

SCANZ NEWSLETTER

SOCIETY OF CRYSTALLOGRAPHERS IN AUSTRALIA AND NEW ZEALAND



<http://www.sca.asn.au/>

No 60, October 2005

FROM THE PRESIDENT

President's Farewell report:

It has been a pleasure and a privilege to lead the Society for the past two years. That time has been very eventful for our crystallographic community with recent developments such as the OPAL Reactor and the Australian synchrotron, as well as the 50th anniversary of the structure determination of DNA (which SCANZ marked with the release of a postcard), and the sad passing of so many world-renowned crystallographers – John Cowley, Maurice Wilkins, Francis Crick, David Blow and Carl-Ivar Branden.

One of my first and most difficult tasks as President was to find a new newsletter editor after Brian Skelton stepped down from the position. He proved very difficult to replace, but fortunately Geoff Jameson from Massey University in NZ took up the challenge (after I tapped him on the shoulder). I want to single him out for thanks for accepting the task so graciously on such short notice and for doing such a wonderful job. Thank you Geoff!

A couple of other things to report on, first is the publication in the IUCr newsletter of an article on Crystallography in Australia And New Zealand. The article is a collation of reminiscences from over twenty five contributors and I would like to thank them personally if not individually for their time and effort. I hope that everyone will read and enjoy the article. Hopefully it will be out soon!

The second item to report on is that the SCANZ executive agreed recently to set aside up to \$2000 pa (beginning in 2005) for projects in Australia and NZ that raise awareness of science or improve our members' access and knowledge of new techniques. Applications will be called for in the next newsletter, and these will be evaluated by a sub-committee with the results published in the following newsletter.

One of the events supported recently was a protein crystallization workshop held in Brisbane in November 2004. I would like to take this opportunity to read out part of the report from the organizer Bostjan Kobe:

With the help of colleagues at the University of Queensland, supporting societies, local institutions and commercial companies I am proud to report on the extremely successful "Protein Crystallization Workshop" that took place at the University of Queensland, Brisbane, on 3 November 2004. The program of the one-day workshop consisted of lectures by invited international speakers (Janet Newman, Yong Yi, Hidong Kim, USA; Joby Jenkins, UK) and several national speakers, who introduced state-of-the-art approaches to protein expression in bacterial and eukaryotic systems, protein purification,

protein crystallization and post-crystallization treatments. In addition, the delegates participated in demonstrations of protein expression screening, crystallization robots and crystallization monitors. There were seventy-one delegates from around Australia and New Zealand. Considering the interest and feedback from this workshop, it may be valuable to consider organizing another workshop on a similar topic in ~2-3 years.

I echo that sentiment: I think it is timely that SCANZ consider running crystallography workshops on a regular basis, just as is done in the US and in Europe. This is especially critical with the Australian synchrotron expected to be operational within the next few years. The Materials and Molecular Structure Network, which held a very interesting two-day satellite meeting prior to Crystal24 thanks in large part to the efforts of Peter Turner, is also considering running workshops, and several people have expressed interest in being involved. I hope that SCANZ will participate and support such ventures.

The last item on the President's report is for me to formally thank the Society, the nominations committee and the SCANZ council and executive for nominating me first to the council and then to the Presidency. It has been an honour and a delight. Thank you,

Jenny Martin

FROM THE SECRETARY

Report on SCANZ-24, Marysville, Victoria, 29 March – 1 April 2005

The majority of SCANZ members, especially NZ members, missed the well-organised and scientifically stimulating SCANZ-24 meeting in Marysville. The meeting was preceded by a two-day meeting of the Materials and Molecular Structure Network.

Rarely has a plenary lecture been given in country and western style.

SCANZ supported a total of 8 students to attend:

Zara Marland (Monash University, Jamie Rossjohn)
Kate Henderson (Monash University, Jamie Rossjohn)
Fleur Tyman (Monash University, Jamie Rossjohn;
declined as travelling to synchrotron)
Lauren Ely (Monash University, Jamie Rossjohn)
Mark Krashnefski (Griffith University, Helen
Blanchard)
Stacy Scott (Griffith University, Helen Blanchard)
Joseph Bevitt (University of Sydney, Cameron Keppert)
Karna Chapman (University of Sydney, Cameron
Keppert)

Natasha Sciortini (University of Sydney, Cameron Keppert).

Life membership was bestowed on Syd Hall, University of Western Australia, and, *in absentia*, on John White, Australian National University. Syd reminisced about the early days of the Bush Crystallographers and overland travel on unsealed roads from Perth to Melbourne and back.

SCANZ Council (secretarial notes; minutes to be confirmed at next Council Meeting): The SCANZ Council met and received reports from the Nominations Committee. President Jenny Martin reported on behalf of Alison Edwards, Ed Tiekink, Ian Grey and Brendan Abrahams on their initiative to set up an endowed prize, the Bernard F Hoskins Prize. This prize would be awarded for the best post-doctoral presentation, poster or oral, at SCANZ meetings, including joint meetings with, for example, the Asian Crystallographic Association, AsCA.

SCANZ General Meeting (secretarial notes; minutes to be confirmed at next General Meeting): Democracy in action led to the following slate of officers and council members being (s)electd by acclamation:

President: Brendan Kennedy
Vice President: Steve Wilkins
Treasurer: Bostjan Kobe
Secretary: Geoff Jameson
Immediate PP: Jenny Martin
Council: Ray Withers
Jose Varghese

A lively discussion on how to encourage greater student attendance at SCANZ meetings ensued. One suggestion was in IUCr years to couple attendance of Ted Maslen awardees to the IUCr meeting with attendance at the SCANZ meeting. Another was to couple the SCANZ meeting with a workshop targetted to students and post-doctoral fellows.

Many thanks are due to Steve Wilkins and Sherry Mayo and for organising SCANZ-24. SCANZ gratefully acknowledges generous commercial sponsorship of this meeting.

SCANZ-25 will be held in early to mid 2007, somewhere near Sydney (with Brendan Kennedy as provisional chair of the Organising Committee). Coordination with opening dates of the Australian Synchrotron and/or OPAL the renovated neutron facility at Lucas Heights will be attempted.

XXth General Assembly and Congress of the International Union of Crystallography, Florence, Italy, 23-31 August 2005

Attendance at the recent IUCr meeting of 10 student members of SCANZ was aided by scholarships from the "Maslen 1987 Scholarship Fund". The students (and their mentors) supported were:

Joseph Beviitt (University of Sydney, Cameron Keppert)
Vincenzo Carbone (Ossama El-Kabbani)
Geoffrey Kong (St Vincents Research Institute, Michael Parker)
Lorien Parker (St Vincents Research Institute, Michael Parker)
Marissa Haywood (University of Melbourne, Brendan Abrahams)
Martin Duriska (Monash University, Stuart Batten),

Natasha Sciortino (University of Sydney, Cameron Keppert)

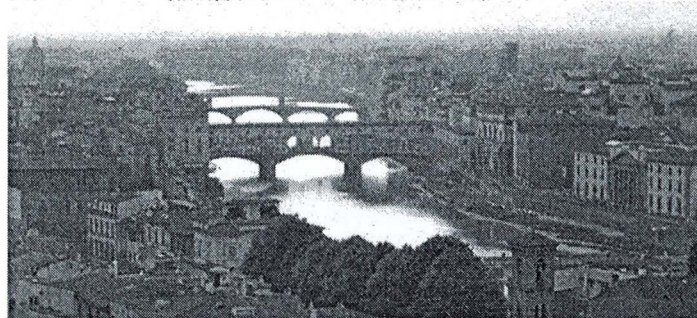
Mihwa Lee (University of Sydney, Mitchell Guss)

Valeska Ting (ANU, Ray Withers)

Andrew Whitten (UWA, Mark Spackman).

Valeska Ting has provided a report of her experiences.

Report on IUCr2005, Florence, Italy (August 23rd - 31st, 2005)



I'd been looking forward to attending the 20th Congress of the International Union of Crystallography since I'd heard about the last IUCr, congress in Geneva at the start of my Ph. D. It just sounded like a huge affair – 2000-plus crystallographers from all over the world, a 9-day scientific program including workshops...and best of all, IUCr 2005 was to be held in Florence, Italy!

Well, the real-life experience did not fail to live up to my expectations!

Florence was nothing short of spectacular as a location for the conference. For one, the conference venue (the Fortezza da Basso) was an actual fortress with battlements and a moat! (Sure beats the Canberra Convention Centre...)



The scientific program for the conference was impressively comprehensive, with enough variety that there was something in it for everyone. The talks I attended were well presented and informative. I really enjoyed the keynote on Strategies and Design principles in Biomineralisation (Lia Addadi). Even though it had little to do with my field, I thought it was fascinating and well worth waiting around for. The Art and Crystallography session was another great idea. The talk on M. C Escher and his links with crystallography I found particularly interesting.

Having the chance to meet so many other crystallographers and to talk with them about their research and their interests

was also very valuable. After presenting my talk in the section on Structures Solved by Powder Diffraction (MS 79), I was approached by a number of people who wanted to ask additional questions or offer advice on different ways to tackle certain issues I'd discussed, which was fantastic!

The social program was equally well managed, with the outstanding events being the Marresearch Traditional Dinner, which was held at a villa on the hills overlooking Florence, and the conference dinner at the Pitti Palace. One thing that was commented on, however, was that in previous years there had been a student mixer so that the younger researchers could meet each other. I was a bit disappointed that this had been omitted from this year's program.

All in all, I feel very privileged to have been able to attend. The IUCr conference was easily a highlight of my short crystallographic career and I'd like to say a big thank you to SCANZ (Ted Maslen 1987 Scholarship) and the Jeffrey Award for grants towards accommodation at and travel to IUCr.

Looking forward to seeing everyone again in Kyoto in 2008!

Valeska Ting
(Australian National University)

Bongiorno! Greetings from the 20th IUCr Congress, Florence, Italy.

We would like to thank SCANZ for giving us the opportunity, through the award of Ted Maslen 1987 Scholarships, to present our research to such a prestigious gathering of crystallographers.

Florence, birthplace of the Renaissance was the ideal place to learn from and meet some of the great minds of crystallography. Not a few of these academics and students were caught determining the symmetries of geometric mosaics within the Cathedral of Santa Maria del Fiore. During 10 days of conference proceedings we gained insights into such diverse topics as the mechanisms of fullerene and nanotube formation, hydrogen storage in molecular compounds, the development of artificial muscle and the role of ultrafast time-resolved X-ray methods in determining reaction mechanisms. Of particular interest was Doris Schattschneider's memoir on M. C. Escher and the crystallographers. Rarely is the art of crystallography so clearly expressed – the works of Escher should be found hanging in any crystallographers study.

The conference banquet, held within the grandiose Boboli Gardens of the Pallazzo Pitti was surreal, with over 1500 guests in attendance, plenty of fresh, hand made pizza, pasta, wine and dancing. We congratulate the IUCr in demonstrating its ability to host an event of such an immense scale. It was great not just to liaise with students and academics working in our field abroad, but to strengthen ties with our colleagues from Australia, some of whom featured quite strongly in their fields of study. It is comforting to know that fellow members of SCANZ remain at the forefront of technical and analytical expertise of crystallography.

Again, many thanks to the SCANZ committee,

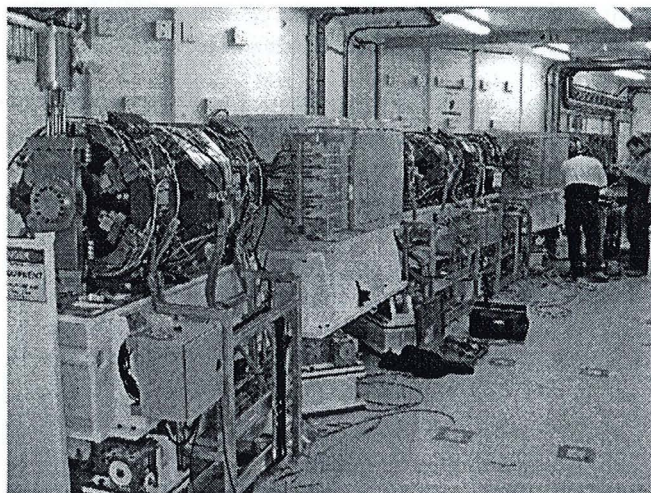
Natasha Sciortino and Joseph Bevitt
(School of Chemistry, The University of Sydney)

AWARDS

Congratulations to Cameron Kepert (University of Sydney) who won the 2005 Malcolm McIntosh Prize for Physical Scientist of the Year. This award is based, partially on Cameron's work on Negative Thermal Expansion materials

AUSTRALIAN SYNCHROTRON

A recent photograph of the interior of the Australian Synchrotron (www.synchrotron.vic.gov.au).



Installation of the magnets in the storage ring. Magnets are colour-coded according to type. The closest (green) is a hexapole magnet, the next closest (red) is a quadrupole magnet, and the large (yellow) magnet is a dipole magnet. Magnets are supplied by CMS Alphatech and Buckley Systems, New Zealand.

A recent workshop 15 September in Melbourne) was attended by investors and potential investors in the beamline funding pool to address issues of governance.

Investors in the beamline funding pool now include Monash University, Melbourne University, CSIRO, New Zealand, Minifab and AAMRI.

Contracts for construction of the protein and powder diffraction beamlines have been announced.

RESEARCH PROFILE

Jenny Martin has been collating for the IUCr profiles of research in Australasia that uses diffraction techniques. In the light of the death of Maurice Wilkins, who pioneered diffraction studies on DNA, it seemed timely to profile Australasia's research activity on diffraction by and structural analysis of fibrous materials. Subsequent newsletters will profile other areas spanned by SCANZ. The following is an abbreviated version prepared by Allan White and Ward Robinson. It is fair to say that Chemical Crystallography has transformed chemistry. The footnotes give the names of the early practitioners and their affiliations.

Chemical Crystallography

Small molecule X-ray crystal structure analysis has been an important component of research in university chemistry departments and government agencies in Australia and New Zealand since the early 1950's, a large number of groups being established throughout Australia and New Zealand during that time and subsequently [1-9]. At the outset the research tended to be focussed on the protagonists' own interests, but, with the growing/widespread recognition of the capabilities, as well as the cost, of the technique, and the constraints of obtaining funding, most groups broadened their activities to encompass the gamut of applicability across the chemical and materials sciences.

The field burgeoned in Australia and New Zealand during the 1960's when computer-controlled diffractometer installations supplanted Weissenberg and precession camera X-ray facilities and the use of electronic computers became widespread. As elsewhere, the technique became an important ingredient in the characterization and identification of crystalline substances across the chemical, materials, natural product and mineralogical sciences, and many antipodean practitioners feature with distinction in the various data-base compilations. Some trained in this system have made careers teaching in it and providing solutions to literally thousands of molecular and ionic structural problems ranging in variety across the spectrum of the past half century of chemical progress.

Amongst the published work you will find very small organic molecules (typical of the 1950's when hand calculators restricted calculations to projections down short axes), simple transition metal salts and hydrates, leading into more complex ones (as coordination chemistry gained popularity in the 1960's and computers enabled three-dimensional calculations), broad front attacks on chemical problems through many chemically related structures (as computing became more straightforward and data acquisition more automated throughout the 1970's) to the very much larger molecules containing hundreds of atoms which occur quite frequently when anti-viral and anti-tumour agents are isolated as natural products and as synthesis reaches new levels of sophistication with the development of supramolecular chemistry, crystal engineering and materials science.

Rationales for these analyses range widely from bio- and pharmaco-logical, to underpinning the understanding of physical effects such as magnetism and electrical properties, and to the understanding of chemical reaction paths, as well as an appreciation of the symmetry and elegance of these structures and processes, to solving structures for more fundamental reasons associated with theoretical and computational development. There may also be a financial imperative driving some of this work, the more so as infrastructure becomes more 'econorat' based. Accounts of this work are represented in most major chemical journals and databases and many of the people who did it can be found all around the world still contributing to science in general and crystallography in particular.

With the advent of powerful CCD instrumentation, backed up by increasing access to synchrotron facilities in the 1990's, and the ongoing increases in costs and in funding difficulties, the widespread dissemination of facilities has contracted [10-17]. Area-detector installations have been widely used in teaching, and their facility in recording of powder patterns has been exploited in uses such as large scale surveys of preferred orientation of cellulose grains in timber microfibrils in both Australia and New Zealand (see Fibre Diffraction below). Neutron studies [18] were instigated at the nuclear reactor at ANSTO.

Instrumentally, the region is well placed for the next decade with area detector and CCD systems dedicated to small molecule work as well as anticipated access to the new Australian synchrotron beamlines.

[1] Queensland: Les Power (James Cook University), Colin Kennard (U of Queensland), Peter Healy and Graham Smith (Griffith U)

[2] New South Wales: Hans Freeman (U of Sydney), Neville Stephenson (U of New South Wales), 'Blue' Barclay (Macquarie U)

[3] ACT: Glen Robertson (Australian National University)

[4] Victoria: David Wadsley and 'Sandy' Mathieson (CSIRO, Vic), John (CB) White and Bernard Hoskins (Melbourne U), Bryan Gatehouse (Monash University) and Maureen Mackay (Latrobe University)

[5] South Australia: Harry Medlin, Mike Snow (Adelaide University), Max Taylor (Flinders University) and Ted Radoslovich (CSIRO, Adelaide).

[6] West Australia: Ted Maslen, 'Judge' Bevan and Brian Figgis (University of Western Australia).

[7] University of Auckland (F.J. Llewellyn, David Hall, and Neil and Joyce Waters)

[8] Massey University (Sylvia Rumball and Ted Baker)

[9] University of Canterbury (Bruce Penfold and Ward Robinson)

[10] James Cook U. Queensland (sharon.ness@jcu.edu.au)

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[16] U. Auckland (g.clark@auckland.ac.nz)

FUTURE CONFERENCES and WORKSHOPS

International Conference on Neutron Scattering November 27-December 2 2006

The next (8th) International Conference on Neutron Scattering will be held in Sydney from November 27. A number of prominent SCANZ members will be speaking at this meeting which includes a tour to the new OPAL reactor at Lucas Heights and a full day mini-symposium on use of neutron methods in Macromolecular Crystallography. A limited number of bursaries are available for students from Australian Universities to attend this conference. More information is available from the conference web-site (www.icns2005.org).

ASRP/AS Users Meeting and XAS Workshop December 5-7

The 2005 annual users meeting of the Australian Synchrotron Research Program will be held in Melbourne December 5-6. This meeting will highlight developments at the Australian Synchrotron – including a tour of the completed building. Two features of this meeting will be discussions by the various beamline advisory groups on the status of the beamlines and the presentation of the first ever ASRP research awards. Given the status of the beamline developments this meeting will provide an ideal opportunity for SCANZ members to have an input into the capability of the diffraction beamlines.

The meeting will be followed by XAS workshop, with expert advice, including a hands on data analysis tutorial on Wednesday December 7. Registration for both of these events is free but numbers, especially for the XAS workshop are limited. Please see <http://www.ansto.gov.au/natfac/2005UserMeeting.html> for more details.

Future AsCA, IUCr and SCANZ meetings

November 2006: AsCA/Crystallographic Society of Japan (Tsukuba, Japan)

Early to mid-2007: SCANZ-25 (NSW)

Late 2007: AsCA (Taiwan)

August, 2008 IUCr-21 (Osaka, Japan)

PROMOTING SCANZ

Members are reminded that \$2000 in funds are set aside each year for activities to promote SCANZ and diffraction sciences in Australasia. The DNA@50 postcards, the Crystal Growing Workshop in Queensland in November 2004, and crystal growing competitions have all benefited from this fund. Please submit applications for the balance of funds allocated for 2004 and for funds allocated for 2005 to the Treasurer, Bostjan Kobe.

SUBSCRIPTIONS

Subscription notices for 2006 are enclosed with this newsletter.

The Treasurer wishes to remind members that annual membership dues for 2005 are to be paid by December 31, 2005. 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, 2006. Members who are over 60 years of age at the time subscriptions are due can elect to become Life Members of the *Society* by paying a one-off amount of five times the current (discounted) subscription rate (i.e. \$100).

Bostjan Kobe

OBITUARIES

Charles Taylor, 1935-2002

John Charles Taylor, MSc(Syd), PhD(NSW), DSc(NSW) died suddenly while playing tennis in Sydney on 30 September 2002. John had spent the whole of his working life as a crystallographer using both X-ray and neutron diffraction methods. He authored or co-authored 99 fully refereed journal publications, 19 lightly or non-refereed publications, various conference papers and 4 seminar/workshop papers and 8 Internal (Lucas Heights) Divisional Publications. John also co-authored a book, "Rietveld Made Easy".

John's start in crystallographic research was in "Old Chemistry" (now the Department of Pharmacy) at the University of Sydney. Under the supervision of H C Freeman, John collected data on the crystal structure of potassium bis-biureto-cuprate (II) tetrahydrate using a Metropolitan-Vickers "Raymax" X-ray generator with a demountable tube. The "Raymax" had arrived from England as a gift shortly after the appointment of R J W Le Fevre as Professor of Chemistry.

John had collected and visually estimated 929 diffracted intensities (another possible 331 were very weak and were not observed) and had manually corrected them for Lorentz, polarization and Tunell effects but not, at this stage, for absorption. John was determined to locate the hydrogen atoms in the anionic complex. Obviously he felt that his collected and visually estimated data was good. The next step truly displays his stubborn determination, patience and persistence. John disappeared to home for quite a few weeks and graphically calculated absorption factors (method of Joel, Vera and Garaycochea, *Acta Cryst.*, Vol.6, 1954) for all of his data. Subsequent cycles of Fourier and Least-Squares refinement (thanks to SILLIAC programs written by H C Freeman) led to the placement of all hydrogen atoms in the structure.

It must be stressed that Sydney University has a long history of X-ray analytical work going back to the early 1930s; D P Mellor and F P Dwyer read their paper regarding *The Crystal Structure of Indium* before the Royal Society of New South Wales, 6 July 1932. This was barely

20 years after the world's first X-ray crystal structure analysis. Mellor provided continuity in structure analysis. This short obituary is important for historical reasons as well as reflecting on the life of John Taylor and his early work (at Sydney University) of which not many people have knowledge. John's work at Sydney was commenced in the era *before computers in Australia* and was completed with the aid of the "SILLIAC", Australia's second and then best electronic digital computer.

These were the days when John and his co-worker John E W L Smith had mentors such as A McL ("Sandy") Mathieson, Janis Fridrichsons, Barrie Dawson and A D (Dave) Wadsley.

After completing his MSc, John transferred to the University of New South Wales using both X-ray and neutron diffraction techniques to determine the structures of ebeline lactone and uranium compounds. In August 1962, John met Mavis McKinnon who was to become his wife. John was awarded his PhD in 1963 for his thesis "Crystal Structure Analysis by X-ray and Neutron Diffraction Methods". In 1981, the University of NSW awarded John the Degree of Doctor of Science in recognition of his research excellence.

As a post-doctorate, he spent several years at Argonne National Laboratory co-publishing papers on neutron diffraction studies of uranium and thorium compounds with, among others, Mel Mueller.

John became interested in the Rietveld method after reading Hugo Rietveld's initial papers on quantification of mineral phases from X-ray powder diffraction, adapting the single crystal program (ORFLS) for profile analysis for his research. This work was the early beginnings of the software program SIROQUANT that allowed multi-phase quantitative analysis of a wide range of materials.

His research was leading edge although to his colleagues the apparent ease with which he succeeded in solving the most complex problems was daunting. This was due largely to his extraordinary high level of intellect. His work on coal minerals was a classic example. To quantify minerals in coal, it was usual to measure the pattern of a low temperature ash to remove organic matter. A problem with this approach is the alteration of some minerals such as pyrite and the reaction of sulfur with calcium-bearing phases. It was suggested to John that a direct analysis of the raw coal would overcome this problem. However a major obstacle was the presence of a high background at low 2-theta angles. John solved this problem "in a few days" by modelling the reflections based on an anthracene derivative. This enabled SIROQUANT to be applied directly to raw coals, providing not only a quantitative estimate of all the minerals but also a measure of the total organic matter present which, in turn, gave the total mineral matter content.

John was the classic individual researcher, best described as the quiet achiever, who shunned the tedium of budgets and management constraints but always delivered on his research. John was also an accomplished pianist and landscape painter of considerable merit. His painting commenced as a relaxation at the age of 40. He leaves a widow, Mavis, and two children, Phillip and Karen.

Chris Kelaart and John E.W. Lambert-Smith

(The Newsletter Editor apologises for the omission in earlier newsletters of this obituary)

FROM THE NEWSLETTER EDITOR

The Editor apologises for the long gap in newsletters, but he has had a number of unplanned and unexpected additional items of responsibility added to his duties, without anything being taken away.

As this is your newsletter, please send any items of news or commentary to the Newsletter Editor.

Society of Crystallographers in Australia and New Zealand

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