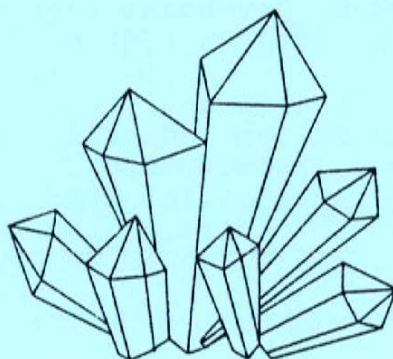


SOCIETY OF CRYSTALLOGRAPHERS  
IN AUSTRALIA

NEWSLETTER No.17



CRYSTAL XVI  
LORNE, VIC.

SEPTEMBER 1988

**SOCIETY OF CRYSTALLOGRAPHERS IN AUSTRALIA**

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 M.F. Mackay (La Trobe Univ.)  
 S.R. Hall (Past President; Univ. of W.A.)  
 H.C. Freeman (Ex officio ANCCr rep.; Sydney)

Nominations M. Sterns (ANU)

Standing Committee: B.M.K. Gatehouse (Monash Univ.)  
 S.W. Wilkins (CSIRO, Chemical Physics)

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

**IMPORTANT MESSAGES**

1. The registration form for the Crystal XVI meeting at Lorne in February 1989 is included with this newsletter; return form ASAP to Dr. Maureen Mackay at La Trobe University if attending.
2. Annual subscriptions for 1989 are now due and a form to accompany payment is included with this newsletter; pay promptly to be eligible for the discount rates!
3. The current term of office for Council Officers expires at the National Meeting to be held in February 1989. Nominations are called for the positions of Vice President, Secretary, Treasurer, and Council (see later in Newsletter). Nominations proposed by the Nominations Committee for all vacancies are presented in this newsletter.
4. The impending resignation of Neil Isaacs as Vice President will cause a casual vacancy, and Council has accepted the recommendation of the Nominations Standing Committee of Prof. John White (ANU) to fill the short-term vacancy. Prof. White will then assume the office of President for the next term.



## COUNCIL NEWS

A meeting of the SCA Council was held in Melbourne on the 27th April 1988. Council news and decisions taken by Council at that meeting and subsequently include:

Professor Jack Dunitz has accepted the invitation to attend the Crystal XVI meeting, to be held at Lorne in February 1989, as the first '1987 Fellowship' recipient. He will also present the Dwyer lecture in Sydney, the Birch lectures at ANU, and an RACI talk in Melbourne on the 22nd February. Prof. Dunitz will also be visiting Adelaide and Perth.

Two eminent protein crystallographers (Drs. J.M. Hogle and R.E. Hubbard) will attend jointly the Protein and Crystal meetings in Lorne.

As per the President's Message in the previous Newsletter, Council intends to award a number of '1987 Studentships' to postgraduate students wishing to attend Crystal XVI and who would appreciate some form of financial assistance. Thus, Council invites applications and it is suggested that students write ca. one page giving a description of their research project and telling what benefits they would anticipate from attending Crystal XVI. Forward to the Secretary by end of October, together with a covering letter from one's supervisor verifying that the applicant is a bona fide student at the time of the meeting.

Council has accepted the offer of an extra SCA representative on the ANCCr, and has nominated Prof. Syd Hall as the SCA representative for the next three years. In return, the Chairman of the ANCCr or his delegate has been invited to attend and participate in SCA Council meetings in an ex officio capacity, without formal voting rights.

Council has commissioned Professor Sandy Mathieson to undertake the preparation of "The History of Crystallography in Australia". This should result in a medium-sized book of, say, 300 pages including photographs. It is envisaged that the project will be completed with release of the book at or prior to Crystal XVII.

## PEOPLE

Prof. Allan White of the Department of Physical and Inorganic Chemistry at the University of Western Australia was awarded the 1987 RACI H.G. Smith Medal for his work in structural inorganic chemistry. Allan has determined the structures of nearly 1000 compounds, and has published more than 500 papers. His structure determinations have been used to make important advances in coordination chemistry, chemical bonding, organometallic chemistry, systematic structural chemistry and in the properties of materials. Congratulations Allan!

A constitutional crisis of some magnitude was precipitated by the news that Neil Isaacs has accepted the foundation Joseph Black Chair of Protein Crystallography at Glasgow University. Neil leaves his present position as senior research fellow at St. Vincents Institute of Medical Research in Melbourne for Glasgow in December. Not only is Australia losing a leading crystallographer and medical researcher, but the SCA is losing its Vice President (and hence next President)! However, congratulations and best wishes must go to Neil, and thanks for his service to the Society.

For all those still pondering the disappearance of Syd Hall, we can report that he has been sighted alive and well in West Germany. Sorry Syd to blow the cover, but the contact address until April '89 is:

Prof. S.R. Hall  
Rontgenlabor  
Max-Planck-Institut für Kohlenforschung  
Lembkestrasse 5  
D-4330 Mulheim a.d. Ruhr  
FRG (West Germany) Fax: (49)208-306 407

We are pleased to welcome four new members - Dr. Katherine Smith works in materials science at ANSTO, with major interests in ceramics and minerals. Also from ANSTO is Ms. Kathleen Hawkins, who works in the areas of transmission electron microscopy and X-ray diffraction. And a third new member from ANSTO is Mr. Robert Knott of the Applied Physics Division, with interests in structural biology and neutron scattering. Ms. Vilma Zubak is an Honours graduate from Hans Freeman's group at the University of Sydney, and is now with Peter Colman and working for a Ph. D. degree from the University of Melbourne.

Dave Stuart and Yvonne Jones of the Laboratory of Molecular Biophysics at Oxford University will be at CSIRO Division of Materials Science and Technology (Clayton, Vic.) for five weeks from the 30th September. Dave has recently been involved in the determination of the structure of the foot-and-mouth virus.



\*\*\*\*\* ANNUAL SUBSCRIPTIONS NOW DUE \*\*\*\*\*

All SCA members are informed that annual membership subscriptions for 1989 are now due. Please use the form below to accompany your payment, and remember that prompt payment will entitle you to the discount rates.

The subscription rates for 1989 are \$20 for full members and \$3 for student members. A discount of \$5 (full) or \$1 (student) applies for members who pay before 1st April 1989.

Some members are in arrears for previous years. If uncertain, the last number on your address label indicates the year to which your subscription is paid up (i.e. 88 for currently financial members). Check, and please take this opportunity to pay all outstanding monies. In the event of any disputes, please contact the Treasurer [Dr. Colin Kennard, ph. (07)377-3296].

.....

Forward to: Dr. C.H.L. Kennard  
Department of Chemistry  
University of Queensland  
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## \*\*\*\*\* COUNCIL ELECTIONS AND BUSINESS MEETING \*\*\*\*\*

Members are advised that a SCA Business Meeting will be held during the Crystal XVI National Meeting of the Society in Lorne, Victoria in February 1989. At present, it is anticipated that the Business Meeting will be held at 1630 on Saturday 18th February 1989.

This National Meeting brings with it the end of the current terms of election of Dr. Peter Colman (President), Prof. Syd Hall (Past President) and Dr. Bob Cheary (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 Prof. Allan White (Univ. of W.A.) for Vice President and Dr. Chris Howard (ANSTO) for Council.

Thus, taking account of pre-determined positions, officers standing for re-election, and new nominations, the proposed composition of Council and Standing Committees for the term beginning February 1989 is:

President:	J.W. White (RSC, ANU) *
Vice President:	A.H. White (Univ. of W.A.) +
Secretary:	G.A. Williams (ARL) #
Treasurer:	C.H.L. Kennard (Univ. of Qld.) #
Council:	J. Graham (CSIRO Mineralogy, W.A.) *
	M.F. Mackay (La Trobe Univ.) *
	C.J. Howard (ANSTO) +
Past President:	P.M. Colman (CSIRO, Protein Chemistry) *
Nominations	B.M.K. Gatehouse (Monash Univ.) *
Standing Committee:	S.W. Wilkins (CSIRO, Mat. Sci.) *
	M. Sterns (ANU) #

\* pre-determined position  
# officer standing for re-election  
+ 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 28th October 1988. If none are received, the candidates nominated above will be deemed to have been elected and will take office at the Business Meeting in February 1989.

G.A. Williams, Secretary



## FORTHCOMING MEETINGS

October 10-14, 1988. Computational Methods in Chemical Design, Molecular Modeling, Theory and Experiment; Schloss Elmau nr. Garmisch-Partenkirchen, FRG. Contact Prof. Dr. Carl Kruger, Max-Planck-Institut, Kaiser-Wilhelm-Platz 1, Mulheim a.d. Ruhr D-4330, FRG.

November 25, 1988. The History of Chemistry in Australia; CSIRO, Clayton. Contact John Spink, CSIRO Division of Materials Science and Technology, Locked Bag 33, Clayton, Vic. 3168

December 19-21, 1988. International Conference on Modulated Structures, Polytypes and Quasicrystals; Varanasi, India. Contact Dr. D. Pandey, School of Materials Science and Technology, Institute of Technology, Banaras Hindu University, Varanasi 221 005, India.

February 16-19, 1989. Crystal XVI Meeting of the Society of Crystallographers in Australia; Erskine House, Lorne, Victoria. Contact Dr. M.F. Mackay, Department of Chemistry, La Trobe University, Bundoora, Vic. 3083

June 13-15, 1989. International Workshop on the Rietveld Method; Petten, The Netherlands. Contact Public Relations Office, NERF, P.O. Box 1, 1755 ZG Petten, The Netherlands. A few copies of the First Circular are available from Geoff Williams, SCA Secretary [tel. (03)433-2211].

July 2-7, 1989. XXVII International Conference on Coordination Chemistry; Gold Coast, Queensland. Contact ICC Secretariat, UniQuest Limited, University of Queensland, St. Lucia, Qld. 4067

July 19-28, 1990. Fifteenth General Assembly and International Congress of Crystallography; Bordeaux, France. Contact Prof. M. Hospital, Laboratoire de Cristallographie et de Physique Cristalline, Universite de Bordeaux 1, 351 Cours de la Liberation, F-33405 Talence, France.

July 29-31, 1990. Application of synchrotron and neutron radiation to the diffraction analysis of nuclear and magnetic structures; Grenoble, France.

July 29-August 5, 1990. Summer School on Crystallographic Computing; Strasbourg, France. Contact Dr. D. Moras, Lab. de Cristallographie Biologique, IBMC, 15 rue Descartes, F-67084 Strasbourg Cedex, France.



## MISCELLANEA

On 11th August, Prof. Allan White delivered the RACI Smith Medal Lecture in Melbourne at La Trobe University. Allan began by querying the structure of  $\text{Ag}(\text{NH}_3)_2\text{Cl}$ , and then led a fascinating journey through a series of far from simple structures of complexes of the coinage metals [Ag(I), Cu(I)] with various amines and halogens. He concluded with some analogous Group I complexes, and the heresy that the Li ion appears larger than Cu(I). We were all left with the view that  $\text{Ag}(\text{NH}_3)_2\text{Cl}$ , if not life itself, is considerably more complicated than we had previously preferred to believe.

Postgrad. students are reminded that a number of '1987 Student-ships' are to be awarded by Council to help with the costs of attending Crystal XVI in Lorne next February. Details of how to apply are given above under 'Council News'.

The Australian Journal of Physics has just published two special conference issues which will be of interest to many readers. The first is X-ray Powder Diffractometry (International Symposium, Fremantle, Australia, 20-23 August 1987), price \$50, and the second is Accuracy in Structure Factor Measurement (International Symposium, Warburton, Australia, 23-26 August 1987), price \$45. These journals are available from the Publications Sales Office, CSIRO, 314 Albert Street, East Melbourne, Vic. 3002. Prices include postage; cheques are payable to 'Collector of Moneys CSIRO'.

**Cambridge Crystallographic Database** - At present it appears that sufficient subscribers have been found at \$750 p.a. (\$1,500 for commercial users) to continue with the database in Australia. This relatively low subscription charge is dependent on 100% participation by all those who have given a commitment. If any have not yet sent the money to David Winkler (CSIRO Division of Chemicals and Polymers) please do so forthwith. The SCA Council will continue to monitor the situation closely to ensure that Australia does not lose access to this valuable resource, if at all possible.

**Membership** - There has been a steady trickle of new memberships. Please put any prospective new members in touch with the Secretary for membership details and application forms.

**New IUCr Commission on Powder Diffraction** - At its August 1987 meeting in Perth, the General Assembly of the IUCr established a Commission on Powder Diffraction. The Australian member of the new Commission is Dr. Rod Hill of CSIRO Division of Mineral Chemistry. The first newsletter of the new Commission was produced in January this year, and those wishing to receive future copies should write to Dr. J. Langford, Dept. of Physics, University of Birmingham, Birmingham B15 2TT, England.

TOWARDS ROUTINE ACCESS TO SYNCHROTRON RADIATION  
FACILITIES BY AUSTRALIAN SCIENTISTS

D.C. Creagh  
Royal Military College, Duntroon, A.C.T.

### Background

For about three years discussions have been held between Australian and Japanese scientists with a view to the provision of an Australian experimental hutch on a beam line at the synchrotron radiation source at the Japanese Centre for High Energy Physics, Tsukuba, Japan.

An Australian Research Grants Committee proposal [Creagh, Barnea & O'Connor (1986)] was not funded but funds were made available to hold a workshop on synchrotron radiation. This was organised by Stephen Wilkins (Melbourne, 1987). It was attended by a number of eminent users of synchrotron radiation from England, U.S.A., Japan and Germany as well as local users and potential users of synchrotron radiation sources.

As a result of this workshop two courses of action have been followed. In the first, another Australian Research Committee proposal for funding has been made [Barnea, Creagh & Sabine (1988)]. This proposal seeks funding to investigate a number of issues connected with the future use of synchrotron radiation sources, for example what sort of instrumentation is required, where might our instrument be sited, and what costs might be involved?

The second was a decision to keep up discussion with our Japanese colleagues on the beam line proposal so that we might best be able to formulate a proposal which serves Australian requirements and fulfils a need to the Photon Factory. A description of the present status of this project forms the bulk of this article.

Unrelated to this is a decision by the National Committee on Crystallography of the Australian Academy to investigate the need for the use of overseas "big science" facilities. Members of the SCA will be aware of the circular letter and questionnaire which Hans Freeman has recently had sent to all members.

It is essential that all members answer this questionnaire fully. If they do not the case for Australian access to synchrotron radiation facilities will be irreparably harmed.

### The Australian-Japanese Proposal

For any proposal to build an instrument at a synchrotron radiation source to succeed it is necessary to determine what instrument is deemed most desirable by the host institution.



After considerable investigation it has been established that the Japanese lack a versatile high-resolution powder diffraction system.

The emphasis here is on the words versatile and high resolution. Each beam station has to provide a proportion of its time for other users and the Japanese believe that its construction would considerably enhance the range of options open to their own researchers. By the same token Australian scientists would have right of access to all the other stations at the Photon Factory.

Expertise exists in Australia for the design of such an instrument and the preliminary design considerations have been addressed by Stephen Wilkins and myself. Sabine (1987) has proposed a design to be implemented at HASYLAB.

The key to versatility in an instrument is the design of the monochromator system. This system must optimise the flux incident on the specimen at a particular wavelength and have provision for the tailoring of the incident beam cross section. At the Photon Factory the beam line we would be offered is beam line 18C which emerges from a bending magnet. The optimum scattering plane from this line is the vertical plane since the beam is linearly polarised in the horizontal plane. This implies that the axes of the principal monochromator elements are horizontal. The monochromator consists of a primary and a secondary stage.

The operational range of the primary monochromator system would be 5 to 25 keV with good harmonic rejection and an energy resolution of better than 2 eV. A choice of silicon or germanium diffracting elements would be available. A schematic diagram of the primary monochromator, available from the author, indicates that by moving the primary axis out of the beam the white beam can pass through into the experimental hutch. This enables experiments such as X-ray topography to be undertaken. Axes 1 and 2 can be rotated and translated under computer control setting the monochromator elements to the appropriate positions for selection of the desired photon energy [Creagh (1988)].

When the beam emerges from the second monochromator it is well collimated in the vertical plane but somewhat divergent in the horizontal plane. Slit systems are usually used to reduce the horizontal divergence. This is a cheap expedient but there is a loss in photon flux. An extension to the design would enable the ability to condense the horizontal divergence of the beam either by totally reflecting mirrors or by sagittal Bragg reflecting collimators.

A secondary monochromator of the condensing Bragg optics type [Wilkins (1987)] would be able to be located in the beam for those applications in which highly collimated beams with small

cross-sectional area are required. Such experiments include high-resolution powder diffractometry and small-angle X-ray scattering.

For the X-ray diffractometer system a high capacity Huber theta-2theta diffractometer (type 422) would be chosen since these are the basic building blocks on which most experimental systems at synchrotron radiation sources are constructed. Both high- and low-temperature specimen holders would be available for use.

A variety of methods for detection of the scattered intensity would be made available. For high-resolution powder diffractometry the choice would be between the following:

the Fuji X-ray plate system [Miyahara et al. (1986)], data from which can be extracted digitally by use of a laser-diode detector flying spot scanner system;

a curved position-sensitive detector system [Shushiguchi et al. (1986)];

a conventional sodium iodide detector mounted on the 2theta arm; and

a solid-state detector system (for use primarily in energy-dispersive white beam experiments).

In the small-angle X-ray scattering mode, the choice would be either a Fuji plate system or a linear position-sensitive detector system.

The overall system is extremely versatile and should enable experiments to be undertaken in all fields of scientific endeavour. Those involved in the study of ceramic materials (high  $T_C$  superconductors, SYNROC etc.) would find the system equally as useful as those involved in the study of biological materials (oncology, biology etc.). A brief summary of the fields of research which could be undertaken by use of such a system has recently been given [Creagh (1988)].

The cost of the proposal is not astronomical. I expect that the total cost, inclusive of all Photon Factory demands, would be not more than \$900,000. There would be no charge for beam use. The cost of the installation is considerably less than the per annum running cost in the Photon Factory of a beam line.

Conditions which may be encountered by visitors to the Photon Factory are first rate; accommodation is excellent and living costs are quite low. The differences in language and culture are apparently great, but in all my visits I have not yet encountered any difficulty in these respects. Also one suffers no jet lag on the trip. It is possible to commence work on arrival, a



situation which does not easily occur with any other synchrotron radiation facility.

### Conclusion

Although a substantial part of the preliminary design of an experimental station has been completed it will never reach completion unless you, the members of the SCA, dedicate some of your time making a response to Hans Freeman's questionnaire.

### References

- Creagh, D.C. (1988) Aust. J. Phys., 43, 2.
- Miyahara, J., Takahashi, K., Amemiya, Y., Kamiya, N., and Satow, Y., (1986) Nucl. Instrum. Meth., A246, 572.
- Sabine, T. (1987) J. Appl. Cryst., 20, 173.
- Shushiguchi, S., Minato, L., and Hashizume, H. (1986) J. Appl. Cryst. 19, 420.
- Wilkins, S. (1987) patent pending.

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**WORLD DIRECTORY OF CRYSTALLOGRAPHERS**  
and of Other Scientists Employing Crystallographic Methods

**Eighth Edition**

Those people interested in having an entry in the eighth edition of the World Directory or modifying their entry from the seventh edition, and who have not already been contacted, are asked to contact the Australian Sub-Editor, Andrew Stevenson, at CSIRO Division of Materials Science and Technology, Locked Bag 33, Clayton, Vic. 3168; phone (03)542-2917. This may be the case if you have changed address or your location has changed its name, and the letter sent hasn't found you yet!

Anyone knowing of someone in Australia (other than SCA members) who might be interested in having an entry in the World Directory is asked to contact Andrew Stevenson or make the person aware of this notice.

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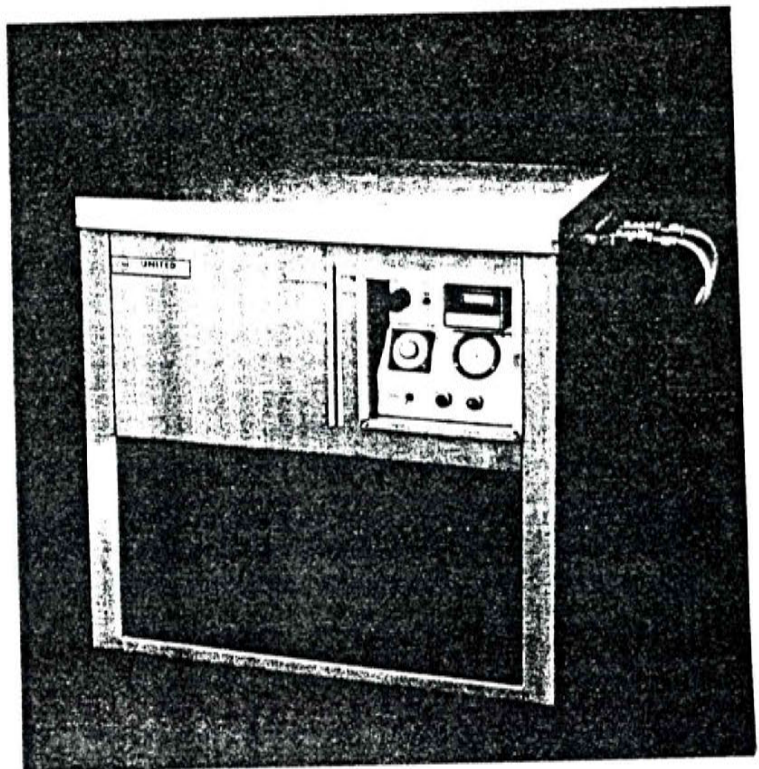
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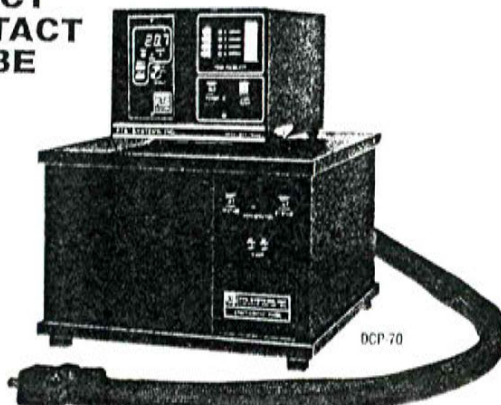
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### RECIRCULATING COOLERS



### DIRECT CONTACT PROBE



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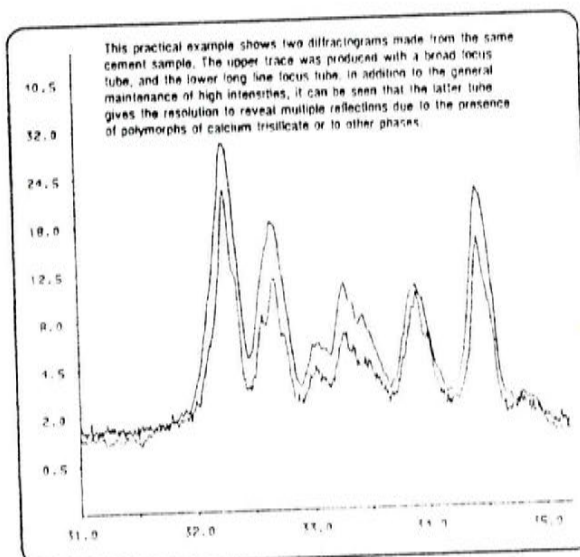
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