

Society of Crystallographers

in

Australia

Newsletter No. 10

December 1984

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OFFICE BEARERS

President: T.M. Sabine (NSWIT)
Vice President: S.R. Hall (Univ. WA)
Secretary: R.J. Hill (CSIRO Min. Chem: 03 647 0211)
Treasurer: M.F. Mackay (LaTrobe Univ.)
Council: W.T. Robinson (Univ. Canterbury, NZ)
F.H. Moore (AINSE, Lucas Heights)
R.W. Cheary (NSWIT)
B.M.K. Gatehouse (Monash Univ.)
(immediate past President)

Standing Committees (*Chairperson)

Electron diffraction: A.W.S. Johnson (Univ. WA)*
J.R.J. Sellar (ANU)
R.A. Eggleton (ANU)

X-ray diffraction: J.M. Guss (Univ. Sydney)*
S.W. Wilkins (CSIRO Chem. Phys.)
J.N. Varghese (CSIRO Protein Chem.)

Neutron diffraction: C.J. Howard (AAEC, Lucas Heights)*
T.J. Hicks (Monash Univ.)
C.H.L. Kennard (Univ. Qld.)

Computing: N.W. Isaacs (St. Vincents Sch. Med. Res.)*
A.D. Rae (Univ. NSW)
T.R. Welberry (ANU)

Nominations: S.L. Mair (CSIRO Chem. Phys.)*
M.R. Snow (Univ. Adelaide)
J. Epstein (Kodak, Vic.)

Newsletter Editor: R.J. Hill
CSIRO Div. of Mineral Chemistry
P.O. Box 124
Port Melbourne VIC 3207

MESSAGE FROM THE PRESIDENT

In 1984 Council considered an offer by the Australian Academy of Science to consider up-grading its sponsorship of the Perth Congress from Category 1 to Category 3. The Perth Organizing Committee considered that certain mandatory requirements of the Academy made its sponsorship at Category 3 level unacceptable to them. After deliberation Council decided to accept the advice of that Committee. A verbatim extract of the minutes is given below.

Item 4. Academy support for the 1987 Perth Congress

Terry Sabine tabled several documents relating to a recent proposal from the Australian Academy of Science to upgrade the status of the Perth Congress from category (i) to category (iii). In addition, the agenda papers contained several letters from Ted Maslen outlining his reactions to the preliminary approaches he had received from the Academy.

In reading these documents Council noted that there were several areas of conflict between the statements from the Academy Conference Executive Officer (Rosemary Green) and those appearing in the Academy Guidelines for the Organization of Conferences forwarded with the letter from Ms Green. In particular, the mandatory areas of involvement of the Academy for category (iii) sponsorship in Ms Green's letter seemed to be more appropriate to those outlined for category (ii) sponsorship in the Academy Guidelines.

In any event, the restrictions imposed by the Academy for sponsorship in either category appeared to be such that they would be unacceptable to the Perth Organizing Committee. This was especially clear in regard to the handing over of financial and organizational matters concerning Congress registrations and accommodation, although Council noted that the Academy's support would be gratefully accepted in areas relating to the Conference program.

In view of the above uncertainties relating to the Academy's proposed level of support, its ability or otherwise to compromise, and the reactions of the Perth Organizing Committee to the recent developments, Council was unable and unwilling to provide a firm answer to the problem. There was, however, a general reluctance to "change boats in midstream", especially since the Academy had not been willing/able to provide more than moral support in the early stages of the organization of the Congress.

Council therefore unanimously resolved to give its full and complete support to the Perth Organizing Committee (and its Program Committee) and to recommend that they proceed with their present handling of the Congress.

Council did, however, note that quite aside from the new proposal from the Academy, recent correspondence from Ted Maslen indicated that a change appeared to have taken place in regard to the financial arrangements originally agreed upon at previous SCA Business Meetings. In particular, a rereading of the Minutes of the 1983 Morpeth meeting revealed that the sum of \$30000 provided by the University of Western Australia has always been referred to as "bridging" funds and/or as an "underwrite". The minutes also specifically state that this money "will

have to be paid back eventually", although "the SCA will not have to pay interest".

Council considers that this latter financial arrangement is the one to which the SCA membership agreed at the Morpeth Business meeting. The SCA has, therefore, always understood the money from the UWA to be a loan and that the SCA would accept all of the losses or all of the profits arising from the running of the Congress. Since the UWA offer will be repaid, the SCA, through its Temporary Standing Committee, assumes full control over all of the funds, while at the same time accepting that the UWA has normal auditing control over the portion which it lent.

[end of extract from the minutes]

The Congress of Crystallography is a major activity in world science. I hope that all Australian crystallographers will participate enthusiastically in making our Congress, the accompanying satellite meetings, and the visits of overseas scientists to our laboratories an outstanding success.

Terry Sabine

NOMINATIONS FOR OFFICERS FOR THE 1985/1987 TERM

In accordance with Rule IV, Section 1 of the SCA Constitution, the Nominations Committee has proposed the following list of nominations for the Offices becoming vacant after the Business Meeting in Adelaide in May, 1985. For the benefit of those members who are not familiar with SCA election procedures, the Council and Standing Committee nominations are for the positions vacated by the longest serving members (i.e., the ones at the top of the lists on page two). The current Vice President (Syd Hall) assumes the Presidency automatically, while Terry Sabine replaces Bryan Gatehouse as the Immediate Past President on Council.

| Position | Nomination | |
|----------------------|----------------|-------------------------|
| Vice President | Peter Colman | (CSIRO, Protein Chem.) |
| Secretary | Rod Hill | (CSIRO, Mineral. Chem.) |
| Treasurer | Maureen MacKay | (LaTrobe Univ.) |
| Council | Jim Graham | (CSIRO, Mineralogy) |
| Electron Diffraction | Les Bursill | (Univ. Melb.) |
| X-ray Diffraction | Brian O'Connor | (WAIT) |
| Neutron Diffraction | Frank Moore | (AINSE) |
| Computing | Max Taylor | (Flinders Univ.) |
| Nominations | Meta Sterns | (ANU) |

The Secretary now invites additional nominations for these positions to be submitted over the signatures of two SCA members not later than January 18, 1985.

CRYSTAL 15 AND THE COMPUTING SCHOOL

Computing School: Sunday evening, May 12 - Tuesday afternoon (14th).

Crystal 15: Tuesday, May 14 - Thursday afternoon (16th).

Those who have not yet sent their Intention to Attend Forms to Max Taylor should do so forthwith because these are going to be the biggest and best two meetings the SCA has ever mounted. And on top of that, it is being held in one of the most beautiful capital cities in Australia, with the best weather, the best beaches, the best wine, the most scenic mountain ranges (Mount Lofty and Flinders), and the best seafood in Australia, all within easy reach of the conference venue. (Not hard to guess where the Editor comes from, is it!)

The Computing School will feature review lectures on the following topics:

data collection methods, matrix operations, Patterson methods, direct methods, isomorphous replacement, anomalous dispersion, non-crystallographic symmetry, least-squares, macromolecular refinement, profile analysis, XTAL, SHELX, maximum entropy, APPLECRYST (microcomputers), and CYBER 205 programming.

As well as the usual short research contributions, the Crystal 15 meeting will give special emphasis to subjects such as:

crystallographic computer graphics,
high accuracy data collection,
structure solution from powder data.

Once again, if you have not already done so, please dig out the Intention to Attend Form from your copy of the last newsletter, or call Max or the Secretary for a new copy, and send it to:

Dr M.R. Taylor
School of Physical Sciences
The Flinders University of South Australia
Bedford Park, South Australia 5042

1987 PERTH IUCr CONGRESS

At the Hamburg IUCr Congress last August the IUCr formerly accepted an invitation from the SCA to hold the XIVth International Congress in Australia in August 1987. We can all now breath a sigh of relief and proceed at full speed with the business of getting it organized.

Ted Maslen, Chairman of the Organizing Committee, and Hans Freeman, Chairman of the Program Committee, met with the IUCr Executive during the Hamburg Congress and, among many other things, approved of the following dates:

| | |
|-----------|---------------------|
| August 12 | Opening ceremony |
| 13-15 | Scientific sessions |
| 16 | Excursion |
| 17-19 | Scientific sessions |
| 20 | Closing ceremony |

Tentative dates for the four satellite meetings associated with the Perth Congress are given below in the section on Forthcoming Meetings.

The Hamburg meeting was a huge success. Credit must be given to the Organizing Committee chaired by Professor Saalfeld, and to Professor Bonse and his International Programme Committee. Thanks are of course also due to the International Union of Crystallography and to Professor Jerry Karle and the Executive Committee. All their hard work is much appreciated.

There were 1519 participants, and more than 150 accompanying persons, that attended the meeting. Many stayed at the Hamburg Plaza Hotel which adjoins the Conference Centre. There were thirty exhibitors at the commercial and non-commercial exhibition. A typical morning consisted of a choice of listening to one or other of the two main lectures from 9 to 10 o'clock, and then from 10:30 to 1 p.m. there were five (and on one day, six) parallel sessions or microsymposia. For those with varied interests, choices were sometimes difficult. On each of six afternoons, from 2:30 to 6 p.m., there were over two hundred posters to be seen! Some of these were works of art. It was a pity there was no specific artistic display and that several posters were missing. The number of presentations, oral and visual, totalled 1398.

The Opening Ceremony on Thursday, 9th August, included P. Brammer's ingenious slide show of minerals and mountains merging into one another accompanied by music, and Professor Bertaut's talk "Commensurate - Incommensurate", after which there was a reception. After two and a half days of crystallography, Sunday afternoon was free: the Kunsthalle was full of crystallographers peering at paintings.

Wednesday was also a day off. Six hundred went by a fleet of luxury coaches on the Conference Excursion to the Mediaeval town of Lubeck and were entertained to a recital by Ernst-Erich Stender at the famous organ of St. Mary's Cathedral. A three course lunch was laid on at Travemünde on the Baltic Sea, after which some participants bought the traditional Lubeck marzipan. Some crystallographers, in their quest for all three dimensions, took the view from the top of the thirty-three floors of the Maritime Hotel, and a few even explored parts which other beers never reach. The day out was a welcome break from four and a half solid days of trying to absorb so much information, and with another two and a half still to go.

On the second Thursday evening (16th) we were again entertained to wine and cheese, this time in the Geological Institute and Museum. Much fine white wine flowed and there was no shortage of cheese. After feeding the multitude, twelve baskets of bread rolls were taken up.

After such a memorable meeting, people are now talking about Perth 1987 and Bordeaux 1990

Moreton Moore

The business of the Union is conducted at the General Assembly which is attended by the Executive Committee of the IUCr and by delegates from various countries. The composition of the Executive Committee for the last three years has been:

President: J. Karle (U.S.A.)
 Vice President: S. Ramaseshan (India)
 General Secretary and Treasurer: K. V. J. Kurki-Suonio (Finland)
 Immediate Past President: N. Kato (Japan)
 Ordinary members: S. Amelinckx (Belgium)
 T. Hahn (Fed. Rep. Germany)
 M. Nardelli (Italy)
 H. Neels (German Dem. Rep.)
 V. I. Simonov (U.S.S.R.)
 M. M. Woolfson (U.K.)

In each country there is an "Adhering Body," usually a scientific society that is responsible for sending delegates to the meeting (the number being determined by the category (I-V) of the adherence). The adhering body in the U.S. is the National Academy of Sciences and our category is V. The various countries represented by delegates, with their categories, are: Argentina (I), Australia (III), Austria (I), Belgium (II), Brazil (III), Canada (III), Chile (I), China, PRC (IV), Czechoslovakia (I), Denmark (I), Egypt (I), Finland (I), France (IV), Germany, Fed. Rep. (IV), Germany, Dem. Rep. (I, this meeting), Hungary (I), India (II, this meeting), Israel (I), Italy (III), Japan (IV), Mexico (I, this meeting), Netherlands (II, this meeting), New Zealand (I), Norway (I), Poland (I), Portugal (I), South Africa (I), Spain (III), Sweden (II), Switzerland (II), U.K. (V), U.S.A. (V), U.S.S.R. (V), Yugoslavia (I). The U.S. delegation consisted of J. P. Glusker (Chairman), S. C. Abrahams, W. A. Hendrickson, W. L. Duax, D. Sayre, with alternate delegates H. A. Hauptman, L. H. Jensen, G. A. Jeffrey, R. E. Newham and C. T. Prewitt.

The following items of business were conducted:

1. The President, J. Karle, noted with sadness the deaths of Sixten Abrahamsson, Gopinath Kartha and Marianna P. Shaskol'skaya
2. The Netherlands reduced their category of adherence from III to II. An appreciation of the great contributions of the Dutch to crystallography was expressed by D. Sayre with the approval of those present. The problem, apparently, was the costs of dues payments. For a similar reason the German Democratic Republic reduced its category from I to I. The category of adherence for India was changed from I to II. The new member of the General Assembly at this meeting was Mexico which entered with a category of I.
3. Some changes in the voting procedures were put forward in order to clarify what a vote of "yes" meant. For most delegates English is not their primary language and sometimes (also even for native English speakers) it may not be clear what is going on. Therefore whenever a

motion was on the floor the text of the motion was displayed by use of an overhead projector.

4. The financial situation of the Union has greatly improved in the last three years as a result of the formation of a Finance Committee and the work of the President.

5. The editor of *Acta*, Sidney Abrahams, reported that two new co-editors, Jan Drenth and Charles Bugg, had been appointed.

6. With respect to *International Tables*, Volume A has sold well. However the point was made to the Executive Committee that Volume I is now unavailable (out of print) and will not be reprinted. Volume A contains direct space data only. Volume B on reciprocal space will not be available for some time. Therefore it was felt that the second part of Volume I should be reproduced in some way.

7. The Commission on Biological Macromolecular Crystallography changed its name to the Commission on Biological Macromolecules.

8. The U.S. proposed a Commission on Small Organic Molecules. The formation of this Commission was hotly debated, mainly on the grounds that there were too many Commissions already. However the motion to form such a commission passed, with the word "Organic" removed from the name. Thus there is now a Commission on Small Molecules. The membership of the new Commission was also extended over that originally proposed. The Commission consists of J. Stezowski (Fed. Rep. Germany), Chairman; W. Duax (U.S.A.); C. Dehanter (Belgium); M. Hospital (France); A. Kalman (Hungary); M. Vijayan (India); S. Neidle (U.K.); B. Oleksyn (Poland); G. Tishchenko (U.S.S.R.); P. Coddling (Canada); and S. Garcia-Blanco (Spain). The terms of reference are:

- (a) to advise the IUCr on organizing or sponsoring sessions on small molecule structural analysis at Congresses and conferences.
- (b) to promote and coordinate scientific exchange between countries in the fields of small molecule structural analysis.
- (c) to cooperate with the Commissions of the Union on matters dealing with small molecule structural analysis
- (d) to cooperate with other international bodies concerning small molecule structural analysis.

9. The compositions of the various Commissions were approved.

10. There will be no dues increase.

11. The donation of \$35,000 by the Japanese Crystallographic Community to the Union's publications was gratefully acknowledged. With the help of this donation a microcomputer with 384K bytes of memory and 15M bytes of hard disc storage (with magnetic cartridge tape back-up) has been installed in the Union Office at Chester.

12. A motion was carried that required the Executive Committee, when planning the Budget for the General Fund, to give high priority to the provision of scholarships to enable talented graduate (i.e., pre-doctoral) students to attend Congresses of the Union.

13. The Fourteenth General Assembly will be in Perth, Australia, 12-20 August, 1987.

14. The Fifteenth General Assembly will be in Bordeaux, France in 1990. Invitations were also received from India, China (PRC), and Spain. In order to choose a site, a delegate vote was taken. It required three ballots with elimination of the site with the lowest number of votes, before France was finally chosen by majority vote.

15. The new Executive Committee is:

| | |
|----------------------------------|---------------------------------|
| President: | T. Hahn (Fed. Rep. Germany) |
| Vice-President: | V. I. Simonov (U.S.S.R.) |
| Immediate Past President: | J. Karle (U.S.A.) |
| General Secretary and Treasurer: | K. V. J. Kurki-Suonio (Finland) |
| Ordinary members: | A. Authier (France) |
| | A. Kalman (Hungary) |
| | E. N. Maslen (Australia) |
| | R. Diamond (U.K.) |
| | M. Nardelli (Italy) |

Y. Tang (China, PRC)

We congratulate them on their election and express our appreciation to J. Karle for his successful three-year presidency.

The U. S. National Committee organized a two hour reception at the U.S. Consulate General in Hamburg for delegates to the General Assembly and all U.S. participants in the Hamburg IUCr meeting. The Consul-General, Mr. Grant Mouser, was there to greet more than 300 guests.

Scientific highlights of the Hamburg IUCr meeting will be reported in the next Newsletter. Contributions will be gratefully received by the Editor (deadline October 31, 1984).

SE ASIAN REGIONAL CRYSTALLOGRAPHIC ASSOCIATION

Much progress has been made on the formation of a South East Asian Regional Crystallographic Association since the matter was discussed at the SCA Business Meeting at Crystal 14. Immediately after this meeting Council acted upon the motion carried at that meeting and sent a letter to 21 people in 18 countries located in the SE Asian region, inviting them to participate in the formation of a Regional Crystallographic Association. A follow-up letter was subsequently sent to all those who replied to the first letter, and a slightly different one to all those that did not, informing them that an attempt would be made to contact delegates during the Hamburg Congress to arrange a meeting.

This meeting was duly called on August 13 at the Hamburg Plaza Hotel, and was attended by 27 delegates from 6 countries, with apologies received from a further 9 delegates from 8 countries. The meeting was chaired by Terry Sabine and minuted by Rod Hill and, by everyone's estimation, was a resounding success, promising a great deal for the future collaboration between participant countries. The two major resolutions carried at this meeting were that the SCA would draft a Constitution for the Association for subsequent distribution among the member countries, and that the Australians and Japanese (initially) would collaborate on the production of a Regional Newsletter. Council of the SCA is currently in the process of finalizing this draft constitution, which will be on display at Crystal 15 for the perusal of members.

SMALL MOLECULE COMMISSION

As indicated in a previous section of this newsletter, a new IUCr Commission on Small Molecules was approved at the Hamburg Congress. The charter members of this new commission are anxious to establish the commission activities well in advance of the next IUCr Congress and have, therefore, solicited the help of crystallographers in Australia. The Secretary of the SCA has received a copy of the minutes of the first meeting of this commission, together with a Feedback Form on the proposed activities of the group. Questions of particular interest include:

- (i) Willingness of individuals to collect intensity data for crystallographers who lack state of the art diffraction equipment,
- (ii) Identification of crystallographers in need of a data collection service,
- (iii) Willingness of individuals or organizations to help with the organization of small molecule crystallography symposia at annual meetings of local Societies,
- (iv) Suggestion of topics for future symposia,
- (v) Identification of examples of the use of X-ray crystallographic data in establishing a correlation between molecular conformation in the solid state and chemical or biological activity, solution conformation, or theoretical calculations,

- (vi) Identification of speakers who could be invited to contribute to a Commission organized symposium.
- (vii) Interest in collaborative projects involving the measurement, storage, retrieval, analysis and utilization of parameters defining X-ray thermal motion.

Any member of the SCA who would like further information, namely, a full copy of the Minutes of the Small Molecule Commission meeting and/or of the Feedback Form should contact the SCA Secretary or

Dr W.L. Duax
Associate Director - Research
Medical Foundation of Buffalo
73 High Street, Buffalo
New York 14203-1196, USA.

MEDIA RELEASE FROM THE ACADEMY

The following Media Release was received by the Secretary in August. It is reproduced here without change.

A bad budget for science

Whatever is Australia's visibility in international sport, its visibility in international scientific bodies is being reduced to that of a third world country. This is one aspect of the government's disastrous science budget. Without adequate financial support from the government, Australia's international scientific reputation will decline with the consequent reduction in Australia's national scientific and technological capacity.

The Academy of Science which conducts relations with International Unions and similar bodies on behalf of Australia was forced last year by lack of government support to cut a number of categories of adherence, and to eliminate some entirely. A significant example is the Scientific Committee for Antarctic Research, to which the Academy no longer subscribes. This largely stills the Australian voice in major scientific affairs. On our present budget this is likely to continue to be the situation.

The financial situation with respect to international dues has deteriorated dramatically since 1978/79. The cost of dues increased by 78% while the increase in the Commonwealth grant was only 27%, less than half the Australian inflation rate.

The scale of support we now offer to our delegates to attend interantional scientific meetings is absurd when compared with present Public Service entitlements and we experience great difficulties in finding people who are able and willing to find their own expenses to fulfil the government's obligations.

As the Minister has acknowledged, the perception of Australian Science overseas has a marked effect on us. International Scientific conferences which are essential to keep Australian scientists up-to-date are less likely to come to Australia if we are thought to be a third rate scientific nation.

It represents only one aspect of the government's contemptuous incomprehension of the long term aspects of science. It is only possible to raise the living standards of all sectors of the community

because of the high productivity resulting from scientific discovery, applied through invention and innovation, which produces goods, services and systems surplus to the needs of the producers and operators. Without the results of science in the last hundred and fifty years, Australia would still be socially about the subsistence level of the days of Governor Macquarie. What of the next century (or twenty years)? It is the science of today which results in capabilities in twenty year's time.

As one example of inept government decisions, the funding of the Australian Research Grants Scheme is about half what it should be. The research this supports is of the creative, breakthrough type, unforeseeable by government committees, and which forms the basis of future innovation. Researchers who depend on ARGS support are facing a continuing crisis.

The pity is that the sums of money required are virtually statistical errors in some other budgets. We in Australia are now busy eating our seed corn, and on behalf of my grandchildren, I protest.

Arthur J. Birch
President
Australian Academy of Science

23 August 1984
[End of Media Release]

This document arrived with an assurance that the Academy's Science Policy Committee is preparing a "Case for Science" for discussion at the forthcoming meeting of National Committee Chairmen and representatives of Scientific Societies in April/May 1985. It also came with a call for support for these initiatives through "public statements, letters to the editors of newspapers, making contact with your local broadcast media, and through any other avenues open to you".

The SCA Council believes that activities of this kind are more appropriately handled by the National Committee of Crystallography (our "political" arm), but resolved to use the newsletter to undertake a survey of crystallographic research in Australia, the results of which will be forwarded to the National Committee for further action. Council therefore asks for a short contribution from all concerned SCA members detailing the relationship between their research and perceived national needs and objectives. That is, an indication of where their research in crystallography contributes, for example, to materials engineering, human and animal health, food production, national security etc. An example of the kind of contribution which Council believes will be of most help is the following:

Structures of two anti-depressant drug molecules, nortryptyllyne and triimipramine, are being determined in a program to assist the structure-activity relationship work at the Victorian College of Pharmacy.

[Name and Institution]

The Editor notes that many of the thesis research topics given in the next section of the newsletter have strong applied aspects and, therefore, also represent examples of the kind of submission required by the SCA survey.

GRADUATE STUDENT CRYSTALLOGRAPHY THESES IN AUSTRALIA

The following is a summary of some of the research work being undertaken by student members of the SCA. The list is an alphabetic arrangement of the material submitted by each individual and only includes slightly more than half of the 18 PhD/MSc students who are currently members.

Tony Brown (Research School of Chemistry, ANU):

An Electron Microscope Study of the Pd-P System.

An electron microscope study of various phases in the Pd-P system has been started. Of particular interest is a phase with the broad range of composition Pb_3P_{1-x} with $0 < x < 0.3$, and a phase with a reported composition of $Pd_{4.8}P$. Both regions of the phase diagram have been explained as random phosphorus vacancies to account for deviations from stoichiometry. However, we believe this is unlikely, and it is hoped that the phases in the composition range Pd_6P to Pd_3P can be described as intergrowths of the Re_3B structure type (Pd_6P) and the Fe_3C type (Pd_3P) in appropriate ratios.

Bret Church (Inorganic Chemistry, Univ. Sydney):

Neutron Diffraction Study of Poplar Leaf Plastocyanin.

A neutron diffraction study of the protein should reveal the positions of hydrogen atoms which, at this stage, have had to be inferred from the X-ray structure analysis. Neutron diffraction data for deuterated plastocyanin have been collected to 1.8 Å resolution at the Brookhaven high flux neutron source by Thomas P.J. Garrett. X-ray counter data to 1.6 Å resolution have also been recorded. The structure is being refined by means of nuclear scattering density difference maps, and by the method of stereochemically restrained joint refinement with the new X-ray and neutron diffraction data. In a related study the structure of Hg(II)-substituted plastocyanin has been refined at 1.9 Å resolution.

Charles Collyer (Inorganic Chemistry, Univ. Sydney):

Structure Analysis of Plastocyanin From a Green Photosynthetic Alga, *Enteromorpha Prolifera*.

This algal protein crystallizes in space group $I4$ whereas the known crystal structure of *Populus nigra* plastocyanin was determined from crystals of space group $P2_12_12_1$. Optimal alignment of the amino acid sequence of this algal plastocyanin with that of poplar reveals 57% homology. These differences are to be investigated by X-ray structure determination. The structure has been solved by the molecular replacement method using refined poplar plastocyanin as a search model. Film data have been collected at the synchrotron source DESY to 1.9 Å. A molecular model was fitted to Fourier maps with the aid of a computer graphics facility. Refinement is proceeding with the use of constrained-restrained least squares.

Sylvano Colmanet (Australian Radiation Laboratory, Vic.):

Structural Studies of Technetium Complexes.

Technetium in its metastable form (^{99m}Tc) has found widespread use as an ideal imaging agent in diagnostic nuclear medicine. The chemistry of technetium is, however, poorly understood. This study involves

synthesis of new technetium complexes and their characterization by single-crystal X-ray crystallography. By this means it is possible to establish the relationship between structure and radiopharmaceutical behaviour.

Christopher Dean (Phys. & Inorg. Chemistry, Univ. Adelaide):

Structural Transformations in Inorganic Crystals.

Potentially martensitic transformations induced by changes in temperature or pressure in various inorganic crystals are being studied. The aim is to identify the transformation mechanism and to determine in which instances the phenomenological theory of martensitic transformations is a veritable description of the geometric mechanisms. Analysis techniques are X-ray diffraction, computing, optical and electron microscopy.

Tom Garrett (Inorganic Chemistry, Univ. Sydney):

Crystallographic Studies of the Copper Protein Plastocyanin.

The structure of copper-free or apo-plastocyanin from poplars has been refined at 1.8 Å resolution. The structural integrity of the protein is maintained despite the loss of the copper atom. A change in the orientation of one ligand suggests a route for the incorporation of copper into plastocyanin. Neutron diffraction data to 1.8 Å resolution has been collected at Brookhaven National Laboratory, USA for use by W.B. Church in his thesis project. The structure of cucumber plastocyanin has been solved by molecular replacement methods and is being refined. There are two molecules in the asymmetric unit (space group $P4_1$). The effect of intermolecular forces on the molecular structures must therefore be different than in poplar plastocyanin ($P2_12_12_1$) and algal plastocyanin ($I4$).

Luke Guddat (St Vincent's School of Medical Research, Vic.):

The Structure of an Fab Fragment of a Monoclonal Antibody.

Single crystal X-ray diffraction techniques are used in solving the three dimensional structure of an Fab fragment of a monoclonal antibody directed against the phosphorylated form of phenylalanine hydroxylase. Phenylalanine hydroxylase is the enzyme used to convert phenylalanine to tyrosine and its deficiency results in the condition phenylketonuria. The Fab fragment is exclusively responsible for the binding to the antigen and so this structural solution will be used to describe the interaction between the antigen and antibody at an atomic level.

Alan Imerito (Dept Physics, Univ. WA):

The Evaluation and Display of Electron Density in Crystalline Materials.

The first part of this work involves a study of the charge density distributions in a number of isomorphous hydrated lanthanide compounds $X(H_2O)_9.(CF_3SO_3)_3$, where X = lanthanides. The aim is to study the bonding of trivalent rare earth cations. The second part relates to the addition of code to the PLOT program of the XTAL system of crystallographic software. The new code will enable colour plots to be

obtained on graphics VDUs and local plotters in real (PLOT) time.
In brief:

Nick Spadaccini (Crystallography Centre, Univ. WA) is using accurate crystal structure analyses to study the effect of interactions involving atoms beyond the first coordination sphere, i.e., not involved in chemical bonds directly.

Ian Castleden (Crystallography Centre, Univ. WA) is studying the use of maximum entropy methods for determining reflection phases.

CURRENT STATUS OF CRYSTALLOGRAPHIC DATA BASES

Please give your attention to the IUCr survey on data bases circulated as a flier with this newsletter.

PERSONALIA / MISCELLANEOUS

John ("Hey guys, give me a break") Parise, currently a Research Fellow with Bruce Hyde in the Research School of Chemistry at ANU, and formerly a student of Frank Moore and Les Power has accepted a new position in the Department of Chemistry at the NSW Institute of Technology, effective from February, 1985. We all wish John well in his new job.

Syd Hall, our Vice President, has been on study leave with Prof Henk Schenk at the Laboratory of Crystallography at the University of Amsterdam since the Hamburg Congress. He will return to Australia in April, 1985.

Dr Garry McIntyre from the Institut Laue-Langevin, Grenoble will be working on X-ray diffractometry with extended face crystals in the X-ray Diffraction Section of the CSIRO Division of Chemical Physics over the summer of 1984/5.

Dr David Stewart from the Laboratory of Molecular Biophysics, University of Oxford will be working in the X-ray Diffraction Section of the CSIRO Division of Chemical Physics on applying maximum entropy to macromolecular structure refinement in March and April, 1985.

At the Hamburg Congress of the IUCr, Aug 10-18, 1984, Dr A.J.M. Duisenberg of the Dept of Structural Chemistry, Univ. Utrecht, Padualaan 8, 3508 TB Utrecht, The Netherlands, handed Sandy Mathieson a printout of a programme update entitled "Concise Explanation of CAD4AJ.LD;Feb-84" by Jan L. DeBoer and Albert J.M. Duisenberg. If any CAD4 user wishes to make a copy of this material (22 pp) it is available from Sandy Mathieson at the CSIRO Division of Chemical Physics, PO Box 160, Clayton, Vic 3168.

Jerome Karle and Herbert A. Hauptman received the A. Lindo Patterson Award of the American Crystallographic Association at its May 1984 meeting in Lexington, Kentucky, in recognition of their major contributions to the theory of direct methods of crystal structure determination. This award honours the memory of A.L. Patterson (1902-1966), who discovered the vector function that bears his name

while he was an unpaid guest at the Massachusetts Institute of Technology during the Great Depression.

The Swedish Royal Academy of Sciences has awarded the Gregory Aminoff Medal in Gold to David Harker in recognition of his fundamental contributions to the development of methods in X-ray crystallography for determining molecular structures of biologically important substances. Harker is currently professor emeritus in the molecular biophysics department of the Medical Foundation of Buffalo where he is studying the nature of coloured space groups.

The 32 Australians who managed, by hook or by crook, to get to Hamburg for the IUCr Congress in August could not claim to have been homesick for long while attending the scientific sessions at the Hamburg Plaza Hotel. Not only could they stand around the message board near the main registration desk at any time of the day or night and be sure to meet at least a dozen other Australians, but they were then surrounded by superb displays of Australiana in the form of Victorian and Western Australian tourist posters. These quite spectacular displays were placed there to advertise the Perth Congress in 1987 and were responsible for countless favourable comments and assurances of attendance in Perth from many non-Australian registrants. The credit for this very successful public relations exercise can be given to Sharman Hill, of the BHP Melbourne Research Labs, and Syd Hall, that dazzling dynamic dance duo of discotheques from Hamburg to Amsterdam. For this service to publicity for the 1987 Congress we we extend to them our grateful thanks.

In the last newsletter Council called for ideas on a logo to be used on all official correspondence of the Society. Since no member produced a contribution Council resolved at its December 6, 1984 meeting to undertake this task itself. However, if any member considers that she or he has something to suggest after all, then the idea should be sent to Frank Moore or Maureen Mackay as soon as possible. You will only have yourselves to blame if you do not like what we come up with!

NEW MEMBERS

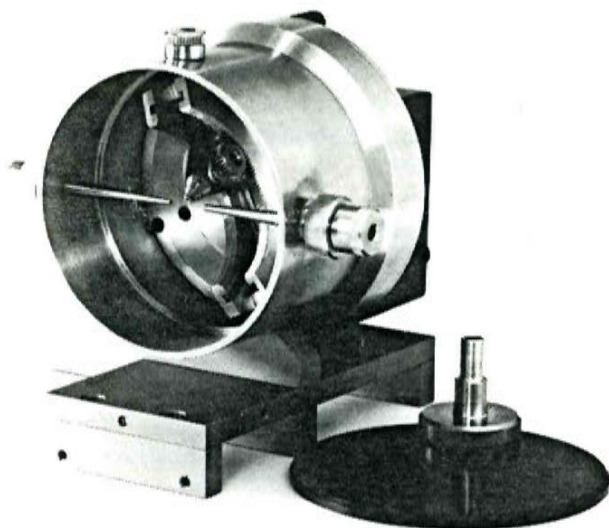
Council of the SCA extends a warm welcome to the following new members:

| | |
|----------------|----------------|
| Mr. A. Brown | (student, ACT) |
| Mr. A. Imerito | (student, WA) |

SUBSCRIPTION RENEWAL FOR 1985

Members are reminded that their SCA subscriptions for 1985 are now due. Please complete and return the dues form which has been included with this newsletter as soon as possible. If your subscription is in arrears (as indicated on the form) you should remedy the matter immediately if you wish to remain on the membership list.

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FORTHCOMING MEETINGS

- Jan 7-11, 1985: Arizona State University Centennial Conference on High Resolution Electron Microscopy, Scottsdale, Arizona, USA. Contact: Dr P.R. Buseck, Centre for Solid State Sciences, ASU, Tempe, AZ 85287, USA.
- Feb 6-8, 1985: 9th Annual Solid State Physics Meeting, Wagga Wagga, NSW. Contact: Dr G.K. White, CSIRO Div. Applied Physics, PO Box 218, Lindfield, NSW 2070.
- Feb 11-14, 1985: Polymer 85 (Characterization and Analysis of Polymers). Melbourne. Contact: Polymer 85, RACI, 191 Royal Parade, Parkville, Vic 3052.
- May 12-16, 1985: Crystal 15 / Computing School, Flinders University/ Haven Motel, Adelaide. Contact: Dr M.R. Taylor, School of Physical Sciences, Flinders University, Bedford Park, South Australia 5042.
- May 26 - June 6, 1985: Static and Dynamic Implications of Precise Structural Information, 11th Course of the International School of Crystallography, Erice, Italy. Contact: Dr P. Murray-Rust, Glaxo Group Research, Greenfords, Middlesex UB6 OHE, U.K.

- June 10-19, 1985: Synchrotron Radiation for X-ray Crystallography.
12th Course of the International School of Crystallography,
Erice, Italy. Contact: Prof L. Riva di Sanseverino, Exec.
Sec., Int. Sch. Cryst., Piazza Porta S. Donato 1, 40127
Bologna, Italy.
- July 28 - Aug 3, 1985: Sagamore VIII - Conference on Charge, Spin and
Momentum Densities, Sanga-Saby Conference Centre,
Sweden. Contact: Prof I. Olovsson, Inst. Chemistry,
Univ. Uppsala, Box 531, S-751 21 Uppsala, Sweden.
- Aug 19-23, 1985: 5th International Congress on Quantum Chemistry,
Montreal, Canada. Contact: Mr K. Charbonneau, Exec.
Sec. 5th ICQC, National Research Council of Canada,
Ottawa, Canada K1A 0R6.
- Aug 26-29, 1985: Steric Aspects of Biomolecular Interactions -
International Symposium, Sopron, Hungary. Contact:
Prof A. Kalman, Dept. X-ray Diffraction, Central Res.
Inst. Chemistry, Hung. Acad. Sci., H-1525 Budapest,
POB 17, Hungary
- Aug 26-30, 1985: 55th ANZAAS Congress, Melbourne, Vic. Contact:
Executive Secretary, 55th ANZAAS Congress, Monash
University, Clayton, Vic. 3168.
- Sept 2-6, 1985: Ninth European Crystallographic Meeting, Torino,
Italy. Contact: Prof G. Ferraris, Dipartimento di
Scienze della Terra, Univerita di Torino, Via S.
Massimo, 22 I - 10123, Torino, Italy.
- July 13-18, 1986: 14th General Meeting of the International
Mineralogical Association, Stanford, USA. Contact:
Prof C.T. Prewitt, Chairman IMA 1986, PO Box 183,
Stony Brook, New York 11790, USA.
- Nov 19-26, 1986: 56th ANZAAS Congress, Sydney, NSW. Contact:
Executive Officer, 56th ANZAAS Congress, GPO Box 873,
Sydney, NSW 2001.
- Aug 12-20, 1987: 14th General Assembly and Congress of the International
Union of Crystallography, Perth, Western Australia.
Contact: Dr E.N. Maslen, Crystallography Centre, Univ.
of Western Australia, Nedlands 6009, Western Australia.
- Satellites: Developments in Neutron Scattering, Sydney, Aug 5-12.
X-ray Powder Diffractometry, Perth, Aug 21-22.
Int. School on Cryst. Computing, Adelaide, Aug 22-29.
Solid State Properties of Minerals, Sydney, Aug 24-26.

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