

Society of Crystallographers

in

Australia

Newsletter No. 4

MARCH 1982

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The following members of the SCA were approved as Office Bearers for 1982/83 at the Annual General Meeting held at Cromwell College, University of Queensland on February 4th, 1982.

President: B.M.K. Gatehouse (Monash Univ.)
Vice President: T.M. Sabine (NSWIT)
Secretary: R.J. Hill (CSIRO Min. Chem.)
Treasurer: M.F. Mackay (LaTrobe Univ.)
Council: Z. Barnea (Melb. Univ.)
W.T. Robinson (Univ. Canterbury, N.Z.)
F.H. Moore (AINSE)

Standing Committees (*Chairperson)

Electron diffraction: D.J.H. Cockayne (Univ. Sydney)*
P. Goodman (CSIRO Chem. Phys.)
A.W.S. Johnson (CSIRO Chem. Phys.)
J.R.J. Sellar (ANU)

X-ray Diffraction: R.B. Fraser (CSIRO Protein Chem.)*
I.E. Grey (CSIRO Min. Chem.)
J.M. Guss (Univ. Sydney)
S.W. Wilkins (CSIRO Chem. Phys.)

Neutron Diffraction: F.H. Moore (AINSE)*
V.J. James (Univ. NSW)
C.J. Howard (AAEC)

Computing: B.J. Poppleton (CSIRO AOC)*
S.R. Hall (Univ. W.A.)
N.W. Isaacs (St Vincents Sch. Med. Res.)
A.D. Rae (Univ. NSW)

Nominations: I.G. Dance (Univ. NSW)*
E.W. Radoslovich (CSIRO Soils)
S.L. Mair (CSIRO Chem. Phys.)
M.R. Snow (Univ. Adelaide)

ITEMS OF NEWS FROM THE 1982 ANNUAL GENERAL MEETING

i) 14th Meeting and General Assembly of the I.U.Cr., 1987

As proposed in an earlier SCA Newsletter (August, 1980), the SCA had its offer to host the 14th I.U.Cr. meeting formally accepted by the I.U.Cr. during the 12th meeting at Ottawa in August 1981. Members should note that while the Australian Academy of Science is willing to help with organizational and secretarial assistance, the financial responsibility for the meeting rests solely with the SCA.

The AGM approved Council's recommendation of Perth as the venue for the meeting. Dr E.N. Maslen has agreed to Chair the Organizing Committee formed to handle arrangements for the Congress. Other members are Professor H.C. Freeman (Program), Dr E.H. Nickel and Dr J. Graham. Correspondence of a specific nature relating to the I.U.Cr. meeting should be directed to Dr Maslen and not to the SCA Council.

ii) Amendments to the Rules of the Society

The AGM approved two amendments to the SCA Rules.

(a) Rule I, Section 1 amended to read (in part):

"The annual membership subscription shall be \$10.00."

(b) Rule I, Section 2 amended to read (in part):

"payment to arrive not later than November 30."

Both amendments are now in effect. Members who have paid in advance have the advantage of the lower rate.

iii) Incorporation of the Society

The AGM approved a motion to proceed with Incorporation of the Society in the State of South Australia, and for Dr M.R. Taylor to be the required Public Officer in this regard (Dr M.R. Snow in his absence). Members should note that the advantages of Incorporation are that it limits the financial liability of individuals, protects the name of the Society, and allows access to a greater range of financial institutions.

iv) The Society Prize

No prize of a trip to the I.U.Cr. meeting in Ottawa was awarded. Council is exploring alternative methods of assisting student members in the future.

v) Cambridge Crystallographic Data File

Although about nine groups around Australia have already agreed to commit \$800 towards the annual fee for this file there is still a large shortfall from the required \$10,000. Members are urged to approach any likely contributor groups within their Organization and to point out the wealth of potential information in the file and the relative ease of its extraction and manipulation for a host of applications in Organic Chemistry systematics.

vi) Crystal XIV Meeting

Mr H.R. Teitze has generously offered to coordinate the organization of the next meeting of the Society in August 1983. The most likely venue is the C.B. Alexander Agricultural College (Tocal) near Maitland about 20 km from Newcastle.

Treasurer's Reports for the 1980 and 1981 Financial Years

The following two statements of the Society's finances for the two financial years prior to the last AGM were presented by Dr M.R. Taylor and accepted by the 1982 AGM.

Statement of Income and Expenditure for the year ended
30th June, 1980

<u>INCOME</u>	\$	\$
Membership Subs.	531	
Savings Bank Interest	34	
Interest on FCA debts.	170	
Surplus from Crystal XII	<u>946</u>	1681
<u>LESS EXPENDITURE</u>		
Stamp duty	<u>6</u>	<u>6</u>
Surplus for year transferred to Accumulated Funds		<u>1675</u>
		<u>1681</u>

Balance Sheet as at 30th June, 1980

<u>ACCUMULATED FUNDS</u>		
Balance as at 30.6.79	3180	
Add surplus for this year	<u>1675</u>	<u>4855</u>
<u>THESE FUNDS ARE REPRESENTED BY CURRENT ASSETS</u>		
ANZ Savings Account	4852	
Petty Cash	<u>3</u>	4855
<u>LIABILITIES</u>		
-	-	-
		<u>\$4855</u>

(Signed) M.R. TAYLOR
Hon. Treasurer

Statement of Income and Expenditure for the year ended
30th June, 1981

<u>INCOME</u>	\$	\$
Membership Subs	607	
Savings Bank Interest	168	
Interest on FCA debts (from 24.11.80)	<u>230</u>	1005
<u>LESS EXPENDITURE</u>		
Stamp duty	6	
Postage	56	
Ottawa Travel Prize Publicity	<u>115</u>	<u>177</u>
Surplus for year transferred to Accumulated Funds		<u>828</u>
		<u>\$1005</u>

Balance Sheet as at 30th June, 1981

<u>ACCUMULATED FUNDS</u>		
Balance as at 30.6.80	4855	
Add surplus for this year	<u>828</u>	<u>5683</u>
<u>THESE FUNDS ARE REPRESENTED BY CURRENT ASSETS</u>		
Finance Corp. of Aust. Ltd. debts (maturing 24.11.83)	3000	
ANZ Savings Investment Account	1892	
ANZ Savings Account	625	
World Directory Account	161	
Petty Cash	<u>5</u>	<u>5683</u>
<u>LIABILITIES</u>		
-	-	-
		<u>\$5683</u>

2/7/81

(Signed) M.R. TAYLOR
Hon. Treasurer

Reminder from the Treasurer

The new Treasurer wishes to remind all those "members" with dues outstanding from previous years, including those who have paid for 1982, that these back dues should be paid as soon as possible, or their membership will lapse.

Report on the Crystal XIII Meeting

The Society of Crystallographers in Australia held their thirteenth meeting at Cromwell College, University of Queensland, from Tuesday 2 February to Friday 5 February 1982. Fifty-eight Crystallographers were registered and came from most Australian States and New Zealand.

A social between the Department of Chemistry of the UQ and Crystal XIII was the first item on the Agenda for Tuesday afternoon. David Hartley, a local businessman who started his own computer software company and now also makes his own hardware gave a talk dealing with the problems of developing and marketing his product in a field as competitive as "The Computer Business".

Wednesday morning saw the start of the Crystallographic papers with sessions on Large and Small Molecule Structure Determination. Featured lecturers were Hans Freeman on "X-ray Absorption Spectra of Oriented Metalloprotein Crystals", Joe Varghese on his enzyme "Neuramidase", and Jenny Glusker from the Institute for Cancer Research, Philadelphia, reviewing "Drug Receptor Interactions".

After lunch Ugur Ortabasi, from the Solar Research Centre of the UQ talked about "Materials Problems Associated with Alternative Energy Applications". The remainder of the afternoon was devoted to a workshop on Powder Methods, organized by Chris Howard and Rod Hill.

One of the highlights of the conference was the ferry trip that evening on the "Captain Cook" sponsored by Philips Scientific and Industrial Systems. This took place from 6.30 to 10.00 p.m., and the members of Crystal XIII saw a beautiful Brisbane by the river.

On Thursday morning the session on Solid State began with another featured lecturer, Stewart Anderson from the Australian National University, reviewing recent work on HRTEM Studies of Solid State Reactions. After this session the Hon. J. Moore, Minister for Business and Consumer Affairs in the Federal Parliament, officially opened the Conference and then discussed problems of science policy informally with those present.

The next session on Physics/Mathematics dealt with current developments in direct methods, disorder and electron diffraction. The afternoon meeting on Mineral Crystallography took place in the Julius Kruttschnitt Mineral Research Centre of the UQ where its director, Alban Lynch, discussed recent CSIRO initiatives in the interpretation of electron probe results for on-stream analysis of ores. Some members of Crystal XIII then went down the mine and inspected the research facilities before returning to Cromwell for the session on Charge Densities and the Annual General Meeting of the Society. The traditional dinner was held that evening at "Dirty Dicks" in Petrie Terrace, Brisbane.

The last day started with a display of Teaching software from Christchurch, and hardware from St Lucia, and a final session on Powder Diffraction featuring a lecture by Terry Sabine on "Structure Refinement from Pulsed Neutron Powder Data".

The choice of Cromwell College in February was a good one. The weather was good, the insect population low, and John Argus, the host at Cromwell, went out of his way to make Crystal XIII successful. Perhaps some of the novel things introduced at the meeting might be considered by others for the future:

- (a) The presentation of a brief oral "abstract" of their paper at the end of the appropriate formal Session by those individuals who had prepared a poster.
- (b) The use of a 15 seater microbus for ferrying purposes.
- (c) Replacement of the traditional biscuits at morning/afternoon tea with sliced pineapple, watermelon, pawpaw, apples, oranges etc.
- (d) Social gathering with an academic Department from the host University.

Colin Kennard

Inorganic Crystal Structure Database (ICSD)

The following information is extracted from a letter recently received from David Brown of McMaster University, Ontario.

Purpose: The ICSD will contain full numerical data for all inorganic crystal structures not included in the Organic Crystal Structure Database (Cambridge File) or in the Metals Data File (Ottawa). In the first instance the database will contain all structures published from 1972 onward.

Organization: The database is edited by Professor Dr G. Bergerhoff, Anorganisch-chemisches Institut, Universität Bonn, FRG and Dr I.D. Brown, Institute for Materials Research, McMaster University, Hamilton, Ontario, Canada, and will be published by the Fachinformations Zentrum Energie, Mathematik, Physik, D-7514 Eggenstein-Leopoldshafen-2 (Dr Behrens).

Content: The information contained in the data base is of a similar kind to that in the Cambridge File and has been organized along similar lines. Although not as fully developed, there is a similar search and retrieval system.

Publication: The database is on the point of going public and is just awaiting negotiation of a final agreement between the German and Canadian bodies regarding the distribution of marketing rights. The cost has yet to be ascertained.

The Society's interest in this database has been duly registered and we will keep the membership informed of its developments.

World Directory of Crystallographers

Those 20 or so members who ordered copies of the Sixth Edition of the Directory and have not yet received them are once again reminded that their copies are available with the payment of \$5.00 to the Treasurer. Those who have not ordered are reminded that spare copies are available, that the Australian Section has been dramatically expanded from the version in the Fifth Edition, and that the Directory as a whole contains a wealth of useful information, particularly for students.

Secondhand X-ray Analytical Equipment

The following Price List of secondhand XRD and XRF equipment has recently been received from Sietronics Pty Ltd, P.O. Box 521, Fyshwick, A.C.T. 2609 (Telephone: (062) 805576).

X-ray Generators:

- | | |
|---|--------|
| 1. Philips PW 1010; 1000 watts, 0.1% stability; valve electronics | \$4450 |
| 2. Philips PW 1010; 1000 watts, 0.1% stability; solid state | \$8950 |
| 3. Philips PW 1011; 1600 watts, 0.1% stability; valve electronics | \$5450 |
| 4. Philips PW 1011; 1600 watts, 0.1% stability; solid state | \$9950 |
| 5. Philips PW 1130; 3000 watts, 0.03% stability; solid state | \$9950 |

Goniometers:

- | | |
|---|--------|
| 1. Philips PW 1050 vertical goniometer, complete with accessories | \$3950 |
|---|--------|

Spectrometers:

- | | |
|--|--------|
| 1. Philips PW 1540; manual, sequential, air path | \$5950 |
| 2. Philips PW 1540; manual, sequential, vacuum | \$8950 |
| 3. Philips AF 50 Auto Assay, multi-channel, air path | \$6950 |

Electronics:

- | | |
|--|--------|
| 1. Philips PW 42.. series modules (ratemeter, timer, scaler, etc.) | \$300 |
| 2. Complete pulse counting chain of PW42.. series modules | \$1500 |

High Tension Tanks:

- | | |
|---------------------------------------|--------|
| 1. PW 1010; 1000 watts, reconditioned | \$2500 |
| 2. PW 1011; 1600 watts, reconditioned | \$3000 |

Sundry Items:

High voltage cables (from \$300); tube towers (from \$350)
X-ray tubes; sample holders, etc.

NOTE: All prices quoted include three months warranty.
All prices quoted are F.O.B., Canberra.

Forthcoming Meetings

- i) Thirteenth Australian Spectroscopy Conference, LaTrobe University, August 16-20, 1982.

Enquiries to: Dr J.B. Peel
Department Physical Chemistry
LaTrobe University
Bundoora, Vic. 3083

- ii) Seventh National Convention of the Royal Australian Chemical Institute, A.N.U., August 23-27, 1982.

For further information contact:
Dr J.H. Bradbury
Chairman 7NC
Chemistry Department
A.N.U.
Canberra, A.C.T. 2600

- iii) Tenth Australian Ceramic Conference, Melbourne Town House,
August 24-27, 1982.

Please contact: Mr Richard Bowman
The Conference Secretary
AUSTCERAM 82
CSIRO
P.O. Box 56
Highett, Vic. 3190

- iv) Fifth Australian Institute of Physics Congress, Canberra,
August 23-27, 1982.

Enquiries to: Professor G.V.H. Wilson
Royal Military College
Duntroon, A.C.T. 2600

Call for Contributions

All members of the Society are invited to submit material for the Newsletter to the Secretary at any time. This material can be of any kind, but information under the general heading of "Personalalia" would be particularly welcome, that is, news of a more personal nature involving visiting scientists, movements of staff, activities of kindred Societies, formation of new research programs/groups, overseas trips/study leave of members, major new equipment acquisitions, etc. No copy will be refused.

Membership Application Form

Please detach the back page of this Newsletter and forward it to any person whom you think may be interested in becoming a member of the Society. This applies particularly to any Graduate students that you may have.

