Reg Killean and I had virtually established the experimental set-up necessary for this task. The experiment which we set up then was actually aimed at determining the polarization ratio, point by point, across the 0002 profile of a sample of pyrolytic graphite. Our source was polarized Cu Kα_1 radiation and we measured the reflected beam for perpendicular and parallel polarization in order to extract the polarization ratio. Almost as an aside, we measured the transmitted beam intensity and derived the value of μ' across the profile[7] and of the diffraction pattern in terms of μ' over the full range of θ.

With a source of highly-monochromated and highly-polarized radiation, the obvious step is to carry out dual measurements of the reflected and transmitted beam simultaneously. Larry Calvert, Reg Killean and I came close to it in the early 1970's but sadly didn't realize the implications of the experiment we had set up. Indeed, we became so engrossed with the apparatus problems of determining polarization ratios that other potential yields from the set-up were not recognized. As Alan Walsh has commented, "Having an idea is not necessarily the result of some great mental leap: it is often the result of merely being able, for one sublime moment, to avoid being stupid".

Well, at the time, we insisted on being stupid and failed to realize that we had all the essentials to explore Darwin's equations experimentally. Not only that but we were working with a specimen which, by its synthesis, should correspond to a classical imperfect crystal, at least in one direction. At long last, the message is clear. We must set up the experiment again and, this time, do the complete range of measurements.

With highly-monochromated, highly-polarized and low-divergence X-rays from a synchrotron, the means for convenient measurement of both transmitted and reflected beams simultaneously is at hand. □

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Membership Dues for 1994

Please send your subscription for 1994 with the enclosed form to the treasurer. Members should note that the SCA constitution directs that persons whose subscription is more than one year in arrears be dropped from the mailing list. Notice is hereby given that members whose subscription is not paid beyond 1992 will not receive the next mailing—and will also miss out on the next IUCr newsletter!

Electronic Mail

The secretary would like to obtain a complete list of e-mail addresses for the membership. This can be used to distribute topical information without having to wait for the next newsletter and it eliminates the cost of postage. Please ensure that this information is included on your subscription renewal form.

Impressions of IUCrXVI in Beijing

'1987' Scholars

Six research students were awarded '1987' Scholarships to enable them to attend the Beijing meeting. The recipients were:
Liping Chung—Physics, University of NSW
James Hester—Physics, University of WA
Tina Izard—Biomolecular Engineering, CSIRO Melbourne
Robyn Malby—Biomolecular Engineering, CSIRO Melbourne
Airlie McCoy—Biomolecular Research Institute, Melbourne
Mark Nieuwenhuyzen—Chemistry, University of Canterbury

One of the conditions of the award was that they write an report on their activities at the meeting. Five of these follow. James Hester has been 'lost' in Russia since the meeting.

"On arrival in Beijing I was surprised to find that the city was not gripped by IUCrXVI fever, but by preparations for 'Beijing 2000'. The airport bus took us along the old bone-rattler road (which ran alongside a brand new freeway) to the conference venue, the complex built for the 1990 Asian Games. A huge billboard saying 'A Billion Warm Hearts Await Beijing 2000' welcomed us.

With so many sessions on protein crystallography, it was inevitable that some of them would clash. I chose 'Hot Structures' over 'HIV proteins and Drug Design' and saw some remarkable structures, for example, the major domain rearrangements in active elongation factor Tu and the soluble lytic transglycosylase from *E.Coli*, 'the protein with a hole'. Of particular interest to me was the 'Immunoproteins and Growth Factors' session, and Mutsi's views on the evolution of cytokines in the session on 'Proteins of Medical Interest and Interactions with Drugs'. I enjoyed the main lectures by Keith Moffat, Michael Rossman, Bill Saenger, Tom Blundell and A Yonath, as much for their personalities as for the content of their talks.

One of the opportunites the conference provided was to broaden the mind by listening to talks on aspects of crystallography not directly related to your area of research. The session on 'Structure of Nucleic Acids and Nucleic Acid Complexes' introduced me to the contribution of crystallography to the development of DNA binding drugs and using DNA as a tool for nanotechnology.

The beer garden was a pleasant place to make new friends and learn about student life around the globe, although the steady rise in price from 6 yuan to 8 yuan to 15 yuan over the course of three nights threatened to bankrupt me by the end of the week.

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Robyn Malby, Airlie McCoy and James Hester

IUCr Beijing continued from page 5

Fortunately I only learnt the truth about the appalling safety record of domestic air travel in China after surviving two CAAC flights on the post-conference tour, one to Xian to see the spectacular terracotta warriors, and one to Hangzhou to see the 'Venice of the East' and Shanghai. Thank you SCA, for a very educational experience, both crystallographically and culturally."—*Airlie McCoy*

"It was an honour and a pleasure to participate in the "XVI Congress and General Assembly—International Union of Crystallography". The amount of information presented at the meeting was staggering: there were 19 plenary lectures, 61 microsymposia of 4-6 talks each, and 120 new posters every day. The abstract book contains over a thousand abstracts. There were 1500 participants.

The quality of the main lectures was very good. Michael Rossman discussed crystallographic methods used to determine large virus structures and also presented impressive electron microscopy results showing for the first time the interaction of rhinoviruses with their receptors. The receptors used by the virus bind in a canyon of conserved residues which is inaccessible to antibodies. He was able to model this interaction with the X-ray structures of the virus and CD4, and show that drugs binding in a cellular cofactor pocket near the canyon should inhibit receptor attachment. Louise Johnson gave an impressively complete overview on drug design based on structural studies leading to her own work on glycogen phosphorylase. By inhibiting this enzyme, the glycogen levels are maintained at higher levels alleviating the effects of impaired glycogen synthase in diabetes type II (non-insulin dependent diabetes). I was impressed by the ambitious effort Ada Yonath is making towards obtaining the atomic structure of the bacterial ribosome. I also enjoyed the presentations by Tom Blundell on the importance of X–ray crystallography in biotechnological programmes, by Claudine Pascard focusing on the wealth of information in data banks concerning preferred crystallographic environment for molecules and the use of this information for designing pharmacaphores once a target protein structure is available, as well as the in-depth discussion by Michael James detailing the rules for hydrolytic enzyme mechanisms learned from crystal structures of proteases.

The quantity and quality of information offered in the microsymposia made me aware of the immense amount of crystallographic research carried out over the world. I was particularly drawn to the two sessions chaired by Guy Dodson and Wil Hol describing new macromolecular structures. These were both structurally and biologically exciting. Pectate lyase described by Richard Pickersgill consists of a novel secondary structure known as a β–coil or β–helix. The polypeptide forms a spiral of β-strands, to give a helix which has three β–sheets as sides.

I learned much from the session on crystallographic teaching chaired with enthusiasm by Jenny Glusker. Henk Schenk gave an extraordinary demonstration of his way of teaching direct methods in which he totally removed the "black box" normally associated with this technique. This was of interest to my own work, as I was able to apply this method for solving the heavy atom structure of a derivative of the protein I am currently working on.

The large number of structures being solved worldwide becomes apparent in the numerous discussion and poster sessions such as "Immunoproteins and Growth Factors", "Viruses", "Enzymes" and "Proteins of Medical Interest and their Interaction with Drugs" or the "Nucleic Acid/Protein Interactions" presented in a session chaired by Tim Richmond. Wim Hol entertained the audience with an excellent talk describing the efforts towards the atomic structure of 2-Oxo Acid Dehydrogenase Multi–Enzyme Complexes. The complex is built around a 24-mer scaffolding in which trimers occupy the corners of a cube.

I really enjoyed the Phasing and Refinement session chaired by Axel Brünger, where Kam Zhang presented an extremely powerful program (SQUASH) which incorporates histogram matching, maximum entropy, direct methods, non-crystallographic symmetry averaging and solvent flattening to give an impressive density modification system which can be used for macromolecular phase refinement and extension.

In Wayne Hendrickson's session on "Anomalous Dispersion Methods", I liked the work by Janet Smith on glutamine PRPP amidotransferase, the largest protein solved by MAD phasing. This should encourage us, having access to the Photon Factory in Tsukuba, to try this method in suitable cases where one has difficulties in obtaining heavy atom derivatives.

I had excellent opportunities to discuss some interesting work with successful scientists in a relaxing atmosphere over lunch or dinner.

During this meeting I was able to learn about many different techniques for X–ray structure determination, about the enormous amount of new structures being solved, I had the unique opportunity to talk to scientists from all over the world about their exciting work and was able to bring back home some excellent programs. I feel deeply indebted to the "Society of Crystallography in Australia Inc." and the "Union of Swiss Societies for Experimental Biology (USGEB)" who generously gave me the opportunity to attend this international scientific experience."
—*Tina Izard.*

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Pictured after the Banquet in Beijing were:
Standing: Max Taylor, Brian Skelton and Hiêú Skelton
Sitting: Dave Rae, Hans Freeman, Monica Hill and Rod Hill

IUCrXVI Beijing continued from page 6

"When we arrived in Beijing on the Saturday the conference began, it was very warm, and the sky was either very overcast or very polluted. I wanted to get to the opening ceremony; the wait taught me that patience is a necessary virtue when visiting China. If it seemed to take an eternity to get to the hotel, booking in was worse. The hotel staff had never heard of Westpac and were very reluctant to accept a bank draft rather than the requested credit card imprint. By the time that was sorted out it was time for the opening reception. While standing in line for food and trying to find somewhere to eat it, I met different people from countries all around the world. The cosmopolitan flavour was enhanced by the folk tunes played by Chinese musicians on their traditional instruments: "Click go the shears" never sounded like that before!

Sunday dawned with the same eerie gloom as the day before: it was somewhat discomforting to walk to the Convention Centre and not to be able to make out the buildings on the opposite side of the road. The thought of presenting a talk that day in the "Hot Structures" session did not lighten my mood. However later that afternoon, with my presentation over, the gloom lifted and Beijing began to show itself in a better light. The Congress proper began for me; there were wonderful presentations by many of the plenary speakers and the choice of parallel sessions made it difficult to choose which of them to attend. The sessions on Nucleic Acid-Protein Interactions, Metalloproteins, Immunoproteins & Growth Factors, Phasing & Refinement of Macromolecular Structures, & Proteins of Medical Interest were particularly interesting.

Macromolecular structures predominated at the Congress in the early part of the week which made it possible for me to see something of Beijing during the latter part of the Congress. Definite highlights for me were: riding a bike along the crowded streets to Ditan Park with a convoy of Australasian crystallographers; tasting the richness of Peking Duck; experiencing the vastness of Tiananmen Square; struggling up the Great Wall, and surveying the decaying splendour of the Forbidden City.

The week was over too quickly; I found myself esconced on the Post-Congress Tour with the chance to meet still more crystallographers from different fields of interest and places of work. We saw the terracotta soldiers in Xian, more pagodas and Buddhist monasteries than I can remember, and I came home with a memorable souvenir from Shanghai; a case of influenza that lasted for three weeks!

Beijing was an unique and exotic setting for an IUCr meeting, and I am grateful to the SCA for giving me the opportunity to go there."—*Robyn Malby.*

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IUCrXVI Beijing continued from page 7

"The IUCr conference occurs every three years. Fortunately for me I was part of the Australian group representing the SCA. Significantly in this time, not only was it highlighted by the attendance of many distinguished crystallographers, but also it was the first time in Beijing, my home town. Over 1,100 abstracts from 50 countries were presented in the congress. General topics covered most of my scientific interests. Particular topics to me focused on the sessions of muscle proteins and the binding studies of the complex structures, since I gave a poster on the binding study of myosin light chain with synthetic peptides.

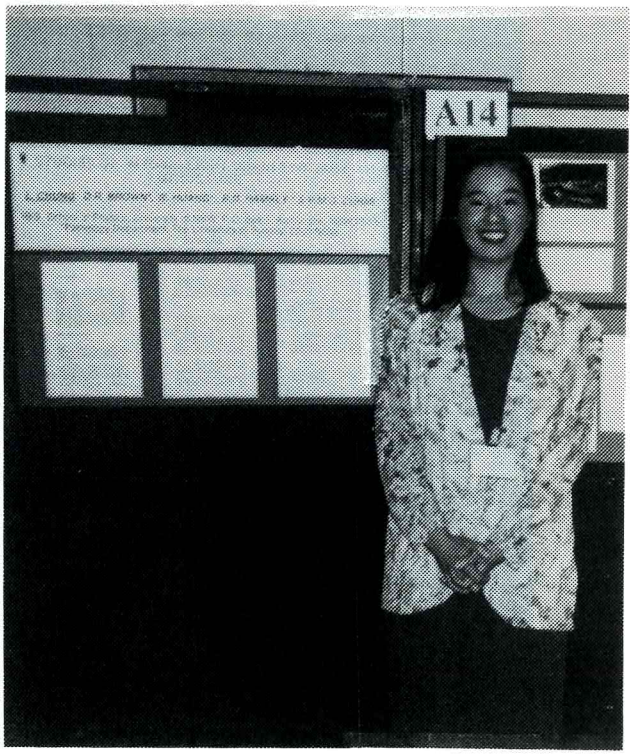
In these sessions, Prof. Michael James who is one of pioneers in solving the structure of troponin C (a member of calcium-binding regulatory proteins involved in muscle contraction) lectured on the contribution of crystallography to the elucidation of hydrolytic enzyme mechanisms. The C/E-1 inhibitor, a good example, represents a distinct family of protein inhibitors of serine proteinases. The packing pattern of inhibitor/porcine pancreatic elastase complex exhibits abundant interactions of molecules, predicting common features of the novel inhibitor family. Dr Rolf Hilgenfeld, representing the protein crystallography group in Frankfurt, talked about some their work on the crystal structure of intact elongation factor Tu (EF-Tu) at high resolution.

In this time at Beijing, I also had a tour of synchrotron radiation source and beam lines at BSRF (Beijing Synchrotron Radiation Facility). I was impressed with their work on synchrotron radiation crystallographical research in materials science and protein engineering.

In particular, I would like to thank the SCA for the award of the 1987 scholarship which enables me to attend the XVI IUCr congress. It was a good experience for postgraduate students keeping eyes open to the whole world. —*Liping Chung.*

"First I wish to thank the Council of the SCA for giving me the opportunity to attend the 16th IUCr Conference in Beijing. This allowed me to see for the first time the scope of the field of crystallography and also to see new developments in instrumentation, data collection strategies and crystallisation techniques combined with current methodology being applied to a wide range of scientific problems.

I was able to see how the techniques developed and used in small molecule crystallography have been improved and extended to much more complicated systems such as proteins, viruses and other macromolecular systems. This is not, however, a one-way street and many of the developments arising from this type of research are applicable to small molecule



Liping Chung with her poster

systems. For example, the development of new detectors and X-ray sources. These developments have made it possible to explore solid state photochemical processes via 'time-resolved' X-ray experiments.

There were many differing approaches to data collection in general and one of the most interesting, to me, was the use of *in situ* crystallisation, using IR laser techniques, to obtain information about 'fragile' crystals. While I can see that this has advantages for these types of crystals it ties up the diffractometer for long periods of time, which is impractical if not impossible for most laboratories where more than one client is being serviced.

I found it particularly useful to meet with the software and hardware manufacturers and discuss their products as this allowed me to talk over some of the problems that I was having and apply their experience and knowledge to these questions. I was also able to make some suggestions for improvements to the software used in the data collection process with these products.

Apart from the crystallographic aspects, the conference allowed me to experience another culture and to see a part of the world that I otherwise may not have. The chance to meet crystallographers from all over the world was especially enjoyable and potentially valuable. I expect to make a career in this discipline and therefore these initial contacts will undoubtedly be useful in the years ahead."
—*Mark Nieuwenhuyzen.* □

An Appreciation of Larry Calvert (Lauriston Derwent Calvert)

Larry was born in Zeehan, Tasmania but subsequently, his family moved to New Zealand where he grew up and received his education. In 1952, he was awarded a Ph D. by the University of New Zealand. His supervisor was Professor Llewelyn. He then joined the National Research Council of Canada, working in its Division of Chemistry in Ottawa. There, he soon became involved in studies of the structure of intermetallic compounds. This subject became a major, if not the major theme of his research activities for the next three decades. He and his colleagues at NRC investigated a wide range of these structures and became acknowledged experts in this area.

As a result of his experience and wide knowledge of this field, Larry was drawn into the onerous task of being Editor for the Inorganic and Metals Section of Structure Reports, a major publication of the International Union of Crystallography. He did this task, not for an occasional volume, but for all those covering 1970 to 1981. Most of this work was necessarily in addition to his own research.

From this experience of overviewing a wide range of different structure types, Larry was drawn to correlating and rationalizing the immense amount of structural information already recorded.

As well as single crystal studies, he became interested in the possibilites offered by the advances in powder data techniques and was drawn into the international activities in gathering powder pattern data, assessing its quality and publishing them for the use of scientists all over the world. These data files are of immense value in identifying solid state phases. In this organization, the International Centre for Diffraction Data, he became a member of the Board of Management. Even when he retired to Lake Entrance in Australia, his contribution continued too be so valuable that he frequently travelled to attend Board meetings in America.

My own closer association with Larry was initiated after the 9th International IUCr Congress in Kyoto in 1972. He, with Eric Gabe, passed through Melbourne and we discussed the possibility of his spending a sabbatical year with the Chemical Physics Division of CSIRO. He spent mid-1973 to mid-1974 in the Division. Together with Reg. Killean of St. Andrews University, we did some work on pyrolytic graphite. Our main aim was to make detailed measurements of the polarization ratio. We got some useful results on other matters concerning pyrolytic graphite, but although we collected a great deal of data, we felt that there was some physical instability in our set-up that we could not identify. So we didn't achieve our aim. That was nearly 2 decades ago. Only in the last few months, an alternative explanation of our results—one of perhaps more general interest—has appeared. It was on these matters that our talks over the phone in his last few months centred on. In the late 1970's, Larry continued his studies of intermetallic phases and his involvement with powder data. As if these interests were not enough, he took on the responsibilities of being Chairman of the Local Organizing Committee for the International Union of Crystallography's 12th Triennial Congress to be held in Ottawa in 1981. Regular attendance at these is usually in the order of 2000 so the task of organization was not trivial.

After the Congress was over, a little later in the 1980's, Larry took retirement from the NRC and came to Australia, settling in Lake Entrance in Victoria. That step did not however mean giving up science. He was involved with the Australia X-ray and Analytical Association and he spoke at the 1989 meeting of the Society of Crystallographers in Australia. Although somewhat isolated in Lake Entrance, he was supplied with a computer/word processor and worked on, co-editing the latest four volume set of Pearson's Handbook of Crystallographic Data for Intermetallic Phases. This was published in mid-1991. (Bill Pearson who did the original Handbook was a colleague at NRC in the early days.)

Larry was an enthusiastic and dedicated scientist, a man of great integrity, a private individual. He had a quiet stubborness which would not give in and yet with it a sweetness of temper.

We here join with his colleagues and friends in Canada, among them Farid Ahmed, Eric Gabe, Yvon Le Page, Maria and Vatek Przybylska, in mourning his departure and our loss.

—*A. McL. Mathieson.*

IUCr Newsletter

A copy of the latest IUCr newsletter is enclosed for all members whose address is within Australia. It is assumed that overseas members will be able to obtain a copy from a local source. If an overseas member cannot obtain a copy by some means, please inform the secretary and a copy will be sent.

CRYSTAL XVIII Medlow Bath 5–8 April, 1994

Henry John Rossell (1936-1993)

In Melbourne, on the morning of Monday October 11, 1993, Henry Rossell collapsed and died suddenly from a heart attack: he was 57 years old, and had not been long retired from his position as Principal Research Scientist in the Division of Materials Science and Technology, CSIRO. He will be long remembered by his friends and colleagues, not only as a scientist of international repute but also as a great character: anyone who has heard him talk, whether formally or informally, will never forget his penchant for wit and comical turn of phrase. He is survived by his widow, Elizabeth, & four adult children, to whom we extend our deepest sympathy.

Henry Rossell graduated with First Class Honours in Physical and Inorganic Chemistry from the University of Western Australia in 1958, where he proceeded to work for his PhD in collaboration with me and the Australian Atomic Energy Commission on the then topical subject of the thorium carbides. It very soon became obvious that he had experimental skills of the highest order, which he retained throughout his working life. Indeed, these were not confined to science, as he demonstrated often in the fields of music and painting.

At the end of 1964, now Dr Rossell, he undertook post-doctoral work with (the late) J.S. Anderson at the Inorganic Chemistry Laboratory in Oxford. During the two or so years that he was there he not only married Elizabeth but embraced with enthusiasm the ancient art of bell-ringing.

In 1967 he returned to Australia as a Research Scientist with the Division of Tribophysics, CSIRO, under the direction of Walter Boas, where he very soon became involved in crystallographic studies of refractory oxides, particularly the so-called "fast-ion conductors", such as lime-stabilized zirconia, with fluorite-related structures. In the earlier stages of this he was associated with (the late) John Sanders and John Allpress, from whom he learnt the techniques of electron microscopy and diffraction. In Rossell's hands, the combination of these with Guinier powder X-ray diffraction methods led to many significant advances, and he became an acknowledged authority on those zirconia-based materials which have assumed such importance in the ceramic industry. His involvement in this work continued to his retirement in 1992 and beyond, but was by no means his only interest.

His sudden death is a great loss to crystallography in general, and particularly to Australian crystallography, where he will be sadly missed as both scientist and friend.

—D.J.M. ("Judge") Bevan, October 17, 1993.

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The photograph of the group at the banquet was kindly provided by Graeme Gainsford. The editor regrets that one of Tina and Mark was not reproduceable.