



# Society of Crystallographers in Australia and New Zealand SCANZ

## Newsletters

### No 49, June 01

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

## FROM THE PRESIDENT

In the last SCANZ *Newsletter* I mentioned the concern that was being expressed about the continuing regional tensions in Israel and the effect that this might have on attendance at the 2002 IUCr Congress scheduled to be held in Jerusalem. Since then the situation appears to have deteriorated even further and the Executive of the IUCr, after extensive consultation, has made the unprecedented decision to change the venue to Geneva. This must be a bitter disappointment for Joel Bernstein and his organising team, who have already devoted a great deal of work to hosting the Congress in Israel. The Israeli team will still be in charge of the organisation in Geneva but in collaboration with a local committee. Further details and a statement from the IUCr President may be found at the web site:- <http://www.iucr.org/iucr-top/cww-top/mtg.iucr2002.html>.



A second piece of news is that Edward Tiekink, who is the SCANZ Public Officer, is about to leave Australia to take up a position overseas, and will therefore be unable to continue to act for us. I would like to take this opportunity of thanking Edward for his contribution to the *Society* and in particular in carrying through the transactions required to change our name to SCANZ. Alan Pring has said that he would be willing to take over from Edward (n.b. the Public Officer has to be a resident of South Australia).

A few weeks ago I attended, as President of one of the member societies, the FASTS forum entitled 'The Innovation Plan - making sure it works'. This included the televised National Press Club Address 'The Next Step for Science in Australia' given by the Chief Scientist Dr Robin Batterham. This was the first time that I had heard him speak and I was duly impressed and agreed with many, but not all aspects, of his vision for the future of Science in Australia. He clearly has the ear of the Government and is a key player in any future developments in Science. It does worry me somewhat that his vision is not the only possible way forward and alternatives seem already to have been excluded.

In addition to Dr Batterham's talk, the day was spent discussing three topics related to the Governments Innovation plan. These were 'The CRC Program', the '2000 additional university places for Science' and the 'Centres of Excellence'. Of the three, the CRC program seems to be in the most satisfactory shape. There seems to be general agreement on priorities and there is in place a healthy system of consultation between bureaucrats and scientists. Discussion on the 2000 additional university places, on the other hand, was very varied, confused and far from satisfactory. There does not seem to be a clear picture of what exactly is intended. The First Assistant Secretary of the Higher Education Division of DETYA (Dr Gallagher) made the perplexing statement that Australia has enough scientists and producing more was not

what was intended! Competition by individual institutions for these additional places is, in the DETYA tradition, via advanced hoop-jumping. Most contentious was the third topic of the 'Centres of Excellence'. Although there was broad agreement of the way forward for the Biotechnology Centres of Excellence, there was strongly divided opinion on the Information and Communication Technology Centre of Excellence. Opposing factions were in favour of a multi-node national centre linked to established institutions or a single Centre placed strategically at one location. Opponents of the latter option were of the view that such a concentration would denude the rest of the country of sufficient expertise in this area to even provide adequate undergraduate teaching capability. For those interested in reading more about the forum see the FASTS web-site:- <http://www.fast.org>.

As I foreshadowed last time, the National Committee of Crystallography deemed that it would be useful to take stock of the state of crystallographic research in Australia and asked me if I would canvas the membership of SCANZ. I undertook to put together a (short) questionnaire and this is included with this *Newsletter*. I would be grateful if you could find time to tick the appropriate boxes for your own situation and return to me as soon as possible. The aim is to find out who is doing what kind of work with what facilities etc. and how this impinges on the new research reactor, the proposed synchrotron, the Australian Synchrotron Research Program, the Government's Innovation Statement, etc.

*Richard Welberry*

## A VISIT TO ChemMatCARS

Colleague Dai (David) Hibbs and I arrived at Argonne National Laboratory late on 22/3/01, just in time to catch the start of an unseasonal cold snap and snow. Sight seeing in Chicago was out of the question, but the Argonne Guest House was warm and next morning Sector 15ID Station C, or ChemMatCARS, was less than a ten-minute walk away. Access required a Certificate of Core Radiological Training awarded on passing a computer based General Employee Radiation Training test, which was probably a little less difficult than deciding which cable TV channel not to watch the night before. Along with the credit card sized certificate, comes a user pass with an identification photograph that perfectly catches the feeling of jet lag. Armed with qualification and identification we went in search of ChemMatCARS and David Cookson. David introduced us to the Sector 15 folks and anyone else that happened to be passing by, and he then gave us our sector specific orientation. Maren Pink of Indiana University was just finishing her last collection and it was not long before we stepped inside the heavy doors of Station C. Dai had worked at Daresbury, but it was my first visit to a synchrotron and it took a little while to adjust to the sight of a goniometer platform mounted on its side. Also surprising was the large size of the detector, which houses 4 discrete 1K CCD chips in a 2x2 array.

Our official beam time was not due to start until 28/3/01 but David had asked us to arrive early in case spare shifts became available; spookily shifts became available immediately. The group that was to have the four days beam time prior to our arrival dropped out because of illness. We were thus to have about 71/2 days of beam time, the first four days or so of which we shared with Victor Young of the University of Minnesota. Well known for his work on twins (<http://www.chem.umn.edu/services/xraylab/>), Victor has made a substantial contribution to the development of ChemMatCARS. Victor was very generous with help and advice and we were fortunate to be working with him, however he showed no mercy when playing pool. Other than a planned day of 'machine studies', we suffered only one beam dump over the following week and that was a couple of hours before a scheduled dump that was accordingly skipped. There was also some beam instability for a couple of hours following a change in fill mode from 'top up' to 'single fill'.

Between us thirty data sets were collected, with frame exposures ranging from one to ten seconds and data set collection times from less than two hours to eight hours. We suppressed correlation for exposure time of less than five seconds, and the presence of zingers may be why we often had to use the twin-resolving program Gemini to index reflections. In general collections were pure phi scans with all other angles of the

SMART Kappa platform at zero. This left a hole in the diffraction sphere that was initially filled for triclinic systems by further psi scans at a different chi setting. As this was not particularly efficient, Victor bravely drove the axes around to find out what omega scans could be used without removing the collimator or putting something solid through the front of the detector.

The smallest crystal I used was an all-organic crystal of approximately 80x40x20 microns; Victor had the smallest which was a metal complex crystal of about 10x2x1 microns. The beam cross section was about 100 microns. The conventional residuals for the 11 structures I obtained range from 3.5% to 14% and the best  $R_{\text{merge}}$  was 6.5%. The  $R_{\text{merge}}$  values are good considering the composite nature of the detector, and the difficulty of getting good spatial and flood field corrections for four discrete chips. An advantage of the composite detector was that at two theta zero and 6 cm from the crystal the two theta diffraction coverage was about  $\pm 56^\circ$ . The composite detector is not well suited to charge density work, and David plans to replace the detector with a SMART 6000 detector later this year.

David Cookson has set up an excellent facility with an emphasis on user friendliness. Innovations since James Hester's visit include beam tracking and recovery software that keeps the user at a safe distance from the 'secret beam scientist business'. The software corrects for minor beam drift, and makes beam dump recovery at 3am relatively painless. Another innovation is the mounting of a large television set and video player above the processing PCs. Currently the video collection is maybe a little too thematic; The Philadelphia Experiment, Phenomenon, The Abyss and Armageddon. Must see TV at any time of day or night is 'beam channel', which presents graphic and text displays of the beam status and schedules; gripping.

If you're planning a visit to ChemMatCARS we recommend Dennis for the airport to Argonne Guest House taxi trip. Coincidentally taking about the same time as the trip, Dennis details his intimate connections with the Chicago Mafia and ultimately the truth behind the assassination of JFK. It's a ripping yarn with plenty of action and some violence; definitely value for money.

We'd like to thank David for his tireless efforts on our behalf, Victor for help and advice, James Hester for pre-visit tips, Brendan Kennedy for suggesting the visit, and Richard Garrett and the ASRP for, well, the money.

Use of the ChemMatCARS Sector 15 at the Advanced Photon Source, was supported by the Australian Synchrotron Research Program, which is funded by the Commonwealth of Australia under the Major National Research Facilities Program. ChemMatCARS Sector 15 is also supported by the National Science Foundation/Department of Energy under grant numbers CHE9522232 and CHE0087817 and by the Illinois board of higher education. The Advanced Photon Source is supported by the U.S. Department of Energy, Basic Energy Sciences, Office of Science, under Contract No. W-31-109-Eng-38.

*Peter Turner*

*Crystal Structure Analysis Facility*

*University of Sydney.*

## **OBITUARY**

**Dr Jim Graham MSc (UWA), PhD (Birmingham), FIP, FAIP**

**Born 13.10.1929 - Died 9.5.2001**

Jim Graham was educated at Scotch College and won a University General Exhibition to attend the

University of Western Australia, where he majored in Mathematics and Physics. In 1951 he graduated BSc, with First Class Honours and then completed an MSc in Physics in 1953. He won a prestigious UWA Hackett Research Scholarship in 1953 to undertake studies for a PhD at the University of Birmingham, sailing to the UK with the assistance of a free passage from the ANZ Shipping Conference. He was awarded a University of Birmingham Research Fellowship and completed his PhD in physical metallurgy, under the legendary Gilbert V. Raynor, Professor of Physical Metallurgy.

Quite soon after completing his PhD, he was lured back to Australia to work as a Research Officer in the Cement and Refractories Laboratories of the CSIRO Division of Industrial Chemistry, Melbourne. He returned to Perth in 1964 to set up microprobe, microanalysis and X-ray diffraction (XRD) facilities in the new Secondary Industry laboratories of the Division of Applied Mineralogy, Floreat Park. Initially, before the new building was completed, Jim came back to his alma mater and spent many months in the laboratories of the UWA Department of Chemistry where the Division had leased some temporary space. He remained in this Division as Principal Research Scientist until 1994, when he retired from CSIRO (Division of Minerals). On retirement, he returned yet again to UWA as an Honorary Research Fellow in the Research Centre for Advanced Mineral and Materials Processing (RCAMMP) and the Department of Chemistry.

Throughout his long and distinguished career as a research scientist he made many significant contributions, published in over 100 papers and technical reports, in crystallography, solid state physics and chemistry of minerals, particularly those hosting the nickel, tantalum and titanium deposits of WA, applied mineralogy, physical methods of analysis and characterisation of minerals, including XRD, electron beam and magnetic methods, quantitative analysis by XRD, and trace analysis using the electron microprobe analysis. He was a superb crystallographer and a rigorous scientist with wide, internationally recognized expertise in clay mineralogy, heavy mineral sands processing, the occurrence of 'invisible gold' in sulfides and the chemical processing of complex mineral oxides. He was also an expert in scientific instrumentation and pioneered the application of a number of 'cutting edge' techniques to the study of minerals in WA, particularly with the electron microprobe.

His strong academic background and his deep commitment to research led him to supervise, or co-supervise, several MSc and PhD students at both Curtin and UWA. On top of all this, he still managed to contribute to professional matters and activities, serving as Founding Member, Chair, Secretary and Committee member of the Australian Institute of Physics and Editor of the Australian Physicist (1980-85), a Founding Member of the Society of Crystallographers in Australia and Committee Member and later Vice President of the International Council for Applied Mineralogy. He was also a member of several committees that organised successful international conferences in Melbourne, Sydney, and in Perth, the International Union of Crystallography Congress and General Assembly (1987) and the International Conference on Applied Mineralogy (1993).

With his long academic and industrial research experience, quick brain, good nature and judgment and calm temperament he was a wonderful mentor to students, colleagues and industry collaborators alike. Even during his long illness, he insisted on coming to work several times a week to help colleagues Frank Lincoln, Terry Parks and student Nathan Webster understand the complex chemical processes occurring in an ilmenite reduction kiln in the Becher process - truly a mark of a dedicated, applied scientist! A deeply religious man, a gentle man and a devoted family man, he is survived by his wife Valerie and daughters Caroline, Dorothy and Margaret.

Vale Jim, you will be missed!

*Frank Lincoln*

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## CRYSTAL FRAGMENTS

Douglas du Boulay (Crystallography Centre, UWA) has taken up a one-year Post-Doctoral Fellowship with A/Prof Nobuo Ishizawa at the Tokyo Institute of Technology at the Yokohama campus. Douglas will be involved in charge density studies of Perovskites.

Peter Junk (Department of Chemistry, JCUNQ) has been appointed Lecturer in the Department of Chemistry at Monash University and expects to start in mid-July.

In January Bret Church (formerly at the Garvan Institute) was appointed the Entigen Senior Lecturer in a new Molecular Biotechnology program at the University of Sydney. A number of appointments in Chemistry, Biochemistry and Biological Sciences have been made possible by the Commonwealth Department of Education, Training and Youth Affairs and industrial partners. Entigen Pty. Ltd. is one of the partners.

Karl Byriel has moved from the Chemistry Department at the University of Queensland to the newly created Institute of Molecular Biosciences, formed by merging the Centre for Drug Design and Development, the Centre for Molecular and Cellular Biology and the Special Research Centre for Functional and Applied Genomics.

Edward Tiekink will be leaving Adelaide University in early July to take up a position of Associate Professor in the Department of Chemistry at the National University of Singapore.

## CRYSTAL XXII

Crystal XXII is nearly upon us! For those of you who have not registered yet, late registrations are still being accepted. Registration forms can be downloaded from the Crystal XXII website <http://www.chemistry.uq.edu.au/crystal22>.

### Program Information

The conference program is now available on the website. The registration desk will open in the late afternoon of Saturday 7 July and a welcome barbecue will be held that evening. The conference program begins on the morning of Sunday 8 July. Program sessions include Biotechnology, Technical Advances, The Solid State, Intermolecular Interactions, Materials and Disorder, Structural Biology and a Poster Session. The 1987 plenary speaker is Professor Sung Hou Kim from Berkeley University and keynote speakers are Jacqui Gulbis (WEHI), Trevor Hambley (USyd), Pat Kelly (UQld), Mark von Itzstein (Griffith U) and Richard Welberry (ANU). The conference dinner is on Monday evening and the program wraps up on Tuesday 10 July with a half day of presentations followed by a farewell lunch.

### Transfer Information

If traveling by plane to Brisbane, you will need to travel from the airport to Runaway Bay, about 40 minutes south. CoachTrans runs a regular coach service from both domestic and international terminals at Brisbane Airport to Runaway Bay. You can purchase your tickets with CoachTrans upon arrival at Brisbane Airport, asking to be dropped off at the Couran Cove Check-In desk at Runaway Bay. When you arrive at Runaway Bay you will need to check in your luggage at the Couran Cove desk and board the catamaran for transfer to Couran Cove. A special price for the catamaran return trip has been negotiated for the conference and this can be booked on the registration form.

For those attending the IUPAC conference and requiring information about travel to the Crystal XXII conference, please contact the local organizing committee by e-mail on [crystal22@chemistry.uq.edu.au](mailto:crystal22@chemistry.uq.edu.au).

*Jenny Martin*

## **BRUKER AXS ACQUIRES NONIUS**

Bruker AXS Inc announced in April that it had acquired the Nonius crystallography business from Delft Instruments. Nonius, with calendar year 2000 revenue of more than \$US8 million, has 42 employees worldwide, and is headquartered in Delft, The Netherlands.

The former Nonius in Delft will become Bruker Nonius BV, and will be the joint European centre for X-ray crystallography. The combined crystallography product lines of Bruker AXS and Nonius will be marketed under the joint brand Bruker Nonius. Bruker AXS manufactures a diverse set of X-ray technology platforms for molecular and materials analysis. In the year 2000, the company had revenue of more than \$US68 million.

## **IUCr XIX**

The 19th Congress and General Assembly of the IUCr will be held in Geneva, Switzerland, August 6-15, 2002 in the Palexpo Congress Centre. The 2002 General Assembly and Congress remains the 'Israeli' Congress, organised in another country by the agreed Committees.

## **AsCA'01**

AsCA'01 is the fourth meeting of The Asian Crystallographic Association (AsCA) and will be held at the Indian Institute of Science, Bangalore, India, during November 18-21, 2001.

The Second Circular, available shortly, will include more information about the scientific and social programs, submission of abstracts and hotel accommodation etc. Further information, including a reply form, is available at the Conference Website: <http://www.iisc.ernet.in/~asca401>.

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