

Society of Crystallographers in Australia



SCA

Newsletters

No 35, September 1997

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

FROM THE PRESIDENT

Two quite notable events have occurred in the past few months. The first concerns what might seem to some members the new obsession of Australian crystallographers with synchrotrons and with synchrotron radiation. The second was a celebration held to mark the "formal" retirement of Hans Freeman.

With time X-ray crystallography has become so accepted in many areas of science that it is no longer considered novel and many practitioners give their first allegiance to their broader scientific discipline, chemistry, physics or biology. Protein crystallographers might, for example, prefer to present their results at meetings of biochemists, virologists or molecular biologists with a common interest in the broader biological context than at specialist crystallographic meetings. Synchrotrons as well as being intense, tunable sources of radiation which span the X-ray part of the spectrum, are increasingly becoming a common interest of a large number of Australian crystallographers. The uses of synchrotron radiation cover a variety of applications from reflectometry and microprobe analysis in the material sciences, to X-ray absorption spectroscopy, small angle diffraction, tomography and crystallography in the chemical and biological sciences.



In 1996 a consortium of Australian universities, CSIRO and ANSTO were successful in being awarded one of the inaugural Major National Research Facility grants. The award of \$12,500,000 over five years is to maintain and enhance the already successful National Beamline facility at the Photon Factory, Tsukuba, Japan and to participate in three beamline consortia at the Advanced Photon Source (APS), being constructed at the Argonne National Laboratories, Chicago, U.S.A. A one-day meeting was held in Melbourne in July to formally inaugurate the Australian Synchrotron Research Programme (ASRP). The minister for Science, Peter McGauran, gave the opening address following a welcome from the Chair of the ASRP board, Professor Helen Garnett from ANSTO. Peter Colman highlighted the importance of synchrotron radiation in the process of rational structure-based drug design. Dr Denny Mills, the executive director of SRI-CAT, outlined the facilities and opportunities available to Australian scientists who wish to participate. Speakers for the remainder of the proceedings demonstrated the wide ranging uses of synchrotron radiation. The Australian community is now invited to submit proposals for the SRI-CAT and to contact members of the ASRP for guidance on access to the other facilities either at the Photon Factory or the APS. The starting point for information is the ASRP web page: <http://www.ansto.gov.au/natfac/asrp.html>.

Another one day meeting held in July marked the *formal* end of Hans Freeman's academic career. As Hans continues his research and teaching as before, this is only a formal milestone not retirement from academic life. Hans was a founder member of the Bush Crystallographers the precursor of the SCA and was the foundation president of the SCA itself. The meeting, organised by Peter Lay, was held in the School of Chemistry of the University of Sydney and set out to showcase where areas of science to which Hans has made major contributions over the past 40 years will head in the next century. A separate report of this meeting is included in this *Newsletter*.

SKETCHES OF CRYSTALLOGRAPHY LABORATORIES

University of Western Australia

The recent passing of E.N. Maslen, the foundation Director of the UWA Crystallography Centre, provides an appropriate occasion for a thumbnail sketch of crystallographic activities at UWA over the past forty years.

Crystallography has a number of independent roots in Western Australia. The first single crystal studies at UWA were under the direction of C. J. B. Clews, who came as Professor of Physics in 1952 from the Cavendish Laboratory, Cambridge. Two pyrimidine structures were determined with Noel E. White, D.E. Jukes and E.N. Maslen in 1956, the latter in his Honours year. Ted proceeded to Oxford as a Rhodes scholar to work with Dorothy Hodgkin on penicillin and cephalosporin derivatives for his Ph.D. which he received in 1960, returning to the UWA Physics Department as lecturer in that year. He took over the diffraction group of Clews, who became Deputy and Acting Vice-Chancellor. In this period, electron diffraction studies were also introduced.

A reflection electron diffraction camera was constructed and used by P.B. Sewell, J.H. Chute and A.E.C Spargo for epitaxy studies under the supervision of L.N.D. Lucas, subsequently Director of the Electron Microscopy Centre established in 1970. His third research student was a later Director, A.W.S. Johnson, who worked on lead films and surfaces. Powder diffraction studies on soil colloids were undertaken by J. Graham in 1953 under the supervision of J. Shearer. In the Chemistry Department, D.J.M. Bevan was appointed in the late fifties followed by B.N. Figgis, B.G. Hyde and A.H. White in the early and middle sixties, together with, subsequently, one of Bevan's Ph.D. graduates, F.J. Lincoln.

The study of crystallography with electrons flourished in the Chemistry Department in the early 1960s with Hyde, Bevan and L. Bursill's acquisition of a Siemens transmission electron microscope which was used to elucidate the structures of refractory oxides. The Centre for Microscopy and Microanalysis currently houses a Philips 430 analytical transmission electron microscope (AEM) with a Gatan Image Filter, an X-ray energy dispersive spectrometer and computer analysis system (EDS) acquired in 1985, a JEOL 2000FX II STEM, a 200kV instrument with an integrated EDS system (1990) plus a variety of scanning electron microscopes.

Maslen brought with him from Oxford a keen interest in the application of computers to diffraction studies, first of all in accessing SILLIAC at Sydney, then locally in 1963, an IBM 1620 followed by a DEC PDP-6 in 1967. The latter was used to control one of the first four-circle diffractometers in Australia, a Hilger and Watts Y-231. In this decade, Ted's interests were directed at the elucidation of organic structures by direct methods, with developing interest in precise diffraction studies and their potential for the study of electron density distributions, while the study of inorganic and coordination compounds was developing solidly in the Chemistry Department. A number of graduates of this era subsequently became influential in initiating structural work in other venues: S.R. Hall, G.B. Robertson, K.J. Watson, in single crystal studies, and B.H. O'Connor and H.M. Rietveld in powder work.

A purchase of another four-circle diffractometer by the Chemistry Department in 1970 (a Syntex) led to the formation of the Crystallography Centre with Maslen as Director and White as deputy. In 1975 S.R. Hall joined the Centre, and in 1993 became Director when Maslen became Head of UWA Physics. A further diffractometer was purchased in 1978 (Syntex P21), followed by two Enraf-Nonius Turbo CAD-4 instruments, one with a rotating-anode generator, in 1987 and 1992. These acquisitions were with ARC support in cognisance of collaborative structural activities with other campuses, such grants also funding the initial appointments of C.L. Raston, and, later B.W. Skelton.

In the late 70's, the Centre's involvement in the development of the XRAY system, and subsequently the XTAL package, together with the precision density and structural chemistry studies, led to the acquisition of an Interdata microcomputer, and a separation from the UWA central computing facility. Subsequent generations of machines have led to the present complement of workstations that include Sun, SGI and DEC machines.

Research activities at UWA have also encompassed single-crystal neutron diffraction experiments, primarily in respect of X-N electron distribution studies, and more recently the use of synchrotron X-ray sources at Tsukuba, and polarized neutron spin density studies at Grenoble, the latter being coupled with the successful local construction of a helium-

temperature instrument by B.N. Figgis.

In 1991 the Research Centre for Advanced Mineral and Material Processing (RCAMMP) acquired a powder diffractometer (Siemens D500) with a high temperature attachment. F.J Lincoln's solid state chemistry group's research includes detailed systematic structural and chemical studies of crystalline Western Australian minerals such as the Fe/Ni, Cu/Ag and Au/Ag sulphides and Pd/Pt and Cu/Ag selenides, the altered beach sand minerals ilmenite and zircon, the rare earth beach sand monazites and xenotimes, and the carbonatite-laterite monazites. This work is being carried out by the combination of X-ray/electron diffraction (principally, convergent beam electron diffraction) and electron microprobe analysis. Profile fitting (Rietveld) refinement methods are used for structure analysis and the quantitative analysis of mineral suites, such as the mineral sands and bauxites, from powder data. Synthesised materials, such as rare earth metal solid electrolytes, magneto-resistive lanthanum manganates, and synthesised mineral-like phases, such as the rare earth substituted monazites and apatite-based ceramic waste forms are also subjected to crystal structure analysis.

Current research activity in the Crystallography Centre includes electron density studies by V. Streltsov and D. du Boulay with synchrotron data collected at the Photon Factory, software development for the XTAL package and the improved scientific data handling methods using the STAR and CIF formats (Hall and du Boulay).

Small molecule X-ray studies (B.W. Skelton and A.H. White) at UWA are diverse, originating in part from collaboration with local, national and international chemists without facilities for this type of work. These include organic, natural products, organometallic, coordination, inorganic and mineral structures ranging in size to 'supramolecular' in scale. This work is closely supported by the XTAL software development. With the recent appointment of Bill Harrison to the Chemistry department structural studies also encompass the synthesis and characterisation of new inorganic phases including porous solids related to aluminosilicate zeolite and the solid-state chemistry of vanadium.

RETIREMENT OF HANS FREEMAN

A symposium was held in the School of Chemistry, University of Sydney on the 22nd July to mark the formal retirement of Professor Hans Freeman. The meeting began with a welcome from the current Professor of Inorganic Chemistry at Sydney, Professor Len Lindoy. He was followed by Dr Peter Colman, who, with Hans, was responsible for introducing protein crystallography into Australia. In pre- and post-lunch sessions collaborators and former students of Hans talked about his contributions, directions of current research and future developments in their area. Thus, Professor Keith Hodgson (Stanford) who has collaborated with Hans for many years talked about EXAFS and protein crystallography. Professor Ed Solomon (Stanford) covered metalloprotein spectroscopy and Professor Ian Dance (Univ. NSW), a former MSc student in Sydney, discussed theoretical modelling of active sites in metalloproteins. Professor Alan Bond (La Trobe) covered metalloprotein electrochemistry and Professor Geoff Sykes (Newcastle-upon-Tyne) metalloprotein electron transfer. This was followed by a most entertaining lecture from Hans himself in which he talked about the development of his work and research interests with frequent reference to (and photographs of) his many students and collaborators.

In the evening a most enjoyable dinner was held in MacLaurin Hall which forms part of the quadrangle of the University. This was attended by many of Hans' former students, current and former colleagues and collaborators. Professor Don Napper gave an entertaining after dinner speech that included the obligatory 'Duck Story' and Hans responded with some more delightful reminiscences. Everyone who attended agreed that the day was a great success and was a very appropriate way to mark the occasion of Hans' retirement.

Trevor Hambley, Mitchell Guss

AsCA'98

This is a preliminary announcement concerning AsCA'98, the third meeting of the Asian Crystallographic Association. The meeting will be held at the Hotel Equatorial Bangi, near Kuala Lumpur in the State of Selangor, Malaysia. The dates of the conference have been confirmed as October 13 - 15, 1998. A homepage with further information on the AsCA'98 meeting has been established at <http://gandalf.otago.ac.nz:800/rweavers/ASCA/asca98.htm> (also accessible through the SCA homepage) and this will be regularly updated with additional information as it comes to hand.

The available accommodation includes:

(1) Hotel Equatorial: Single/Double Superior RM180 per room per night; buffet breakfast RM20 (US\$1 = RM2.50 approximately).

(2) Metro Kajang Hotel: Single US\$50; Double US\$65 (including breakfast; prices quoted are current rates, subject to change. The hotel is located 12 kilometres from the Conference venue).

(3) The Universiti Kebangsaan Malaysia (UKM) student hostel. This is located approximately 4-5 kilometres from the Conference Venue and will probable cost in the vicinity of US\$20 per night.

The members of the Local Organising Committee are: A. Hamid Othman *Chair*, Chen Wei, *Secretary/ Treasurer*, Lo Kong Mun, Bohari Yamin, Musa Ahmad, Yang Farina, Fun Hoong Kun, and Ng Seik Weng.

The members of the International Organizing Committee are: Prof. Shih-Lin Chang (Taiwan) *Chair*, Prof. Su Jin Chung (Korea), Prof. Lu-Hua Lai (China), Dr. Krishan Lal (India), Dr. Hamid Othman (Malaysia), Prof. Jim Simpson (New Zealand), Dr. Mark Spackman (Australia), and Prof. Hideo Toraya (Japan),

The International Program Committee consists of Professor T. Yamanaka (Japan) *Chair*, R. Cheary (Australia), Fun Hoong-Kun (Malaysia), G. Jameson (New Zealand), K. Miki (Japan), M. Guss (Australia), K. Ohsumi (Japan), M. Sakata (Japan), Se Won Suh (Korea), Yu Wang (Taiwan), R. Withers (Australia), and J.J. Vittal (Singapore), with other members to be advised.

Jim Simpson

SUBSCRIPTIONS

The Treasurer wishes to remind members that annual membership dues for 1998 are to be paid by December 31, 1998. 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, 1998.

Sagamore XII

The Twelfth Sagamore Conference on Charge, Spin and Momentum Densities was held in Waskesiu, Saskatchewan, Canada from July 27 to August 1, 1997. A total of around 115 delegates attended including several from Australia. Mark Spackman (University of New England) presented a lecture and Nicholas O'Toole and Victor Streltsov (University of W.A.) presented posters. The conference was held at the southern end of Lake Waskesiu, where the resort community spreads along the sandy beach for a kilometre. Bird colonies fishing in the lake, friendly ground squirrels, mosquitos and bear traps between cabins, where some participants lived, reminded us about the plentiful animal life of this park and reflected its position in central Canada. The weather conditions allowed the conference participants to attempt recreational swimming in the lake between sessions, which were wisely organised in the early mornings or late afternoons. Fermiology and momentum densities studies dominated during the first two days of the conference but electron densities studies in organic substances were more prevalent later. There were very interesting presentations on interaction densities and charge densities in large organic molecules with data measured with area detectors. The accurate synchrotron charge densities in the study of inorganic materials could not overpower the large number of studies on small organic molecules.

Victor Streltsov

SCA HOMEPAGE

Have you visited The Society of Crystallographers in Australia website at <http://www.sca.asn.au>? This contains information on conferences, the Society's Constitution, and the list of Council members with postal addresses, telephone and fax numbers and e-mail addresses. Past and current *Newsletters*, including all the Sketches of Crystallographic Laboratories that have been included in recent issues, have been tabulated. An Application for Membership form is also included. There are also links to other sites of crystallographic interest including FASTS, IUCr, ACA, the Photon Factory, and Crystallography World Wide. Of particular interest is the link to Educational Material which contains information suitable for lectures and courses. Recent additions to the website have included a section on jobs available in crystallography and a link to the homepages of crystallography laboratories in Australia. While reports of Crystal XX

have appeared in the *Newsletter* some photographs taken in Queenstown have been included on the SCA homepage.

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