

SOCIETY OF CRYSTALLOGRAPHERS IN AUSTRALIA

NEWSLETTER No.20



Boooloomlnbah, University of New England, N.S.W.

CRYSTAL XVII
3-5 APRIL 1991

JULY 1990

SOCIETY OF CRYSTALLOGRAPHERS IN AUSTRALIA

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Newsletter Editor:	Geoff Williams Australian Radiation Laboratory Lower Plenty Road Yallambie, Vic. 3085 [tel. (03) 433-2211; FAX (03) 432-1835]

IMPORTANT MESSAGES

Perhaps the most important information to be gleaned from this Newsletter is that planning for the Seventeenth Meeting of the SCA at the University of New England, Armidale, NSW is well underway and the dates are now firm, viz. April 3-5, 1991. Please be prepared to respond promptly to the second circular which will be with members later this year.

It is also worth mentioning that our National Committee for Crystallography (ANCCr) has foreshadowed a review of the Organisation(s) of Crystallography in Australia. The ANCCr is appointed by the Australian Academy of Science to report and give advice on all matters affecting (i) international relationships in science, and (ii) the special interests of the Australian crystallographic community. The review may consider the advantages and disadvantages of having three professional societies (SCA, ANBUG and ASBUG) in a relatively small scientific community, and the possibility of overlap between the international activities of SCA (through its membership of the Asian Crystallographic Association, AsCA) and the international responsibilities of ANCCr. Members views on these issues are welcomed.

With this Newsletter are included two flyers, one giving details of the Crystal 17 meeting of the SCA (for noticeboards) and the other from the Federation of Australian Scientific and Technological Societies (FASTS) detailing current activities.

First announcement for

CRYSTAL XVII

THE SEVENTEENTH MEETING OF THE SOCIETY OF CRYSTALLOGRAPHERS IN AUSTRALIA

3-5 APRIL, 1991

UNIVERSITY OF NEW ENGLAND
ARMIDALE, NSW

Venue and Accommodation

The conference will be held on the campus of the University of New England, largely in Mary White College. The accommodation facilities are excellent; the tariff will be approximately \$53 per day (includes cooked breakfast, buffet lunch, three-course dinner, morning and afternoon teas, towel, linen and daily room service). Firm rates and details of non-resident tariffs for meals will be provided in the second circular (with registration forms) due out in late 1990. There will be a registration fee of approximately \$70.

Speakers

To date several overseas speakers have been invited to deliver key lectures, including J.B. Forsyth (Rutherford Laboratory, SERC, UK), A. Hewat (ILL, France), G.V. Gibbs (Virginia Tech, USA) and J.C.H. Spence (Arizona State University, USA). Additional overseas speakers are planned if we can obtain funding, and it is expected that further key lectures will be delivered by invited local participants.

Contact

Dr. Mark Spackman, Department of Chemistry, University of New England, Armidale NSW, 2351.

Tel. (067) 73 2722

Fax: (067) 71 1563

Telex: 166050

email: mspackma@gara.une.oz.au

COUNCIL NEWS

'1987 Scholarships'

Nine postgraduate student members of the SCA were successful with applications for '1987 Scholarships' to fund their travel to attend the IUCr Congress in Bordeaux. The nine '1987 Scholars' are:

Tony Brown	(Mark Spackman)	Univ. of New England
Joanne Etheridge	(Alex Moodie)	RMIT
Barry Fields	(Hans Freeman)	Univ. of Sydney
Jackie Gulbis	(Maureen Mackay)	La Trobe Univ.
Kate Hawkins	(Ian Mackinnon)	Univ. of Qld.
James Hester	(Ted Maslen)	Univ. of W.A.
William Shepard	(Ed Baker)	Massey Univ., N.Z.
Louise Vilkins	(Max Taylor)	Flinders Univ.
Vilma Zubak	(Peter Colman)	CSIRO, Biotechnology

1987 Scholars have been requested to write collectively on the Congress in general, and on some specific sessions of interest, to share with SCA members via the SCA Newsletter. Scholars were encouraged to seek extra funding from other sources for the non-travel costs, and many have taken the opportunity to spend time at other institutions of particular interest. Council is pleased that SCA funds were available for such a sound investment in the future of crystallography in Australia.

Financial statements prepared by the Treasurer, Colin Kennard, and the administrator of the '1987 funds', Ted Maslen, are attached for the information of SCA members. Formal audited statements will be presented at the Business Meeting to be held at Armidale in April 1991. Ted Maslen has requested that the arrangements for supervising the 1987 funds be altered to include three trustees (at present two), with two signatures being sufficient to operate the Trust Fund account. This change has been approved in principle by the SCA committee, with either Syd Hall or Allan White to be nominated as the third trustee.

The Asian Crystallographic Association (AsCA) has proposed that an inaugural AsCA meeting be held in 1992, possibly in Singapore. This would be organised jointly by the SCA and the Crystallographic Society of Japan (CSJ) and would incorporate the next SCA National Meeting ('Crystal 18') and an SCA Business Meeting. The SCA executive has responded favourably to the proposal, and has suggested Syd Hall as the SCA representative to liaise with the Japanese. Further planning will take place at Bordeaux. As an IUCr Regional Associate, AsCA is eligible for IUCr grants for funding the travel of young scientists to such a meeting.

The Australian Academy of Science has initiated the Australian Foundation for Science as a means of bringing additional resources of people and money to promoting science and technology in Australia, and of increasing the contribution of science to national welfare. The Academy is particularly keen for support from the many scientific societies, research institutions and individuals. ANZAAS has already decided to join the Foundation at a high level. In order to present the case for supporting the Foundation to other scientific bodies, a presentation is planned in Melbourne on 25 July. The SCA secretary will attend.

FINANCIAL STATEMENTS

The following statements have been received from the Treasurer, Colin Kennard, and from the administrator of the 'Perth Funds', Ted Maslen.

SCA accounts, 31 May 1990

Unicredit accounts (five)	\$24418.24
AGC	\$14000.00
CGS	\$ 3000.00
Payment of FASTS annual dues	<u>-\$ 437.50</u>
	<u>\$40980.74</u>

The only other outgoing for the financial year was a \$5000 transfer to the 'Perth account' for the SCA contribution to '1987 Scholarships'.

SCA earned \$3164.98 from Unicredit up to May 1990.

XIVth IUCr Congress a/c #381413

Balance at 30/6/89

Bank	\$ 2554.48	
Partnership Pacific at call	\$ 10000.00	
Commercial bills at cost	\$110815.66	
Balance		\$123370.14

Income

Commercial bills	\$ 14392.43	
Bank interest and investments	\$ 5031.26	
Total income from investments		\$ 19423.69
SCA grant for Travel Scholarships		\$ 5000.00
Total		\$147793.83

Expenditure

Government and bank charges	\$ 15.27	
Travel scholarships	\$ 21113.80	
Total expenditure for 1989/90		\$ 21129.07

Assets at 30/6/90

Bank	\$ 6664.76	
Investments	\$120000.00	
Balance at 30/6/90		\$126664.76

CRYSTAL XVII

Crystal XVII will be held at the University of New England, Armidale, N.S.W. between April 3 and 5, 1991 (i.e. a few days after Easter). Some details are given in the loose announcement distributed with this Newsletter. For those of you who have never been to Armidale, or who know very little about it, Mark Spackman has provided the following enticement:

Armidale is a city of some 22,000 people, situated on the New England plateau. The city is 980 metres above sea level, 560 km by road from Sydney and 440 km from Brisbane. The Armidale campus of the University of New England is 5 km north-west of the city centre, amid attractive rural surroundings. Early April is a beautiful time of the year; the weather is usually cool to mild, with average maximum daily temperatures of 22°C and overnight minima of 9°C.

The countryside around Armidale is largely sheep and cattle properties, but nearby are magnificent gorges, waterfalls (Wollomombi, Dangars, Ebor) and National Parks (New England, Cathedral Rock, Oxley Wild Rivers, Guy Fawkes, Dorrigo). A couple of hours drive due east of Armidale is the beautiful sub-tropical New South Wales north coast and the delights of Coffs Harbour, Nambucca Heads, South West Rocks and the spectacular beaches in between. Armidale is serviced by frequent flights from Sydney and Brisbane on Eastern Australian Airlines (a regional affiliate of Australian Airlines) and State Rail XPT train service to Tamworth with a bus connection to Armidale.

WORLD DIRECTORY

Bulk Orders for the Eighth Edition of World Directory of Crystallographers

The IUCr advise that work on this new edition of the Directory is now reaching completion. Dr E.N. Maslen, Assistant Editor of the Eighth Edition of the Directory, has assembled a very comprehensive team of sub-editors throughout the world. These sub-editors have supplied new entries and updates which have been added to the database for the Seventh Edition which was published in 1986. Camera-ready copy is being prepared from this updated database.

The final production costs will depend on the number of entries in the Directory and the number of copies printed. The Directory is being offered at a price of US\$5.00 for block orders. The price for individual copies will be appreciably higher. To keep the cost per copy to a minimum, the number of copies required must be known before printing.

Could individuals or groups please make their needs known to Professor H.C. Freeman as soon as possible (send no money at this stage):

World Directory,
Professor H.C. Freeman,
Department of Inorganic Chemistry,
The University of Sydney,
N.S.W. 2006

FAX: (02) 692-3329

PEOPLE

Louise Vilkins, a Ph. D. student in chemistry at Flinders University, is already making good use of her '1987 Scholarship' fare to Europe. She took part in a NATO Advanced Study Institute on charge density in Spain at the end of April and is currently working with Bryan Craven on her thesis research at the University of Pittsburgh. After attending the Bordeaux meeting, she will return to Adelaide to complete her degree. She was recently awarded the Doreen McCarthy Bursary by the Australian Federation of University Women to assist her with her overseas travel.



The SCA Treasurer, Colin Kennard, is planning to spend two months at the university in Kuala Lumpur after Christmas helping to set up a Nonius CAD-4 diffractometer. This follows the successful commissioning of a similar diffractometer in Colin's own department.

Peter Colman has become interim director of the new Biomolecular Research Institute to be based at Melbourne's internationally renowned medical research precinct, centred on Parkville's Royal Parade. The new Institute, established jointly by CSIRO and Victoria's Strategic Research Foundation, will work on a new generation of drugs with a view to developing new pharmaceuticals. Effort will concentrate on the structure and chemistry of biological molecules and, in particular, binding to proteins and DNA. As such it is a macromolecule rather than small molecule initiative. The Institute will ultimately offer some new positions as well as better research facilities for scientists from the CSIRO, Melbourne's universities and other research institutions. The Institute is seen as a centre where scientists from many disciplines can exchange ideas and pursue research with equipment that their individual institutions could not afford.

The Biomolecular Research Institute represents a cornerstone in plans by the Victorian and Federal governments to establish a local pharmaceutical industry to capitalise on Australia's skills in medical and biological research. The lack of such an industry has, in the past, seen many promising research developments languish or go overseas. (Compiled in part from a recent report by Graeme O'Neill in 'The Age')

We note with pleasure that Syd Hall has been appointed as Co-Editor of *Acta Crystallographica*.

New Members. We welcome three new members:

Miss Wen Huo, a student of Ward Robinson at the University of Canterbury, has interests in crystal structure analyses in general and in the chemistry of Hg compounds.

Mr James Hester of the Crystallography Centre at the University of W.A. is pursuing Ph. D. studies in electron density analyses.

Dr Paul Curmi is a protein crystallographer recently returned to Australia to take up a position at the University of N.S.W. Dr Curmi is also a user of synchrotron radiation.

LETTERS TO THE EDITOR

An occasional page which will appear whenever there is anything to go on it. To set the ball rolling, Rod Hill argues for taking ourselves more seriously.

Dear Editor,

Many of those members of the SCA who know me well will realise that it is not my bent to complain, criticise or castigate. However, recent events have moved me to reluctant but irresistible action.

Is it not bad enough that the SCA has such a naive and trivial logo decorating the front cover of its 'Official Record' (i.e. Newsletter), without further demeaning the Society and its Membership by the use of the term 'Bush Crystallographers'?

Are we so terrified of success and recognition that we must ridicule ourselves in the full light of day? How can we command respect and attention from others when we show such little respect for ourselves?

There is a time and a place for frivolity and friendly disrespect in the true Australian tradition, but the first page of the SCA Newsletter is certainly neither. Please, please, remove 'Bush Crystallographers' from future editions!

R.J. Hill
CSIRO Mineral Products

HODGKIN PRIZE

In celebration of Professor Hodgkin's 80th birthday, the British Crystallographic Association (BCA) are pleased to announce the creation of the 'Hodgkin Prize', an annual recognition of her great contribution to our field and to science in general.

Nominations for this Prize are welcomed from any part of the crystallographic community and the award will be made at the time of the Spring Meeting of the BCA. Periodically the award will recognise specifically the achievements of young crystallographers.

The BCA is counting on the generosity of Dorothy's many friends and colleagues to make this Prize financially worthwhile as well as prestigious. All donors will be named within the prize scroll and it is hoped that many will wish to be associated with this splendid and permanent tribute to Dorothy's scientific achievements. In order that the first award may be closely associated with Dorothy's 80th birthday, the first presentation of the 'Hodgkin Prize' will be made at the Sheffield Meeting of the BCA in Spring 1991.

Please forward contributions as early as possible to the Treasurer, Dr. Ian Langford, Department of Physics, The University, Birmingham B15 2TT, U.K.

MISCELLANEA

Members are reminded that subscriptions for 1990 are now overdue and will attract the penalty rate (i.e. \$20 for full and \$5 for student members). If you are in this category, please save the Society the stamp and trouble of chasing you up by sending your arrears to the Treasurer, Dr. Colin Kennard, forthwith.

The Crystallography Centre at the University of Western Australia is expecting delivery in July of a new CAD-4 diffractometer. This will restore the functional diffractometer situation at the Centre to two.

For those of us (few in number, it would seem?) unable to afford a new CAD-4 or such like, the option is to revamp an older diffractometer. This is the path which has been taken at the Australian Radiation Laboratory where, over the space of two years, a 23-years old Siemens AED diffractometer has undergone a complete overhaul. The mechanical side of the diffractometer was in excellent condition but the electronics (control interface and counting) and computer control (originally a PDP-8 with 4K of memory) were outdated and regularly gave problems. The solution chosen was to build new motor-control electronics and interface, and to use standard NIM detector HV and pulse counting modules. The power of the new system comes from the choice of a PC (AT clone) to control all the basic diffractometer functions and to run data collection. Software has been developed from first principles to perform an automatic peak search and cell determination, thus aiding greatly the ease of setting up a crystal for data collection. Anyone contemplating such a project, or interested in using any of the software or electronics which have been developed, can contact Geoff Williams on (03) 433-2211.

Anyone interested in using the Inorganic Data Base is invited to contact Colin Kennard at the University of Queensland on (07) 377-3296.

Elsewhere in this Newsletter, the nickname of 'Bush Crystallographers' raises some contention. I was not present when the name was coined, although I have a suspicion it may have been at the Bendigo meeting of the Society. If anyone is prepared to admit they are old enough to remember, a letter telling the yarn would be gratefully published ... Editor.

Another always vexatious issue is that of the SCA logo - an arrangement of needle-like crystals pointing strongly upwards (towards truth and enlightenment?). This particular design was chosen from an array of 12 alternatives presented to members by the previous Secretary, Rod Hill, in a poll conducted through the Newsletter in 1985.

FELLOWSHIPS

Studentships for BCA Course

The Chemical Crystallography Group of the British Crystallographic Association is running its third Intensive Course on Structural Analysis. The intention is to encourage standards of technical excellence through lectures and tutorials covering both the theoretical background to, and the practical applications of, modern techniques. The course, aimed primarily at young postgraduate and post-doctoral workers, will enable them to undertake further analyses with confidence and competence. The course will take place at Aston University, Birmingham from 18-24 March 1991, and will be divided into four major sections:

data collection and processing;
structure solution;
structure refinement;
analysis of results.

Some grants are on offer to cover costs of meals, accommodation and fees. These will be awarded in strict order of receipt of application. Application forms and other details are available from Dr. David Watkin, Chemical Crystallography Laboratory, 9 Parks Road, Oxford OX1 3PD (FAX: 0865 272690).

Postdoctoral Fellowships and Exchanges

Japan: under 35 years of age;
period of 12 months commencing between 1/4/91 and 31/3/92;
return airfare, monthly stipend, plus allowances.

U.K.: under 30 years of age;
2 year tenure, commencing between April and October 1991;
return airfare(s), stipend, plus some research costs.

Japan: short- or long-term exchanges;
support for collaborative work;
airfare plus allowances/remuneration.

China: short- or long-term exchanges as above.

U.K.: short-term exchanges as above.

France: Rhone-Poulenc Fellow for a senior Australian scientist;
for travel to France during 1991 for collaboration;
return airfare plus \$500 per week for 6 weeks.

All the above are for research in any field of natural science. Further details and application forms from the International Exchanges Officer, Australian Academy of Science, GPO Box 783, Canberra ACT 2601; (06) 247-3966.

POWDER DIFFRACTION

In Newsletter No. 4 of the IUCr Commission on Powder Diffraction, there is a fascinating article on powder diffraction facilities at ISIS. ISIS, at the Rutherford Laboratory in the U.K., is the most powerful pulsed spallation neutron source in the world. A High Resolution Powder Diffractometer (HRPD) at ISIS has proved invaluable for profile refinement using data from crystals of complex molecules with large unit cells and for ab-initio structure solution. There is also a medium resolution high intensity diffractometer. Further details including applications for beam time from The ISIS Facility, Rutherford Laboratory, Chilton, Didcot, Oxfordshire OX11 0QX, U.K.

FORTHCOMING MEETINGS

July 19-28, 1990. Fifteenth General Assembly and International Congress of Crystallography; Bordeaux, France. Contact Dr. M. Hospital, Laboratoire de Cristallographie et de Physique Cristalline, Université de Bordeaux 1, 351 cours de la Libération, F-33405 Talence, France; telefax 56/800837.

July 29-31, 1990. Complementary Applications of Diffraction by Neutrons and by X-ray Synchrotron Radiation; Alpe d'Huez (nr. Grenoble), France. Contact Dr. M. Marezio, Cristallographie, CNRS, BP 166X, F-38042 Grenoble cedex, France.

July 29-31, 1990. Symmetry in Physical Space and in Superspaces: Quasicrystals, Incommensurate Phases; Chatenay-Malabry (nr. Paris), France. Contact Prof. Weigel, Ecole Centrale, F-92295 Chatenay-Malabry cedex, France.

July 29-August 5, 1990. International School on Crystallographie Computing; Bischenberg (nr. Strasbourg), France. Contact Dr. J. C. Thierry, IBCM, 15 rue Descartes, F-67084 Strasbourg cedex, France.

November 5-9, 1990. International Symposium on Crystallography and Molecular Biology; Sao Paulo, Brazil. Contact Prof. Y. P. Mascarenhas, C.P. 369, 13.560 Sao Carlos-SP, Brazil.

March 18-24, 1991. Third Intensive Course in X-Ray Structural Analysis of Small and Medium Sized Molecules; Chemical Crystallography Group of the BCA; Birmingham. Contact Dr. D. Watkin, Chemical Crystallography Laboratory, 9 Parks Road, Oxford OX1 3PD, U.K.

April 3-5, 1991. Crystal 17, Seventeenth Meeting of the Society of Crystallographers in Australia; Armidale, N.S.W., Australia. Contact Dr. M. A. Spackman, Department of Chemistry, University of New England, Armidale, N.S.W. 2351, Australia.

August, 1991. Sagamore X Conference on Charge, Spin and Momentum Densities; Konstanz, F.R.G. Contact Prof. W. Weyrich, Fakultät für Chemie, Universität Konstanz, Postfach 7733, D-7750 Konstanz 1, F.R.G.

August 12-16, 1991. PICXAM Pacific-International Congress on X-ray Analytical Methods; Honolulu. Contact Dr. E.B. Kho, Department of Chemistry, University of Hawaii-Hilo, 523 W. Lanikaula Street, Hilo, Hawaii 96720-4091.

August 25-30, 1991. Thirteenth European Crystallographic Meeting; Ljubljana, Yugoslavia. Contact Prof. L. Golic, Department of Chemistry and Chemical Technology, E. Kardelj University, 61001 Ljubljana, P.O. Box 537, Yugoslavia.

August 31-September 2, 1991. Biomolecular Structures and Dynamics; Otocec, Yugoslavia. Contact B. Kojic-Prodic, Institute Ruder Boskovic, 41001 Zagreb, P.O. Box 1016, Yugoslavia.

September 2-3, 1991. Synchrotron Radiation in Crystallography; Trieste, Italy. Contact L. Randaccio, Dipartimento di Scienze Chimiche, Università di Trieste, Piazzale Europa 1, 34127 Trieste, Italy.

September 1-8, 1993. Sixteenth General Assembly and International Congress of Crystallography; Beijing. Contact Prof. M.-c. Shao, Institute of Physical Chemistry, Department of Chemistry, Peking University, Beijing 100871, China.