

subs posted  
8/11/78

A message from your President:

September 11, 1978.

Dear SCA Member,

I have just returned from the Warsaw meeting and report briefly on matters concerning the Society of Crystallographers in Australia.

The Eleventh International Congress was held at the Palace of Culture and Science and attended by about 1500 participants. To my knowledge there were 21 Australian crystallographers at the meeting and we behaved ourselves, fairly well. The scientific programme consisted of a General Lecture each morning from 9.00 a.m. to 10.00 a.m., followed by four parallel Oral Sessions from 10.20 a.m. to 13.00 p.m. Poster sessions were held each day from 14.30 p.m. to 18.00 p.m. There was a very well organised Exhibition of Crystallographic Equipment together with a separate Non-Commercial Exhibition of crystallographic data files, photographs concerning visual aspects and the teaching of crystallography, crystallographic equipment etc. There was also a Book Exhibition. The Congress had a lot to offer and copies of the programme and abstracts should be available from any of the Australian delegates. There will be a report at our next meeting, Crystal 12.

The General Assembly met on four occasions and considered 24 items of business. China and the Arab Republic of Egypt were admitted as new member countries of the Union. The Union also considered applications for membership of the Union as Associated Organisations. The International Organisation for Crystal Growth (IOCC) was subsequently admitted as a Scientific Associate of the Union and the European Crystallographic Community (ECC) as a Regional Associate of the Union. Representatives of such Associate Organisations may attend General Assemblies of the Union to take part in the discussions, but not in the voting.

This decision suggests that other countries or scientific bodies may form Regional Groupings (viz. Australia, Japan, China and India) to enter into more formal arrangements with the International Union. The roles of the Australian Academy, the National Committee for Crystallography and the Society of Crystallographers in Australia would have to be clarified in order to proceed with such an affiliation.

It was agreed that the Eleventh General Assembly could both set the time and place for the Twelfth General Assembly for 1981 and provisionally set the time and place for the Thirteenth General Assembly for 1984. The invitations from Ottawa, Canada (1981) and Hamburg, West Germany (1984) were accepted. Australia did not formally bid for the 1984 meeting since the Australian Academy was not prepared to support an invitation without the formal agreement of the SCA to co-sponsor and share the organisation. Informal discussions at Warsaw indicated that Australia would be a most acceptable venue for the Fourteenth General Assembly. Would you please inform the secretary whether you wish us to become so involved. Perhaps you could include your reply with your subscription. I believe we have the expertise and enthusiasm to make 1987 a year to remember.

N.C. Stephenson  
President, SCA,  
N.S.W. Institute of Technology,  
P.O. Box 123,  
Broadway, N.S.W. 2007

Secretary's Notes:

The Constitution of the Society, as revised at the Bendigo Meeting, is enclosed. The dates for the next meeting of the Society, Crystal XII, have been arranged by your Officers in conjunction with two other meetings of possible interest to you as follows:

- [1] Crystal XII, Canberra, Wednesday 30th January - Saturday 2nd February 1980. Organiser: Mr. George McLaughlin, Research School of Chemistry, A.N.U., P.O. Box 4, A.C.T. 2600.
- [2] RACI COMO Division Meeting, University of New South Wales, Sunday 3rd February to Thursday 7th February 1980. Organiser: Dr. Ian Dance, Chemistry School, Univ. N.S.W., P.O. Box 1, Kensington, N.S.W. 2033.
- [3] X-Ray Analytical Society Meeting (to be held in Canberra at the same time as COMO). Organiser: Dr. V. Manners, Building 4, N.S.W.I.T., P.O. Box 123, Broadway, N.S.W. 2007.

It is hoped that this conjunction of meetings will be helpful for members from outside NSW to minimise their travel costs. George McLaughlin would like to hear of theme suggestions and of possible visitors for Crystal XII. Contact George directly.

The National Committee for Crystallography has considered the question of applying to hold the 1987 Congress in Australia. The Academy of Science would accept financial responsibility for the Congress but would wish the Society to join with it in sponsoring the event. I imagine that the brunt of the organisation would fall heavily on either Canberra, Melbourne or Sydney members. An opportunity for you to express an opinion on whether we should seek sponsorship for the 1987 Congress appears on the subscription slip. The opinions of Sydney, Melbourne and Canberra people are especially sought.

To help form your opinion, I have drawn up a partial list of arguments for and against:

- FOR
  - (i) Debt to scientific community discharged.
  - (ii) Brings upwards of 1000 active scientists into the country which will raise the standard of the subject.
  - (iii) Brings money into the country.
- AGAINST
  - (i) Very heavy burden on those running Congress. At least 20 people will lose two years research effort and a lesser contribution from forty more.
  - (ii) This will occur at a time when the universities will be very strained to meet their teaching and research commitments if current trends continue.
  - (iii) We are a small crystallographic community and perhaps should have smaller specialist symposia such as the one on Real Atoms in Real Crystals held some time ago in Melbourne.

A reminder that the joint meeting in Honolulu of the Chemical Societies of the USA, Australia, NZ and Japan takes place from 1st to 6th April 1979. Several of the symposia will interest Crystallographers and abstracts are to be in by 13th October 1978. Recent issues of *Chemistry in Australia* have

details. This meeting will be preceded by an International Meeting on Modulated Structures, March 22-25, at Kailua-Kona (contact Prof. Charles N. Caughlan, Dept. of Chemistry, Montana State University, Bozeman, Montana 59717), and by the American Crystallographic Association Meeting at the University of Hawaii, March 26-30 (the Program Chairman is Arthur Camerman, University of Washington, Seattle WA 98195).

Dr. Peter Goodman of the Committee on Electron Diffraction has asked me to circulate the enclosed information on space-group determination by electron diffraction. He and Andy Johnson have collaborated with various inorganic crystallographic laboratories since the Bendigo meeting in solving space-group problems intractable by X-ray methods. They are prepared to undertake further problems in collaboration (P.O. Box 160, CLAYTON, Vic. 3168).

Dr. Bruce Poppleton and the CSIRO have been putting up the Cambridge Data file on the CSIRO CDC7600 and the full file is now available. Interested users can obtain information from Bruce, CSIRO Division of Applied Organic Chemistry, P.O. Box 4331, MELBOURNE, Vic. 3001.

I hope the next mailing will appear in May 1979 with the first Crystal XII circular. Please let me know of material you want circulated before 1st May 1979. We could also advertise positions vacant and surplus equipment for sale or trade.

The Society now has 163 members: new members can be joined in accord with Article III, Section 1 of the Constitution and their name, address, interests and fee, should be sent to the Treasurer.

M.R. Snow  
Secretary, SCA

Department of Physical & Inorganic Chemistry,  
The University of Adelaide,  
ADELAIDE, S.A. 5001

#### Treasurer's Notes:

The first annual statement of the Society's finances is enclosed. The accumulated funds are in a healthy state, and income of at least another \$1500 can be expected before the Crystal XII meeting. Two thousand dollars has been invested with the Finance Corporation of Australia Limited (a wholly-owned subsidiary of the Bank of Adelaide) in debenture stock at 10½% interest p.a. paid quarterly, maturing on 21/4/80.

A number of members who joined in the first year (1976) and who have not paid a subscription since then, are being circularised for the final time before the provisions of the constitution will be applied.

M.R. Taylor  
Hon. Treasurer, SCA

THE SOCIETY OF CRYSTALLOGRAPHERS IN AUSTRALIA

Statement of Income and Expenditure for the year ended  
30th June, 1978

<u>INCOME</u>	\$	\$
Membership Subs.	823	
Membership Subs. paid at Bendigo	56	
Savings Bank Interest	27	
Interest on FCA debs.	40	
Crystal XI - Surplus	<u>511</u>	1457
 <u>LESS EXPENDITURE</u>		
Stamp Duty on Cheques	10	
Stationery	<u>2</u>	<u>12</u>
Surplus for year transferred to Accumulated Funds		<u>1445</u>
		<u>\$1457</u>

Balance Sheet as at 30th June, 1978

<u>ACCUMULATED FUNDS</u>	\$	\$
Balance as at 30.6.77	878	
Add surplus for this year	<u>1445</u>	<u>2323</u>
 <u>THESE FUNDS ARE REPRESENTED BY CURRENT ASSETS</u>		
Finance Corp. of Aust. Ltd. debs.	2000	
Bank of Adelaide Savings Account	320	
Petty Cash	<u>3</u>	<u>2323</u>
 <u>LIABILITIES</u>		
-	-	<u>-</u>
		<u>\$2323</u>

10/9/78

(signed)

M.R. TAYLOR  
Hon. Treasurer

## SPACE-GROUP DETERMINATION BY ELECTRON DIFFRACTION - I.

Electron diffraction provides a means of space-group determination independent from that provided by X-ray diffraction. The electron diffraction method proceeds from the fact that a set of reflections (belonging to a zone) can be excited simultaneously and that n-beam scattering is important in first order. The characteristics of n-beam scattering permit a unique determination in most cases. This is true even under the restriction commonly met in electron diffraction, namely the availability of only one principle setting, determined by a particular cleavage habit. Space-group symmetry elements can be identified from convergent beam diffraction pattern symmetries. Vertical mirror planes and vertical rotation axes are directly identifiable in the zone-axis pattern, while the elements of centro-symmetry, horizontal two-fold axes and horizontal mirror planes are identifiable indirectly, from symmetries imposed on particular diffraction orders.

Convergent beam electron diffraction analysis is of particular value in detecting slight deviation from symmetry. This is because of amplification of the asymmetric element in the pattern by dynamic scattering in a sufficiently thick and perfect crystal, and because of the sensitivity of the eye to small deviations from exact pattern symmetry. It is therefore particularly suited to detecting slight deviations from an ideal structure such as frequently occur in mineralogy.

The only indeterminacies in the electron diffraction method are those associated with n-fold axes with  $n > 2$ . These arise because there is no general requirement, with dynamic scattering, for the systematic reflections  $00l$  ( $l \neq m.n$ ), associated with a horizontal n-fold screw axis, to be absent though they would generally be very weak under conditions which avoid exciting a full zone of reflections.

Finally, it is necessary to appreciate that the electron diffraction method actually measures the symmetry properties of the crystal as a whole\* with its relationship to the incident beam, rather than simply the unit cell symmetry of interest to the crystallographer. The main complications which this introduces are those due to stacking faulting, and to highly tilted crystal surfaces. It is therefore necessary to use an unfaulted crystal region, and crystal orientations which correspond, or are close to, perpendicular beam incidence on the single crystal platelet, dependent upon the precision required in the result.

References: Goodman: *Acta. Cryst.*, A31, 804-810 (1975).

Buxton, Eades, Steeds and Rackham: *Phil. Trans. Roy. Soc. (London)* A354, 137-244 (1977).

Jones, Rackham and Steeds: *Proc. Roy. Soc. (London)* A354, 137-244 (1977)

Goodman: *Inst. Phys. (London) Conference No. 31*, 1978).

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Footnote: \*For the purposes of these measurements the crystal may be regarded as a plate of infinite extension, *i.e.* the sideways boundaries (lying outside the region of irradiation) have no influence on the symmetry of the pattern, and we are only concerned here with horizontal, external or internal, boundaries.