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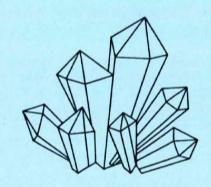
SOCIETY OF CRYSTALLOGRAPHERS IN AUSTRALIA

NEWSLETTER No.22

AsCA'92 CONFERENCE
SINGAPORE

13-16 NOVEMBER 1992
incorporating

SCA National Meeting



MARCH 1992

SOCIETY OF CRYSTALLOGRAPHERS IN AUSTRALIA OFFICE BEARERS

President:	A.H. White (University of WA)	25 A T 25 S A T 1	09-380-3144 09-380-1005
Vice President:	D.C. Creagh (ADFA, ACT)		06-268-8801 06-268-8786
Secretary:	G.A. Williams (ARL, Vic)	20 C MARCH - 100 M.C.	03-433-2211 03-432-1835
Treasurer:	C.H.L. Kennard (U. of Qld)	17 Table 12 Table 17	07-365-3662 07-365-4299
Council:	M.F. Mackay (La Trobe U.)		03-479-2520 03-478-5814
	C.J. Howard (ANSTO, NSW)		02-543-3111 02-543-9265
	W.T. Robinson (U. Canterbury, NZ)		64-3-642465 64-3-642110
ANCCr rep.: (ex officio)	H.C. Freeman (U. of Sydney)		02-692-2757 02-692-3329
Past President:	J.W. White (RSC, ANU)	tel. fax	06-249-3578 06-249-0750
Nominations Standing Committee:	B.M.K. Gatehouse (Monash U.) S.W. Wilkins (CSIRO, Vic) M. Sterns (ANU, Canberra)		
Newsletter Editor:	Geoff Williams Australian Radiation Laboratory Lower Plenty Road, Yallambie, Vic. 30	085	

IMPORTANT MESSAGES

Annual membership subscriptions for 1992 are now due. Please use the form at the back of this Newsletter to accompany your payment.

The first AsCA Conference (AsCA'92) will be held in Singapore from Saturday November 14 to Monday November 16, 1992. A copy of the Second Circular is mailed with this Newsletter. The next Business Meeting of the SCA will be held during this Conference. Student members of the SCA are advised that SCA funds are available on a competitive basis to support student attendance at AsCA'92. Applications should be made to the AsCA'92 Conference Office (Perth) before 1st June, as detailed on page 10 of the Second Circular.

Individual members of the SCA are invited to submit nominations, over the signatures of two members, for vacancies on Council which arise after the Business Meeting in November 1992. See page 7 for details.

COUNCIL NEWS

Summary of Council & Business Meetings 4th & 5th April 1991

The following summary is taken from the draft minutes of the three meetings held at Armidale. A copy of the draft minutes is available on application to the Secretary.

4th April Council Meeting

Treasurer's Report 1989-1991: The proposed motion ('Item 4b') for the Business Meeting was considered, and altered by the Treasurer, Colin Kennard, to read 'Cheques must be signed by two out of three members authorised by Council'. Council agreed to support this as a motion of the Business Meeting, and thus binding on Council, rather than as an amendment to the SCA Constitution. In this manner, the motion could be seen as amending the motion of the Business Meeting of 18 February 1989 which required cheques to be subject to two signatories of which one must be the Treasurer and the other a member of the Council.

The Treasurer is to investigate the provision for payment of membership subscriptions by credit cards. It was emphasised that benefits from making payments easier must be balanced against costs to the SCA. Colin expressed a need for a policy of maintaining SCA capital.

Ted Maslen reported on the Perth trust fund, summarised the level of income, and suggested a spending level of ca. \$6.5k to \$7k per year as appropriate.

Crystal 17 Costs: Council ratified the use of SCA funds (\$6000) to sponsor the attendance of overseas visitors Professor H. Hashizume, Dr J. Bruce Forsyth, and Dr Alan Hewat at Crystal 17. Other costs, largely associated with six '1987 Studentships', were \$1080 for travel and \$2200 for 10 registrations.

ANCCr: Hans Freeman reported on ANCCr matters. It was proposed (Chris Howard, seconded Geoff Williams) that John White be nominated as the SCA representative on the ANCCr for a term of three years expiring in April 1994. This was accepted unanimously by Council, and John White indicated his willingness to accept the nomination. Allan White, as President of SCA, will also be a member of ANCCr until the next SCA Business Meeting in November 1992.

AsCA: Syd Hall reported on AsCA matters. He indicated a need for SCA support for student attendance at the AsCA'92 conference in Singapore in November 1992. Syd also requested a loan (bridging finance) of \$2000 from the SCA, on the basis that the CSJ would provide a similar loan and that these loans would be repaid if possible, with profits from the conference being the property of the Asian Crystallographic Association. A need was expressed for publicity about AsCA'92 through AsCA and other newsletters.

Council discussed underwriting AsCA'92, and considered the maximum liability in the event of cancellation to be A\$10,000 on the basis of the 20 March 1991 'Summary of Planning Meeting'. Council would expect any such liability to be shared equally with the Japanese (CSJ). Under the conditions of this assumption, Council agreed to commit the SCA to jointly underwrite the AsCA'92 conference with the Japanese. After AsCA'92, Council expects the loan of \$2000 to be repaid to the SCA, with the balance of any profit to go

to the Asian Crystallographic Association. Council asked Syd Hall to request an equal commitment in this regard from the Japanese. Subsequently, the Japanese have agreed to match the SCA commitment to funding the meeting, including the sharing of any loss.

ANBUG/ASBUG: Council expressed the general opinion that there would be a certain 'tidiness' in bringing these two special-interest groups under the SCA umbrella. A letter from Rod Hill to John White of 16 August 1990 was considered, in which Rod as President of ANBUG asks for the SCA Council's attitude towards formal (re)instatement of ANBUG and/or ASBUG as Permanent Standing Subcommittees of the SCA. Council feeling was somewhat positive, expressing no objection if either group wished to initiate reinstatement.

Next Crystal Meeting: The gap between Crystal 17 in April 1991 and AsCA'92 in Singapore in November 1992 will be 19 months, with the IUCr Congress in Beijing in August 1993 a further 9 months away. The suggestion was put for a Crystal 18 meeting in February or September 1994, possibly in Canberra (or Sydney?). A final decision was deferred until after canvassing views at the Business Meeting.

FASTS: Membership of FASTS is to continue at the increased contribution level of \$3.90 per member. In response to a circular from FASTS requesting appointment of an SCA representative to interact with FASTS, Council nominated Richard Welberry. Richard subsequently indicated his willingness to fulfil this role.

4th April Business Meeting

In Attendance: 42 members of the SCA, plus observers Professors Hashizume and Spence and Drs Alan Hewat and John Barry.

Membership of FASTS: Colin Kennard summarised the activities of FASTS over the past few years and the question of dual payments (by people who are members of two contributing societies) was discussed but not resolved. Terry Sabine supported FASTS as being effective, and moved a motion that the Society continue membership of FASTS, to be reviewed in two or three years; seconded Sandy Mathieson. The motion was carried on a show of hands. The need for a representative, ideally in Canberra, was raised and Richard Welberry agreed to continue in this capacity.

President's Report: John White discussed the following points:

- members have been kept informed of Society news, and in particular of SCA finances, via the Newsletters;
- funds from the Perth Congress allowed the Society to sponsor travel of nine students of crystallography to Bordeaux, and it was worthwhile having these students at the Congress;
- the SCA participated in the ASTEC report 'Small Country Big Science' through John White's involvement with ASTEC;
- the SCA is involved with the inaugural AsCA meeting to be held in Singapore in 1992;
- the Society is not quite maintaining the real value of its funds resulting from profit on the Perth Congress;
- and congratulations were recorded to Peter Colman on his election to the Australian Academy of Science.

Treasurer's Report: The Treasurer's report was presented by Colin Kennard. The motion 'Cheques must be signed by two out of three members authorised by Council' was moved by Colin Kennard, seconded by Steve Wilkins, and carried on a show of hands. John White queried what the Society is doing to increase numbers. Geoff Williams replied that an active recruiting drive is in place and many new members have recently been added from universities in S.E. Asia and from current students at universities. An earlier invitation to Australian crystallographers not SCA members but listed in the 7th World Directory brought a disappointing response, with the conclusion that SCA membership already includes essentially all established crystallographers who would wish to be members.

Report from ANCCr Chairman: Hans Freeman presented a verbal report of the main activities of the National Committee for Crystallography. Membership is as follows:

Hans Freeman chairman

Judge Bevan Rod Hill Chris Howard John White

SCA representative

Allan White SCA president

One issue addressed was the number of organisations of crystallographers in Australia. The ANCCr concluded that it was not the National Committee's job to stop anyone from meeting, and is satisfied to have raised this issue at this stage and put it on the agenda for future discussion.

The 'Big Science' report of the ANCCr has had a successful result in that the government has recognised the need for Australian access to neutron and synchrotron radiations. Two types of travel grants are in place, both administered by ANSTO; \$150K will be available from July 1991 from DITAC funds for (say) 20 visits to overseas facilities. The preference is for groups to include a student in such visits to overseas facilities.

Inaugural AsCA Conference: Syd Hall presented the current situation re the inaugural AsCA meeting (AsCA'92) to be held in Singapore on 14-16 November 1992. The compositions of the various organising committees were presented. Financial arrangements were discussed; the Conference is to run with an overall budget of \$40K, with a maximum registration fee of \$250 to include the reception and banquet. A sum of ca. \$8000 has been negotiated with the SCA Council to provide student scholarships. Various accommodation options and costs were presented. Any profit from the conference will go to AsCA.

In response to a series of questions, Syd indicated that the budget is based on 200 participants. Support from UNESCO will be investigated. question related to whether the SCA is underwriting AsCA'92 and to what John White summarised the SCA Council position on the total SCA commitment, which is as follows: Council is prepared to underwrite AsCA'92, and considers the maximum liability in the event of cancellation (worst case) to be A\$10,000 on the basis of the 20 March 1991 'Summary of Planning Meeting'. Council would expect any such liability to be shared equally with the Japanese (CSJ). Under the conditions of this assumption, Council would agree to commit the SCA to jointly underwrite the AsCA'92 conference with the The SCA would provide a loan (bridging finance) of \$2000 to Japanese. AsCA'92, on the basis that the CSJ will provide a similar loan. AsCA'92, Council expects the loan of \$2000 to be repaid to the SCA, with 'the balance of any profit to go to the Asian Crystallographic Association. Council has asked Syd Hall to request an equal commitment in this regard from

the Japanese. (Subsequently, the Japanese have agreed to match the SCA commitment to funding the meeting, including the sharing of any loss.) A motion ratifying this Council position was moved by Dudley Creagh, seconded Jose Varghese. This motion was carried unanimously.

Scientific Program for AsCA'92: Ted Maslen presented the draft scientific program. It is expected that invited speakers will come from the Asian region. In response to questions, Ted indicated that young crystallographers will be encouraged (on merit) to participate in the program. The possibility of running a workshop or teaching school just before or after the meeting was raised, with Ted expressing the view that this may detract from the scientific standing of the meeting.

Crystal 18: There was much discussion about the date and venue - Sydney or Canberra? Autumn 1994 seemed a preferred time. Max Taylor put the suggestion of New Zealand, and this was supported by Ward Robinson who expressed a willingness to organise Crystal 18 in Christchurch. Steve Wilkins suggested the logo 'the SCA abroad'! The preferred time for a New Zealand meeting was February 1994.

Nominations Committee Report: The President, John White, expressed thanks from the Society to retiring Councillors Peter Colman and Jim Graham; John White then presented the report of the Nominations Committee, welcoming the new members Dudley Creagh (Vice President) and Ward Robinson (Council). The Nominations Committee remains unchanged with members Bryan Gatehouse, Steve Wilkins and Meta Sterns.

On taking the chair, the incoming President Allan White expressed his thanks to the organisers of Crystal 17, Mark Spackman and his henchmen, indicating that the conference had been a resounding success with a record attendance. Allan indicated that on this basis we can look to the future with optimism. Allan also expressed thanks to John White for a sterling effort as President, and to Geoff Williams and Colin Kennard as Secretary and Treasurer, and expressed satisfaction with having a New Zealander on the Committee.

5th April Council Meeting

Next Crystal Meeting: The suggestion was made at the Business Meeting that Crystal 18 be held in New Zealand in 1994 at either Easter or mid-June. Council felt that there was considerable disquiet amongst members at the number of crystallography meetings to be held offshore in the next three years. Hans Freeman suggested Sydney as a possible venue for Crystal 18. The general consensus of Council was that Crystal 18 should be held within Australia and that New Zealand be considered for Crystal 19. A final decision was deferred until the Council meeting to be held in Singapore in November 1992.

SCA Archives: Geoff Williams suggested that the SCA establish a reasonably stable repository for archival material. In his experience a large amount of material is collected by the Secretary/Newsletter Editor, which should be archived at the end of each term of office. Council agreed to the establishment of an SCA archive, and an approach to Rod Hill at CSIRO was suggested. Rod subsequently agreed to provide space for the archive.

Financial Arrangements: Following the passing of the Treasurer's motion ('Item 4b') at the Business Meeting of 4 April 1991, Council authorised Graham Smith of the Department of Chemistry, Queensland University of Technology, to act as the third signatory for SCA cheques. The other two signatories are the Treasurer Colin Kennard and Colin Raston.

Council Elections and Business Meeting

Members are reminded that a SCA Business Meeting will be held during the Asian Crystallographic Association Conference AsCA'92, which is in effect the next National Meeting of the SCA, to be held in Singapore on November 13-16 1992. Agenda items for this Business Meeting should be submitted to the Secretary.

This National Meeting brings with it the end of the current terms of election of Associate Professor Allan White (President), Professor John White (Past President), Dr Colin Kennard (Treasurer), Dr Geoff Williams (Secretary) and Dr Maureen Mackay (Council). To fill the vacancies thus created the Nominations Committee, in accordance with Article IV and Rules III and IV of the SCA Constitution, will provide a list of nominations which will be mailed to members in May of this year. Individual members of the SCA are invited to submit additional nominations, over the signatures of two members, for these vacancies. Such nominations should reach the Secretary by 30 June 1992.

Financial Matters

Due primarily to some skilful organisation by Mark Spackman, CRYSTAL 17 held at Armidale last April was not only able to return to the SCA the \$1000 loaned to start the conference off, but also returned a small profit of ca. \$30. Council considers this a very satisfactory conclusion to what was a most successful meeting.

SCA financial reports for the years ending 30 June 1988, 1989 and 1990 have been audited and all found to be in order. Details can be obtained from the Treasurer, Dr Colin Kennard.

Photon Factory Management

The installation of the Australian beam-line at the Photon Factory in Tsukuba is approximately on schedule. A number of research groups have started to make use of other facilities at the Photon Factory. Funds are available to support travel by Australian investigators for this purpose. The current memberships of the various committees involved in managing our activities at the Photon Factory are as follows:

Photon Factory Management Committee: Dr David Cook, Chairman (ANSTO), Ms Pauline Barratt (DITAC), Dr Peter Colman (CSIRO), Associate Professor Dudley Creagh (University College, UNSW), Professor Hans Freeman (AAS), Professor Graham Rigby (ARC) & Professor John White (ANU).

Technical Committee: (responsible for getting the Australian beam-line running) Associate Professor Dudley Creagh, Chairman, Dr Richard Garrett, Secretary (Project Scientist), Dr John Boldeman (ANSTO), Professor John White & Dr Stephen Wilkins (CSIRO).

<u>Program Committee</u>: (responsible for assessing proposals to use the Australian beam-line and applications for funds to support travel to Photon Factory) Professor John White, Chairman, Dr Peter Colman, Associate Professor Dudley Creagh & Professor Hans Freeman.

Summary of Profile of Australian Crystallography, November 1991

Of 100 responses received by 31 December 1991, seven were from SCA members overseas (incl. New Zealand). The following summary is of the remaining 93 responses from crystallographers currently practising in Australia.

Institutions:	University CSIRO Industry Other Tert Government Other	iary	62 17 4 2 7	
Age:	21-30 31-40 41-50 51-60 61-65	ų	21 20 26 18 6 2	
Position:	Postdoctor Tenured pr Contract pr Free-lance	ate student ral rofessional professional	3 14 6 53 10 5	
Techniques/Instrumen		Sealed-tube X-ray Rotating-anode gen Synchrotron X-ray Neutron source (HI Neutron source (O/ Powder diffractome Single-xl diffract Low-angle diffract Small-angle scatte X-ray absorption s Electron diffracti	erator source FAR) S) ter/camera ometer/camera ion ring pectroscopy	76 26 23 29 16 59 59 6 11 5
Professional Bodies:		IUCR Commissions Committees Advisory bodies Editorial boards		8 14 4 11

E-MAIL AND FAX ADDRESS LIST

As a precursor to the proposed computer-readable World Directory, member countries of AsCA have been asked to compile an e-mail and fax address list of crystallographers. Somewhere, in a conversation about this to Syd Hall, I said 'yes' at the wrong time, so I find myself the compiler of this list in Australia. The project is being coordinated by Professor H Hashizume.

Please do one of the following before April 7

1. If you have an e-mail address*, please send me a message immediately and include in it information in the following format:

Last name: e.g. Taylor

Title, first name, other initials: Dr Max R

Institution: Flinders University of South Aust.

E-mail address: chmrt@cc.flinders.edu.au

Fax number: (08) 201-3035

2. If you have access to fax <u>only</u> please send me a message via fax (you can include a list of names, etc. with this if several crystallographers use the same number).

* If you have '.oz' in your address then you are probably still using the old ACS network address. It may be worthwhile checking with your site manager to see if there is a standard AARnet address available to you (i.e. ___.edu.au).

Max Taylor

RADIATION SAFETY

ICRP reduces occupational dose limit

Recently, the International Commission on Radiological Protection (ICRP) agreed on new recommendations on the dose limit for occupational exposure. The previous limit (set in 1977) of 50 millisievert (mSv) in a year has been reduced to 20 mSv per year, averaged over five years with the further provision that the dose should not exceed 50 mSv in any single year. The limit for public exposure remains 1 mSv in a year.

The dose limits do not apply to natural sources of radiation or to the medical exposure of patients. The new recommendations come from consideration of new data and a new interpretation of earlier information which indicates with reasonable certainty that some risks associated with ionising radiation are about three times higher than they were estimated to be a decade ago.

The ICRP's system of radiation protection is based on three main principles: that practices causing exposures should be justified; that protection arrangements should be optimised; and that the individual exposures should be restricted by dose limits or source-related dose constraints. The new recommendations continue to stress the importance of keeping exposures 'as low as reasonably achievable'; that is, it is not generally sufficient simply to meet the limits but operators should continue to reduce exposures if this can be achieved without undue cost.

INTERNATIONAL UNION OF CRYSTALLOGRAPHY 16th IUCr CONGRESS

Beijing, 21-29 August 1993

CALL FOR PROGRAM PROPOSALS

The program will consist of 14 Main Lectures, 42-46 Microsymposia and 4 General Lectures. On most days there will be 2 Main Lectures, Microsymposia, 2 to 3 Open Commission Meetings and a poster session. scope of the Congress will be defined by the following topics:

- 01 Instrumentation and Experimental Techniques (X-rays, Neutrons, Electrons)
- 02 Methods of Analysis, Computing and Graphics
- 03 Crystallography of Biological Macromolecules
- 04 Crystallography of Biological Small Molecules
- 05 Molecular Modelling and Design for Proteins and Drugs
- 06 Crystallography of Organic Compounds
- 07 Crystallography of Organometallic and Coordination Compounds
- 08 Inorganic and Mineralogical Crystallography
- 09 Physical and Chemical Properties of Materials in Relation to Structure
- 10 Surfaces, Interfaces and Thin Films
- 11 Amorphous, Imperfectly Ordered and Quasi-periodic Materials
- 12 Defects, Microstructures and Textures
- 13 Diffraction Physics and Optics
- 14 Crystal Growth
- 15 Molecular Structure Determination by Methods other than Diffraction
- 16 Symmetry and its Generalizations
- 17 Data Handling and Communications
- 18 Crystallographic Teaching and the History of Crystallography
- 19 Industrial Crystallography

The Program Committee has issued a call for proposals for:

- topics and speakers for Main Lectures,
- (ii) topics, chairpersons and speakers for Microsymposia,
- (iii) additions or changes to the list of Congress topics (given above), &
- (iv) other matters concerning the scientific program.

Experience suggests that it will assist the Program Committee if proposals under the above headings are collated and forwarded by the National Committee for Crystallography. Proposals should be sent immediately to the Chairman of the National Committee (Professor Hans Freeman, Department of Inorganic Chemistry, University of Sydney, NSW 2006).

Satellite Meetings

- 1. Hefei School on Crystallographic Computing
- 2. Neutron Scattering
- 3. Powder Diffraction
- 4. Synchrotron Radiation in Crystallography
- 5. Symposium on Molecular Structure

First Circular

Copies of the First Circular are available from the Secretary of the SCA, Geoff Williams; (03) 433-2211 n.b. deadline for return 30 September 1992.

International Union of Crystallography

NOMINATIONS FOR THE EWALD PRIZE

The International Union of Crystallography is pleased to invite nominations for the Ewald Prize for outstanding contributions to the science of crystallography. The Prize is named after Professor Paul P. Ewald, in recognition of his significant contributions to the foundations of crystallography and to the founding of the International Union of Crystallography. Professor Ewald was the President of the Provisional International Crystallographic Committee from 1946 to 1948, the first Editor of the Union's publication Acta Crystallographica from 1948 to 1959 and the President of the Union from 1960 to 1963.

The Prize consists of a medal, a certificate and a financial award, and is presented once every three years during the triennial International Congresses of Crystallography. The recipients to date are as follows:

Year	Place	Recipients
1987	Perth, Australia	Professor J.M. Cowley and Dr A.F. Moodie
1990	Bordeaux, France	Professor B.K. Vainshtein

The third Prize, for which nominations are now being invited, will be presented at the XVI Congress in Beijing, China, in August 1993.

Scientists who have made contributions of exceptional distinction to the science of crystal-lography are eligible for the Ewald Prize, irrespective of nationality, age or experience. The Selection Committee will give careful attention to the nominations of outstanding scientists who have not yet won a major prize. Either an exceptionally distinguished scientific career or a major scientific accomplishment may be recognized. Current members of the Prize Selection Committee and the President of the Union are not eligible. No restrictions are placed on the time or the means of publication of the nominee's contributions. The Prize may be shared by more than one contributor, but not more than three, to the same scientific achievement.

Nominations for the Ewald Prize should be submitted in writing, preferably using the Ewald Prize Nomination Form and accompanied by supporting documentation, to the Executive Secretary of the International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England, from whom copies of the Nomination Form, the names of the Selection Committee and advice on the submission of nominations may be obtained. The closing date for nominations is 31 August 1992.

President

General Secretary

PEOPLE

New Members. We welcome 21 new members:

Professor Hiroo Hashizume, Research Laboratory of Engineering Materials, Tokyo Institute of Technology, Yokohama; Professor Hashizume is also a member of the Executive of the Crystallographic Society of Japan.

Dr Alan Hewat, of the ILL, Grenoble, whose work in neutron powder diffraction and on superconductors and phase transitions is well known to many by virtue of his invited talk at Crystal XVII.

Dr Mel Fehlmann, Institute of Crystallography, Zurich, with major interests in topography and the use of synchrotron radiation.

Dr Wei Chen, Department of Chemistry, University of Malaya, Kuala Lumpur, a small-molecule crystallographer.

Dr H.K. Fun, School of Physics, Universiti Sains Malaysia, Penang.

Ms Tina Izard, CSIRO Division of Biomolecular Engineering, Parkville; studying for a Ph. D. in protein crystallography; keen horse-rider.

Mr David Nation, School of Physical Sciences, Flinders University of South Australia; a Ph. D. student studying copper coordination compounds and small-molecule crystallography with Dr Max Taylor.

Ms Bee Kwan Gan, a Ph. D. student at Curtin University of Technology, Perth.

Ms Rebecca Berrigan, Ph. D. studies at Monash Chemistry (characterisation of thin films by X-ray techniques) in between working in Japan for NTT (synchrotron experiments at the Photon Factory) and throwing javelins.

Dr Siegbert Schmid, a member of the Inorganic Solid State Chemistry Group at the Research School of Chemistry, ANU.

Dr J.C. Taylor, CSIRO Coal and Energy Technology Division, whose main crystallographic interests encompass X-ray and neutron powder diffraction.

Mr Andrew Urban, CSIRO Division of Mineral Chemistry, with interests in the Rietveld method and mineral and metal oxide structures.

Dr John Zdysiewicz, Editor, Australian Journal of Chemistry.

Dr Walter Kalceff, Department of Applied Physics, University of Technology, Sydney; with major interests in neutron diffraction (extinction/absorption) and magnetic structures.

Mr Bruce Kerr, chemist at Callide B Power Station, Biloela, Queensland.

Dr Doug Todd, X-ray Centre, Metallurgy Building, The University of Newcastle.

Ms Nicola Scarlett, who is employed at CSIRO Division of Mineral Products and is studying for a Ph. D. at the School of Chemistry, University of Melbourne; main interests being mineralogy and organometallic chemistry.

Mr Anthony Bartel, Department of Physics, Swinburne Institute of Technology (Melbourne) who is undertaking Ph. D. studies.

New Members (continued)

Dr Elizabeth Sutherland, a research fellow at the University of Melbourne interested in organometallic chemistry.

Dr Jonathon White, School of Chemistry, University of Melbourne, with major interests in correlations of structural parameters for organic molecules with reactivity in solution, particularly stereo-electronic effects.

Ms Michaele Hardie, a Ph. D. student at the School of Chemistry, University of Melbourne, whose interests are in synthetic and structural studies of inorganic compounds comprising infinite polymeric frameworks.

Professor John White, FAA

The SCA offers congratulations to its immediate Past President, John White, on his election, last year, to the Australian Academy of Science.

Not THE David Phillips!

David Phillips, Professor of Chemistry, Imperial College, London, is visiting Australia in May to give the Questacon National Lecture Tour. Most of us crystallographers are perhaps more familiar with Professor Sir David Phillips of the Laboratory of Molecular Biophysics, Oxford. The visiting David Phillips was formerly Wolfson Professor of Natural Philosophy in the Royal Institution. The lecture is titled 'A Little Light Relief - uses of Light in Modern Medicine' and will be presented in Melbourne (May 16), Canberra (May 18), Adelaide (May 20), Sydney (May 22) and Brisbane (May 25). More details can be obtained from Sandy Clugston at DITAC on (06) 270-2811.

DAVID WADSLEY

The Naming of the X-ray Laboratory at CSIRO Mineral Products

The CSIRO Division of Mineral Products (formerly Mineral Chemistry) has an outstanding tradition of scientific excellence in the fields of solid state crystal chemistry, mineralogy and crystallography, all dating back to the early 1950's.

The development of this reputation and tradition owes much to one man - the late Arthur David Wadsley. In recognition of his outstanding contribution to science and the Division, it was decided to dedicate the X-ray Laboratory to his memory by naming it the 'A.D. Wadsley Laboratory'.

The dedication ceremony was held on 8 April 1991, in the presence of David's family and many of his friends and colleagues. During the ceremony, David's widow Mrs Joan Wadsley unveiled a commemorative plaque for the Laboratory, while Dr Alan Reid, Director IMEC, and Dr Robert Roth of the National Bureau of Standards of USA, reminisced about David's life and career. On the following four pages, guests at the ceremony are detailed in the list and commemorative photographs, and some snippets from records of David Wadsley's life and career are given.

ATTENDEES

Mr W.J. Asker Mr J.A. Aylmer Dr T. Biegler Dr L.A. Bursill Dr R.I. Garrod Dr B.M.K. Gatehouse Dr P. Goodman Dr D.F.A. Koch Prof A.M.Mathieson Miss J. McKenzie Ms M. Mercurio Dr A.F. Moodie Prof. J.D. Morrison Mrs E. Newnham Dr D.A.J. Rand Dr D.E. Scaife Dr T. Scott Dr E.R. Segnit Dr H. Sinha Mr H.R. Skewes Mr P.R. Smith Mr J.A. Spink

Dr M. Fehlmann Prof H.C. Freeman Dr J. Graham Prof B.G. Hyde Dr P. Leverett Mr. C. D. Priday

Out-of-State Guests

Prof D.J.M. Bevan

Dr A.F. Reid Prof A.E. Ringwood Dr.R.S. Roth

Prof T.M. Sabine Dr P. Smith

Prof N.C. Stephenson

Family members

Dr J.A. Wunderlich

Sir Alan Walsh

Dr R. Woods

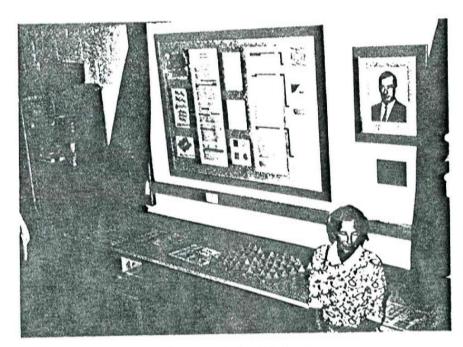
Mrs J.D. Wadsley Mrs P. Dodd & family Mrs P. George & family Mr R. Wadsley

Organising Committee

Dr I.J. Bear Ms C. Calle Ms P. Converse Dr I.E. Grey Dr R.J. Hill Mr I.C. Madsen Ms L. McRae Dr W.G. Mumme Mr J.A. Watts



Colleagues of Dave Wadsley at the Dedication



Mrs J. D. Wadsley in front of display + plaque



A.D. Wadsley 1918 - 1969

Readers may be interested in the following snippets from records of David Wadsley's life and career.

David Wadsley was born in Hobart, Tasmania, on 1 August, 1918. His early training was as a metallurgist. At the age of 16 years he joined the Electrolytic Zinc Company and, during subsequent tertiary studies at the University of Tasmania, twice returned to work at the Company's plants at Risdon and Rosebery. In the final year of his B.Sc. course he gained a high distinction in primary metallurgy and subsequently studied secondary metallurgy at the Hobart Technical College while completing his honours year. He gained his M.Sc. at the University of Tasmania in 1941 and, after a period as the Munitions Supply physicist at Laboratories, joined the CSIR Minerals Utilization Section in February 1943. His first project concerned the wartime use of Australian pyrolusite in dry cells. Pyrolusite is a mineral form of manganese dioxide. Wadsley's applied work was thorough but unspectacular, and in 1946 he unsuccessfully sought permission to do further study overseas. Forced back to an investigation of the structures of manganese dioxide, he developed an interest in X-ray crystallography. This was the beginning of his life's work on the crystal chemistry of non-stoichiometric compounds and a brilliant academic career unfolded.

At that time non-stoichiometric compounds were considered to be single phases which could retain their identities over wide ranges of chemical composition. The range of composition in a non-stoichiometric compound was attributed to random defects in the crystal lattice, such as vacant atom positions or additional atoms inserted between regular atom positions — called interstitial atoms.

Wadsley started to question the universal applicability of this concept. In this he was influenced by the work of Swedish scientists. Pioneering studies by Magneli had established that the non-stoichiometric tungsten and molybdenum oxide systems did not consist of single phases of continuously variable composition, but that each contained a

homologous series of discrete phases. To account for these series of phases, Haag and Magneli, in 1954, published a "block" theory in which it was postulated that in these systems blocks of basic structure were separated by planes of ordered defects. These defect planes accommodated a change in the ratio of metal atom sites to oxygen atom sites in the structure; the number of these defect planes determined the chemical composition of the compound.

Although it was the Swedish crystallographers who first postulated these planes of ordered defects to explain the structures they were investigating, it was Wadsley who immediately grasped the significance of the theory and saw its scope. He realized that it gave a rational explanation for the proliferation of complex structures in non-stoichiometric compounds which he and other workers were discovering. In his 1955 review article in the Royal Australian Chemical Institute's Reviews of Pure and Applied Chemistry, he introduced his concept of crystallographic shear, which was to form the basis of much of his research in the following decade.

In 1967, Wadsley was awarded a D.Sc. by the University of Tasmania for his crystal structure work on manganese oxides.

It is interesting to note in connection with later work in the Division on the beneficiation of ilmenite, that the Swedish scientist, Dr Sten Andersson, and his colleagues established that the non-stoichiometric titanium-oxygen system was also a homologous series of compounds.

Wadsley's work at this point began to follow two clearly defined paths. In addition to his studies of the classical "non-stoichiometric" binary and temary oxide systems, he commenced an investigation of the effect of impurity atoms on oxide structures. He was now seeking, not only a rational picture of defect structures in general, but also a pre-determined route to the synthetic creation of the apparently complex, yet quite specific, structures which he was predicating. This latter theme stemmed from his interest in the alkali-metal vanadium bronzes in the early 1950s.

In both projects he was pressing the use of high-resolution X-ray diffraction

equipment to its limit, and, in 1958, he defined the broad lines of his research programme in the Liversidge Research Lecture. It became evident that he was no longer postulating changes within the structural polyhedra, but rather changes in the grouping of the polyhedral entities; comer-sharing, edgesharing and face-sharing became his tools of trade, and the work of Andersson on the titanium oxide systems began to influence his thinking.

In 1960, Sten Andersson arrived in Australia. The visit resulted in a dynamic leap forward in Wadsley's programme. Their first joint publication mounted a direct attack on traditional concepts. The influence of this collaborative period with Andersson spread to Graham, Allpress, Stephenson and Gatchouse, who were all working in other Australian research laboratories. When in 1962, Wadsley, by invitation, presented his ideas on order and disorder in non-stoichiometric metal oxides to a symposium of the American Chemical Society, a controversy which had been simmering for several years flared up. This controversy was led by Dr Robert Roth of the National Bureau of Standards of U.S.A. Roth, a scientist of international standing, then commenced a series of experiments, the results of which confirmed Wadsley's point of view. Roth's conversion was as complete as it was Granted leave by the National dramatic. Bureau of Standards to work with Wadsley in Australia as guest scientist for 12 months, he triggered off a group of publications that rivalled the original Andersson series in range and significance, and together they placed the long-postulated "block" principle on a sound experimental basis. It also opened the way for fruitful collaboration with Gruehn and Schafer at Munster.

In 1965, Wadsley was awarded the Royal Australian Chemical Institute's H.G. Smith Memorial Medal for contributions to chemical crystallography.

Another visit by Andersson to Australia in 1966 resulted in further fruitful collaboration. Wadsley's international stature continued to grow. It is noted in Divisional files that during 1966 requests from foreign scientists who wished to work with Dr Wadsley's research group averaged more than one per month.

By the time of the Werner Centenary Lectures in 1967, he was able to enunciate two new rules that he had used to predict the structure of previously unsuspected mixed-oxide phases of niobium and tungsten. These rules were to supplement and modify indeed to contradict, the 40 year old Pauling principles for delineating the structure of crystalline solids. In a further advance in 1968, Allpress, Sanders and Wadsley used electron microscopy and electron diffraction to directly measure the spacing of crystallographic shear planes.

It was in these years also that he started a study with Alan Reid and A.E. Ringwood (Professor of Geochemistry, Australian National University) of silicate systems under high pressure, in order to increase the knowledge of the phase relations at depths between 200 - 900 km in the earth's mantle,

At the end of 1968, following correspondence and an invitation from the Nobel Committee, Ivan Newnham, Chief of the Division, drafted a nomination. The opening paragraph of that nomination, which is in the official files of the Division of Mineral Chemistry, reads:

"Dr Wadsley is nominated for the award of the 1969 Nobel Prize for Chemistry, firstly on the grounds of his discovery of two major rules which can be used to predict the structure of, and develop methods of synthesis for, new solid state compounds, and secondly on the grounds of his improvements in the techniques of crystal structure analysis which have provided the experimental evidence to support his theoretical predictions".

Tragically, on the 6th of January 1969, David Wadsley suffered a massive heart attack while chairing the opening session of an International Conference in Canberra; he died shortly afterwards in the Canberra hospital. The Nobel Committee confirmed that the Nobel Prize cannot be awarded posthumously, so the nomination was never completed.

As a final comment on David Wadsley's career, we can not do better than to quote from Dr Sten Andersson's obituary to him:

"The rapid development of solid state chemistry during the last several years (of his life) clearly shows that he was a person with a grip on chemistry and down-to-earthness that was very impressive. He was indeed guided by the intuition that comes from profound knowledge and experience, skill, and intelligence".

CAMBRIDGE STRUCTURAL DATABASE

The Cambridge structural database is now available at Flinders University for access by bona fide users via AARnet.

If you wish to make use of this facility please contact me via e-mail, whether you have enquired about it before or not. Before being allowed access via the network you will be required to fill out an agreement form supplied by Cambridge.

e-mail:

chmrt@cc.flinders.edu.au

Max Taylor

WORLD DIRECTORY

The SCA placed a bulk order for 70 copies of the new (8th edn.) World Directory of Crystallographers, and these have been made available to members at \$10 per copy; a considerable saving on the single-copy price.

A few copies are still available, and anyone wishing to purchase should send a cheque (made out to SCA, \$10 per copy which includes cost of postage) to Geoff Williams. Four copies which arrived in unsaleable condition are offered free of charge to any student members who would like one - apply to Geoff Williams, and these will be dispatched on a first-come basis.

TRANSACTIONS OF THE AMERICAN CRYSTALLOGRAPHIC ASSOCIATION

The following transactions of the ACA are still available, for US\$25 per volume, plus postage and handling (US\$3 for one or two volumes). Orders to Polycrystal Book Service, P.O. Box 3439, Dayton OH 45406, USA.

Volume	25	Molecular Recognition and Protein-Carbohydrate Interactions	1989
Volume	24	NMR & X-Ray Crystallography: Interfaces & Challenges	1988
Volume	23	Neutron Diffraction	1987
Volume	22	Hydrogen Bond: New Insights on an Old Story	1986
Volume	21	Structure Determination with Synchrotron Radiation	1985
Volume	20	Molecules in Motion	1984
Volume	19	Small Angle Scattering	1983
Volume	18	New Crystallographic Detectors	1982
Volume	17	Diffraction Aspects of Orientationally Disordered Crystals	1981
Volume	16	Structure & Bonding: Relationships b/w Quantum Chem & Cryst.	1980
Volume	15	Chemistry & Physics of Minerals	1979
Volume	14	Str. Aspects of Homogeneous, Heterogeneous & Biol. Catalysis	1978
Volume	13	Fifty Years of Electron Diffraction	1977
Volume	12	Instrumentation for Tomorrow's Crystallography	1976
Volume	11	Applied Crystal Chemistry & Physics	1975
Volume	10	Liquids & Amorphous Materials	1974
Volume	9	Biophysical Applications of Crystallographic Techniques	1973
Volume		Experimental & Theoretical Studies of Electron Densities	1972
Volume		Mechanisms of Phase Transitions	1971
Volume	6	Intermolecular Forces & Packing in Crystals	1970
Volume	5	Crystal Structure at High Pressure	1969
Volume		Low Energy Electron Diffraction	1968
Volume	3	Thermal Neutron Scattering Applied to Chem & Solid State Phy	1967
Volume		Machine Int. of Patterson Functions & Alt. Direct Approaches	
Volume		Accuracy in X-Ray Intensity Measurements	1965
	1977	- 1月7月7日 1777 1777 1777	

SOCIETY OF CRYSTALLOGRAPHERS IN AUSTRALIA COUNCIL ELECTIONS AND BUSINESS MEETING

Members are advised that a SCA Business Meeting will be held during the AsCA'92 Conference in Singapore. This Meeting will be held in Room C of the poster area at 1800 on Monday 16th November 1992 preceding the Farewell Banquet at 1930. The annual meeting of the Crystallographic Society of Japan will be held at AsCA'92 at the same time.

This Meeting brings with it the end of the current terms of election of Professor Allan White (President), Professor John White (Past President), Dr Geoff Williams (Secretary), Dr Colin Kennard (Treasurer) and Dr Maureen Mackay (Council). To fill the vacancies thus created the Nominations Committee, in accordance with Article IV and Rules III and IV of the SCA Constitution, has nominated Dr Ian Grey (CSIRO) for Vice President, Dr Max Taylor (Flinders Univ.) for Secretary, Dr Graham Smith (QUT) for Treasurer, and Dr Mark Spackman (Univ. of New England) for Council.

Thus, taking account of pre-determined positions, officers standing for reelection, and new nominations, the proposed composition of Council and Standing Committees for the term beginning November 1992 is:

President: D.C. Creagh (University College, ACT) *

Vice President: I.E. Grey (CSIRO, Port Melbourne) †

Secretary: M.R. Taylor (Flinders Univ.)

Treasurer: G. Smith (QUT) †

Council: C.J. Howard (ANSTO, NSW) *

W.T. Robinson (Univ. of Canterbury, NZ) *
M.A. Spackman (Univ. of New England) †

J.W. White (Research School Chem., ANU) *

ANCCr representative:

(ex officio)

Past President: A.H. White (University of WA) *

Nominations M. Sterns (ANU, Canberra) *

Standing Committee: B.M.K. Gatehouse (Monash University, Vic.) *

S.W. Wilkins (CSIRO Materials, Vic.) ‡

† new nomination

The invitation is now extended for any member to submit additional nominations for any of the positions for which vacancies will occur, i.e. for all but pre-determined positions.

Nominations must be submitted to the Secretary, over the signatures of two members, by the 30th June 1992. If none are received, the candidates nominated by the Nominations Committee will be deemed to have been elected and will take office at the Business Meeting in November 1992.

G.A. Williams, Secretary Australian Radiation Laboratory, Lower Plenty Road, Yallambie, Vic. 3085

^{*} pre-determined position

^{*} officer standing for re-election

BUSINESS MEETING - PROPOSED AGENDA

- 1. Apologies.
- 2. Minutes of previous Business Meeting, 4th April 1991, Armidale.
- Business arising from the Minutes:
 membership of FASTS to be reviewed.
- 4. President's Report.
- Treasurer's Report.
- 6. Report from the Chairman, National Committee for Crystallography.
- Report from Syd Hall on the inaugural AsCA meeting.
- 9. Date and venue for the Crystal 18 Meeting.
- 10. Any other business.
- 11. Report from the Nominations Committee and transfer to the new Council.

IMPORTANT MESSAGES - MAY 1992

Subscriptions Now Due

Members are reminded that subscriptions (\$20 full member, \$3 student member) for 1992 are due and should be paid immediately (see p.21, March Newsletter). Many members are one year in arrears, and such outstanding dues should be paid at the same time.

** Please Note **

A number of 'members' are more than one year in arrears and, technically, are no longer members of the Society. Such non-financial members are clearly ineligible to nominate or vote in the coming Council elections. If you are in this situation (the last two digits on your address label indicate the last year for which you are paid up) then it can be rectified by sending the appropriate outstanding dues plus 1992 subscription to the Treasurer.

Send subscriptions to:

Dr Colin Kennard

Department of Chemistry University of Queensland St. Lucia, QLD 4067

Abstracts for AsCA'92

True to tradition, Australians are leaving their Abstracts for the AsCA'92 Conference to the last minute. The organisers would appreciate receiving our Abstracts as early as possible please ... deadline July 15th.

MISCELLANEA

Travel Grants for Access to Major Overseas Research Facilities

The International Science & Technology Advisory Committee (ISTAC) travel grants initiated by DITAC as a direct result of the ANCCr 'Big Science' Report in 1989 are now administered by ANSTO on behalf of DITAC. The new title of the grants is Access to Major Research Facilities Program Grants. Applications should be addressed to the Executive Director, ANSTO, Private Mail Bag 1, Menai, NSW 2234.

It is of the utmost importance that the Program continues to receive a steady stream of applications for high-quality research at advanced radiation (synchrotron and high-flux neutron) sources by Australian crystallographers and their postgraduate students. If crystallographers do not demonstrate an urgent and legitimate need for the funds, others will.

Synchrotron Research Update

SPring-8: New Synchrotron Radiation Source

Japan Atomic Energy Research Institute (JAERI) and The Institute of Physical and Chemical Research (RIKEN) are building a new synchrotron radiation source at Nishi-Harima district in Hyogo Prefecture, 100 km west of Osaka. The facility, named SPring-8 (Super Photon Ring-8 GeV), plans an 8 GeV storage ring with a 1436 m circumference, an injector linac of 1 GeV and an 8 GeV synchrotron. The design of the storage ring has recently been finalised. Construction work started in 1990 and the first stored beam is foreseen in 1998. Out of the 51 planned beamlines, 10 will be commissioned in the first period. For further details, contact Dr Hiromichi Kamitsubo, Director General, JAERI-RIKEN SPring-8 Project Team, 2-28-2 Hon-Komagome, Bunkyo-ku, Tokyo 113, Japan.

Australian Proposal

Dr Ted Maslen (Crystallography Centre, Univ. of W.A.) is seeking ARC support to investigate the feasibility of establishing a small synchrotron radiation facility tailored to Australian needs. It has been suggested that this would be an appropriate national project. Relevant points are:

- · demand is growing faster than synchrotrons are being built;
- an examination of experiments being performed at the Photon Factory indicates that while none could be done with conventional X-ray tube sources, only ca. 15% use the full potential of the synchrotron beam.

Third generation synchrotrons provide ca. 10^6 times as many photons as conventional sources. The proposal is for a less-ambitious facility (eliminating superconducting magnets as it is now technologically feasible to use new permanent magnets, and with improved wigglers, undulators and insertion devices). For example, a conventional synchrotron of 4-5 m diameter and providing intensities 100 to 10,000 times those of conventional sources might cost ca. \$70 million. Ted would like expressions of interest from those in Australia interested in using such a facility, or knowledgeable on aspects of design. Contact Ted on (09) 380-2727 or fax (09) 380-1118.

FORTHCOMING MEETINGS

May 26-29, 1992. IUCr CPD Conference 'Accuracy in Powder Diffraction II'; Gaithersburg, USA. Contact Dr R.J. Hill, Division of Mineral Products, CSIRO, P.O. Box 124, Port Melbourne, Vic. 3207

May 29-June 7, 1992. NATO Advanced Study Institute 'Modern Perspectives in Inorganic Crystal Chemistry'; Erice, Italy. <u>Contact</u> L. Riva di Sanseverino, Dept. Mineralogical Sciences, Bologna University, 1 40126 Bologna, Italy.

June 1-7, 1992. IUCr Veszprem School on Crystallographic Computing; Veszprem, Hungary. Contact Dr Kalman Simon, Hungarian Chemical Society, H-1027-Budapest, Fo u. 68, Hungary.

August 2-8, 1992. European Crystallographic Meeting ECM 14; Twente, The Netherlands.

August 3-7, 1992. 41st Annual Denver X-Ray Conference: Applications of X-Ray Analysis; Colorado Springs, USA. <u>Contact</u> Dr Paul Predecki, Dept. of Engineering, University of Denver, Denver, CO 80208, USA.

August 17-21, 1992. ICAS International Conference on Anomalous Scattering; Malente/Hamburg, Germany. Contact R. Frahm, Hamburger Synchrotronstrahlungs-labor at DESY, Notkestr. 85, D-2000 Hamburg 52, Germany.

August 30-September 5, 1992. The 4th International Conference on Biophysics and Synchrotron Radiation 'BSR92'; Tsukuba, Japan. Contact Prof. N. Sakabe, Photon Factory, KEK, Oho, Tsukuba, Ibaraki 305, Japan.

November 14-16, 1992. Asian Crystallographic Association Conference 'AsCA'92'; Singapore. Contact Prof. N. Kasai, Department of Applied Chemistry, Osaka University, 2-1 Yamadoka Suita, Osaka 565, Japan.

May 31-June 2, 1993. International Conference for Applied Mineralogy 'ICAM'93'; Perth. Contact Dr J. Graham, CSIRO Division of Mineral Products, P.O. Wembley, Western Australia 6014.

August 21-29, 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.

September 26-October 2, 1993. Australian X-Ray Analytical Association Conference 'AXAA-93 Solutions to Everyday Problems'; The University of Queensland, Brisbane. Contact Tony Raftery, (07) 864-3271.

4th International Conference on Biophysics and Synchrotron Radiation

Following the successful conferences at Frascati (1986), Chester (1988), and Stanford (1990), the 4th International Conference on Biophysics and Synchrotron Radiation will be held August 30 - September 5, 1992 in Tsukuba.

The aims of the conference are to stimulate new ideas for further advances in biophysics and to act as a forum for the exchange of information. The scientific program will include plenary lectures and oral and poster presentation sessions in both biophysical subjects and technical aspects. Further information is available from Prof. Hans Freeman or Geoff Williams.