



# Newsletter

of the ASIAN CRYSTALLOGRAPHIC ASSOCIATION.

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January 1988

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## Introduction

This is the first Newsletter of the recently constituted Asian Crystallographic Association (ASCA). This issue contains information about the formation and the objectives of the ASCA, and some details of the Perth IUCr Congress and associated meetings. Future newsletters will provide up-to-date information about what is happening in the crystallographic world, and particularly in our region. The ASCA Newsletter will be published twice a year and distributed via the national Societies or IUCr Committees in the Asian region bounded by Japan, Korea, China, India, Pakistan, Australia and New Zealand.

It was decided at the first meeting of the ASCA Council in Perth that the Newsletter would be

the main activity of the ASCA for this triennium. It meets the prime objective of our Association -- the promotion of crystallography in the region -- and can be done at relatively small cost to ASCA members. We are aware that many recipients of this Newsletter do not have easy access to the news bulletins of other crystallographic societies, and especially those of North America and Europe. It is our intention to include where possible brief excerpts from these journals as well.

In the longer term the ASCA sees its function as a coordinator of cooperative research efforts in the region; a promoter of crystallographic resource sharing; and a sponsor of regional scientific meetings. These activities will follow naturally from these initial communications, and can be introduced when there is a better understanding of the effort and the finances involved.

We are all aware of the rapid developments taking place in the electronic communication, especially those involving computer networking and telecommunication (FAX) links. It is inevitable, even for those without current access to this technology, that these developments will bring our crystallographic activities closer together. It is already feasible, for example, to collect a complete set of diffraction data in one laboratory; to transmit it electronically to another laboratory; and to solve and refine the structure, all in the same day! And, of course, these laboratories need not be in the same country! Significant difficulties, other than the obvious technical ones, still remain before this level of cooperation can be achieved globally within our region. These are mostly to do with funding -- who pays for what, and how much! Promoting and coordinating this type of

cooperation, especially at the governmental level, is a function that the ASCA will be able to help with. In general governmental agencies are more receptive to providing funds for proposals put forward by an international organisation, that can act on behalf the recipient countries involved.

In closing this message, I would like to say how much the ASCA Executive, M A Viswamitra, Jimpei Harada and I look forward to the challenge of steering this organisation in its fledgling years. The formation of this associa-

tion has been discussed and planned for almost a decade, and has also involved the determined interest of a number of crystallographers, including in particular, Jimpei Harada, Rod Hill, Sadao Hoshino, Norio Kato, Ted Maslen, Terry Sabine, R. Srinivasan and Tang You-qi. It was very gratifying for all concerned to see the ASCA finally come into being.

Syd Hall  
ASCA President

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## Formation of ASCA

The possibility of an Asian regional crystallographic group was mooted almost ten years ago. With the formation of the European Crystallographic Committee for coordinating activities in Eastern and Western Europe, and the fact that the American Crystallographic Association had become the de-facto regional organisation for Canada and other countries in the America's, it was suggested that a similar organisation would be beneficial to the Asian region.

Early informal discussions centered on defining the boundaries of the regional group. Overlap with the ECC or the ACA was considered undesirable, and the boundaries should be as simple as possible geographically. It was decided that the region would be defined by a 'circle' passing through Japan, China, India, Pakistan, Australia and New Zealand. Other crystallographic communities enclosed in the region included Bangladesh, Hong Kong, Korea, Malaysia, Philippines, Singapore, Sri Lanka, Taiwan and Thailand.

Representatives from most of these countries attended an informal meeting at the 1984 IUCr Congress in Hamburg to discuss the formation of a regional group. The meeting was chaired by the then President of the Society of Crystallographers in Australia, Terry Sabine. At this meeting it was resolved that the SCA should prepare and circulate a draft constitution for consideration at the 1987 Perth IUCr Congress. Rod Hill, who was Honorary Secretary of the SCA, was made responsible for coordinating the drafting, circulation and updating of the constitution. Prior to the Perth Congress three drafts of the constitution were circulated for comment and adjustment.

On Friday August 14 1987 a meeting of regional representatives approved the draft constitution, and the Asian Crystallographic Association came into being. The ASCA Constitution, which is shown elsewhere in this Newsletter, provides for three categories of membership. Category I allows for one representative on the ASCA Council who has one vote. Category II allows for one Councillor with two votes. Category III allows for two Councillors with a total of four votes. Membership dues are zero for Category I, one unit for Category II and two units for Category III.

The first meeting of the ASCA Council on Monday August 17 1987 elected the Executive members of the ASCA, composed of a President, a Vice President and a Secretary Treasurer. Most business at the ASCA Council meeting centered on activities for the 1988-1990 triennium, and the budget needed to fund these activities. After considerable discussion it was decided that a biennial Newsletter would be the prime function for ASCA in the initial years, and other activities would follow from this. The 1988-90 unit membership fee was set at 120 Australian dollars per annum.

The ASCA Executive and the Council for the 1988-90 triennium are as follows:

### ASCA EXECUTIVE

President: Sydney Hall  
Vice President: M A Viswamitra  
Secretary Treasurer: Jimpei Harada

## ASCA COUNCIL

**AUSTRALIA**  
Peter Colman  
Sydney Hall

*Category III*  
C.S.I.R.O.  
University of W.A.

**CHINA**  
Fang Ming Miao

*Category II*  
Tianjin Normal Univ.

**HONGKONG**  
Ting-Fong Lai

*Category I*  
University of Hong Kong

**INDIA**  
Krishan Lal  
M.A. Viswamitra

*Category III*  
National Physical Lab.  
Indian Institute of Science

**JAPAN**  
Jimpei Harada  
Sadao Hoshino

*Category III*  
Nagoya University  
University of Tsukuba

**KOREA**  
Young Ja Park

*Category I*  
Sook Myung Women's U.

**MALAYSIA**  
Abdul Hamid Othman

*Category I*  
University of Kebangsaan

**NEW ZEALAND**  
Graeme Gainsford

*Category II*  
D.S.I.R.

**PAKISTAN**  
Anwar ul Haq

*Category I*  
A.Q. Khan Research Labs

**PHILIPPINES**  
Wyona Patalinghug

*Category I*  
De La Salle University

**SRI LANKA**  
R Gunawardane

*Category I*  
University of Peradeniya

**TAIWAN**  
Yu Wang

*Category II*  
National Taiwan Univ.

**THAILAND**  
P Phavanantha

*Category I*  
Chulalongkorn University

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## ASCA COUNCIL 1988-90



*ASCA Council pictured following their first meeting on August 17. From left, seated: M A Viswamitra (Vice President), Sydney Hall (President) and Jimpei Harada (Secr. Treasurer). Standing: Krishan Lal, Fang Ming Miao, Wyona Patalinghug, Abdul Hamid Othman, Sadao Hoshino, Peter Colman, A Q Khan, Graeme Gainsford, Richard Gunawardane, Ting-Fong Lai, Phathana Phavanantha, and Yu Wang.*

# CONSTITUTION of the ASIAN CRYSTALLOGRAPHIC ASSOCIATION

## 1. Name

The Asian Crystallographic Association (ASCA) is hereafter referred to as "the Association".

## 2. Objectives

(a) The objective of the Association is to contribute to, and to promote, the advancement of crystallography and allied subjects in Asia.

(b) The Association adheres to the objectives of the International Union of Crystallography (IUCr).

## 3. Membership

(a) Membership shall be open to those countries and regions (which are hereafter referred to as "countries") within the Asian region bounded by Japan, Korea, China, Pakistan, India, Australia and New Zealand.

(b) A member country shall choose, with the approval of the Council, one of the three categories of membership set out in Articles 4(a) and 5(a).

## 4. Council and Executive

(a) The Association shall be administered by a Council consisting of Councillors from each member country. The number of Councillors from a country and the voting power given to each Councillor shall be in accordance with the membership category, as follows,

Category	I	II	III
Number of Councillors	1	1	2
Total number of votes	1	2	4

The Councillors representing each country shall be appointed by the National Crystallographic Society of that country, or if such an organization does not exist, by the National Committee affiliated with the IUCr. If neither of these bodies exists, the member shall be co-opted by the Executive from among the practising crystallographers in the country.

(b) The Council shall elect a President, Vice President and Secretary-Treasurer. The Executive Committee consists of those three members elected.

(c) Executive members shall hold office for one three-year term, after which elections

shall be held. No member of the Executive shall serve more than three terms. The President shall serve for one three-year term and shall not be eligible for re-election as President.

(d) The Council and Executive shall meet at least once in every three years, preferably at the triennial IUCr Congress. A quorum for meetings of the Council shall consist of not less than one half of the current membership eligible to vote. All members of the Executive must be present at a meeting of the Executive Committee. Notice of meetings of either body shall be circulated to all Councillors at least six months in advance.

(e) If the Councillor for a particular country is unable to attend a meeting of the Council or Executive, an alternate may be appointed by the National Society or National Committee of that country.

## 5. Finances

The finances of the Association shall consist of the following.

(a) Membership dues in accordance with the category, as follows,

Category	I	II	III
Number unit contributions	0	1	2

The unit contribution, stated in terms of a specific currency, and the category of the member country, shall be approved by the Council at the triennial meeting.

(b) Gifts received by the Association with the permission of the Executive Committee.

(c) In the event of dissolution of the Association, its funds shall be dispersed among the member countries in accordance with their accumulated number of unit contributions.

## 6. Changes to the constitution

Proposals for changes to the constitution shall be communicated in writing to the President at least six months prior to a Council meeting. A change to the constitution shall require a two thirds majority vote of all those eligible to vote at Council meetings. Voting may be recorded by mail or proxy.

## **XIVth CONGRESS ON GENERAL ASSEMBLY OF INTERNATIONAL UNION OF CRYSTALLOGRAPHY PERTH, AUSTRALIA, 12-20 AUGUST 1987**

The Meeting in Perth, August 12-20, 1987, was attended by more than a thousand people from around the world, many more than expected and this made for a very convivial atmosphere. The campus of the University of Western Australia was delightful with a view of the city across the water, yacht clubs and pelicans from the water's edge as part of the campus. Green parrots, peacocks and flame trees were everywhere and the sun shone most of the time. A most amazing sight was the kangaroo paw flower which is found only in this part of the world. These sights made the campus a most photogenic and interesting site for a meeting. One Californian remarked, as the parrots squawked, that the trees looked the same but they didn't sound the same. Coffee in the museum was excellent and the aboriginal art, some available as posters through the generosity of Robert Holmes à Court, were enjoyed by the participants particularly since some were reminiscent of electron density maps.

At the opening ceremony the first P.P. Ewald Memorial Medal was presented to J.M. Cowley and A.F. Moodie for their contributions to the development of techniques and instrumentation in the field of electron microscopy. Then Brian Matthews gave a Bragg Lecture, entitled "Crystallography in the Life Sciences" reminding us that W.H. Bragg taught in Adelaide. Of particular interest was his description of the Laue photographs taken with synchrotron radiation by Louise Johnson showing the progress of an enzyme-catalyzed reaction, that of glycogen phosphorylase b. Her poster on the subject noted that a stationary crystal Laue photograph with a millisecond exposure will give up to 70% of the data to 3Å resolution on a single photograph. Brian also discussed the work on the photosynthetic reaction center and the cold virus which have been so interesting. He then talked about studies from his own laboratory on the structural effects of protein mutations.

The general program for the meetings reflected the multidisciplinary character of crystallography. The Program Committee consisting of A. Authier, U. Bonze, C.-I. Bränden, V.A. Koptsik, K. Kuchitsu, R.E. Newnham and C.K. Prout, with H.C. Freeman as the Chairman, are to be congratulated on an excellent scientific program which was greatly appreciated by the participants. Our only

regret was that it was not possible to attend all the plenary lectures.

On the Thursday, David Blow gave a talk on site-directed mutagenesis and structural studies to probe and modify enzyme action. His themes, using tyrosyl-t-RNA as an example from his laboratory, were improvement of the action of the enzyme and improvement in the stability of the enzyme. At the end he philosophically noted that we should discuss how good a thing it is to have many crystallographers working on the same enzyme as is done now, rather than the way it used to be when crystallographers undertook problems no one else was working on. Recent advances in powder diffraction were described by A.W. Hewat, particularly the data obtained by the use of neutrons or synchrotron radiation.

John M. Thomas talked about zeolites, the minerals that froth when heated with a blowpipe. Their catalytic activities were the main focus of the investigations by a variety of physical techniques that he described. The unique geometry of the "active sites" of zeolites makes them of great interest to the X-ray crystallographers but there are extensive problems in the analysis of their structures. G. Materlik gave a comprehensive review of the present status of X-ray surface crystallography. These two plenary talks covered areas that might have been of interest to the same people.

The talk of Saturday by J. Glusker accented small molecule crystallography and the insights it has given into biological activity. The main themes were structure, recognition and reactivity. Dan Schechtman gave a talk on quasi-periodic crystals. This was also the subject of a subsequent symposium with reviews by Marjorie Senechal and A. Janner.

The symposia that took up the rest of the morning each day after the plenary lectures were useful and well-attended. It was not possible to attend all and some had such a packed audience that it was hard to get in. Topics covered included molecular complexes and protein engineering. In the protein-nucleic acid symposium Stubbs noted that sometimes filaments are all you have to work with and showed us some nucleic acid-protein interactions, computed by  $6F_o - 5F_c$  maps,

for TMV. The surrounding of a calcium ion were also revealed. Maxine McCall gave an overview of drug-nucleic acid interactions.

An evening session on relatively high temperature superconductors went on late into the night. This has been an exciting area in the last year. Sam LaPlaca led us through the general physics of the process. In the normal state the magnetic flux lines will penetrate a sample but in superconductors this is not so and that is why projects involving levitation can now be contemplated. Most of the crystal structures determined were perovskite-like. There were many informative papers given on the subject but the exact reason that these materials are superconducting did not appear to be fully understood at this time.

On Sunday there was an outing to York by steam train (the Hotham Valley Railroad). The journey took 3-1/2 hours each way so that there was plenty of time for chatting with crystallographers who filled the entire train. A buffet lunch was held in the town hall and then we were able to walk through the town and its environs which were pretty, especially down by the river Avon.

The next day Hans Deisenhofer talked about the photosynthetic reaction center and M. Hirabayashi discussed lattice defects studied by high resolution electron microscopy. The concept of electronic publishing was discussed in some detail in an *ad hoc* session chaired by K. Prout of Oxford University (England). This addressed the idea of journal distribution on ROM (Read Only Memory) compact discs (CDs). A demonstration in the commercial exhibition, developed by Oxford University Press and IBM (England), presented very impressive color graphics as an integral part of the data contained on the compact disk and the software associated with it.

In the evening there was a symposium in honor of Jerry Karle and Herb Hauptman.

On the Tuesday, Alwyn Jones, with his characteristic good humor, talked about proteins and the use of computer graphics in their structure analyses. X-ray characteristics of superlattices and epitaxial layers were described by M. Sauvage-Siniken.

During a session on IUCr journals Sidney Abrahams was thanked for a decade of dedicated service to the crystallographic community as Editor of *Acta Crystallographica*.

Recent developments in computer technology, with exciting hardware developments, were the themes behind two microsymbiosia: these involved "crystallographic micro-computing" organized by H. Huml and "computer graphics for crystallography" organized by Bob Langridge. Two associated sessions were held on crystallography in the design of molecules with specific biological properties. In one of these P.W. Codding described the interplay between the results of crystal structure determinations and molecular mechanics.

The poster sessions and instrument displays were held in the gymnasium and provided an excellent area for meeting colleagues, discussing work and planning new projects. The abstracts of papers will be published as a supplement to *Acta Crystallographica*, Volume A43.

At the Thursday closing session Ted Maslen gave a good talk on views of running a meeting. He noted that elastic deadlines are the antithesis of good management as they create more problems than they solve. They penalize the majority to help the minority. Since 60% of the abstracts came after the deadline, he thought deadlines were too unrealistic. Unstructured discussion in meetings is one of the most wasteful methods of expending human resources. Committee meetings should be no longer than absolutely necessary. Scientists should be freed from the chore of committee meetings since their real role is interacting with colleagues and younger people. He gave a list of ways to implement this.

We all dispersed to other parts of the world, other meetings or home but the general message from all we have met is that it was a very informative and exciting meeting.

*J P Glusker and J J Stezowski*

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*Extract from the ACA Newsletter (Oct 1987)*

## XIVth GENERAL ASSEMBLY

The General Assembly met for business on three occasions during the Perth meeting. The dates were: August 13, 14 and 18, 1987. The U.S. delegation was composed of R.F. Bryan, Chairman, W.L. Duax, J.P. Glusker, W.A. Hendrickson and L.H. Jensen. Alternate U.S. delegates were S.C. Abrahams, C.E. Bugg, G.A. Jeffrey, I. Karle and B.W. Matthews.

The following items were discussed and acted on, where appropriate.

1. No dues increases were considered necessary because of a reasonably good financial picture at this time. This is a result of the formation of the hard-working Finance Committee initiated when Jerry Karle was President.
2. Bulgaria was admitted as a member and the voting category of South Africa was changed from 1 to 2.
3. The three sections of Acta Crystallographica will be kept in their present form and there are tentative plans for a rapid communication section, possibly, for a machine-readable section, for special issues on important topics and to provide more timely indexes. John H. Robertson is retiring as Book Review Editor and his place will be taken by Robert Gould.
4. The Commission on Crystallographic Studies at Controlled Pressures and Temperatures, started in 1969, was dissolved.
5. The Commission on Powder Diffraction was formed. Ray Young presented the case for the formation of this Commission. It will consist of a Chairman and six elected members (see the report by Ray Young that follows).
6. There was discussion of disbanding Commissions that do not provide a report of their work during the three-year period.
7. This General Assembly asks the Executive Committee to report to the XVth General Assembly concerning the desirability of creating a Commission on Crystallographic Information to replace the present Commissions on Journals, Structure Reports and Crystallographic Data. This was a motion from the Australian delegation which passed. The aim was to focus on the total picture of crystallographic information and not on the separate aspects of it.
8. The XVth General Assembly will be held at Bordeaux, France, July 19-28, 1990. A. Authier will be Chairman of the Program Committee and M. Hospital will be Chairman of the Organizing Committee. Satellite meetings are tentatively being planned on computing, neutron diffraction and magnetic scattering.
9. The XVIth General Assembly will be held in Beijing, People's Republic of China in August, 1993. The invitation of the United States lost in the voting by a narrow margin.
10. The umbrella organization that oversees the International Unions, including the IUCr, is called ICSU and it is mainly concerned with the promotion of science. Since science is the seeking after truth and has nothing to do with politics the following was approved after a discussion of some problems that IUCr had been having. The General Assembly urges the Executive Committee to continue monitoring situations as they develop and to take all steps to ensure that there is neither discrimination against any members of the IUCr nor handicap to the pursuance of their activity as scientists.
11. The Asian Crystallographic Association became a Regional Associate of the Union after a discussion of the name since Australia is also a member. The Chairman is Syd Hall.
12. A Committee to oversee the IUCr/Oxford University Press Book Series has John H. Robertson as Chairman, members V. Simonov, M. Glaser, J. Glusker and Howard Stanbury. Two more members will be chosen. Several books are in press, being edited or written or under consideration. The Australian delegation proposed the following motion which passed (30 for, 15 against, 22 abstentions): "Conference Proceedings shall be published in the IUCr Crystallographic Symposia only in cases where the individual contributions have been subjected to refereeing at the same standards as apply to contributions to the Union's journals."
13. The new President of IUCr is Mario Nardelli, Italy. The new Vice-President is Y.-q. Tang, People's Republic of China. The new Secretary-Treasurer is A. Hordvik, Norway. New Executive Committee members are: P. Coppens, USA, S.A. Semiletov, USSR and R. Diamond, U.K. We congratulate them.

*J P Glusker*

**In the next July issue.....**

- \* Who's who in our national societies
- \* Survey of equipment in the region
- \* News of research and meetings

## Asian Structural Chemistry Workshop in Perth

A group of crystallographers from South East Asia attended a post IUCr Congress workshop at the University of Western Australia last month. Syd Hall, Allan White and Brian Skelton of Chemistry conducted the workshop, which provided a refresher course on all stages of structural chemistry and crystallographic analysis. The workshop was financed by a number of donor agencies through the Asian Coordinating Group for Chemistry operating under the auspices of UNESCO.

Participating in the 6-week workshop were Narongsak Chaichit (Silpakorn U. Thailand), Abdul Hamid Othman (U. Kebangsaan Malaysia), Chaveng Pakawatchai (Prince of Songkla U. Thailand), Wyona Patalinghug (De La Salle U. Philippines), Phathana Phavanatha (Chulalongkorn U. Thailand), Sidik Silong (U. Pertanian Malaysia) and Uncharee Tooptakong (Silpakorn U. Thailand). Yao Jia-xing (Academia Sinica Beijing) who was working at the Crystallography Centre during this period also assisted with the activities of the workshop.

Each participant collected data on several structures and carried out all of the necessary structure analysis calculations. During the course of the workshop 21 structures were solved and refined. Some of the analyses were done using the XTAL System installed on an IBM PC - Definicon co-processor. This combination provides a low-cost computing facility appropriate for many of the crystallography groups in the region.

## News from India

◊ A regional workshop on Data Bases is being held at the National Information Centre for Crystallography, University of Madras, January 18-23 1988. The theme of the workshop is the "data storage, retrieval and dissemination in Science, with special reference to chemical and molecular biosciences". Details of this meeting will appear in the next newsletter.

◊ M A Viswamitra of the Indian Institute of Science in Bangalore has been awarded the prize by the International Centre for Theoretical Physics (UNESCO) for his contributions to third world science. Prof Viswamitra was also

elected as a member to the Third World Academy of Sciences in Trieste, Italy.

## News from Japan

◊ The 1987 Annual General Meeting of the Crystallographic Society of Japan, in conjunction with a symposium on Advanced Materials and Crystallography, was held at the Hotel Sunroute Nagaoka in Nigata, November 9-11. There were more than 250 participants and 139 papers presented. The JCS prizes were given to Kenzi Hiraga (Tohoku U.) for the development of high resolution electron microscopic method for studying quasi-crystals, and to Tomitake Tsukihara (Tottori U.) for the application of X-ray structure analytical methods to the study of the evolution of biomolecules. The Seiji Nishikawa commemorative talk, entitled "Micro World of the Alloy Semiconductor", was given by Akio Sasaki (Kyoto U.)

◊ A book on the history of crystallography in Japan is presently being compiled by a CSJ committee chaired by Tosio Sakurai (Shinshu U.). It will be published later this year.

## Meeting Diary

- Jun88* ACA annual meeting. Philadelphia.
- Jun88* Sagamore IX. Charge Spin Momentum Density. Luso-Bucaco, Portugal.
- Jul88* Conf. Neutron Scattering. Grenoble.
- Aug88* Int. Liquid Crystal Conf. Paderborn.
- Aug88* ECC annual meeting. Vienna.
- Aug88* SRI-88 Conf. Synchrotron Radiation Instrumentation. Tsukuba.
- Oct88* Computational Methods & Chemical Design. Elmau FRG.
- Nov88* CSJ annual general meeting. Osaka.
- Feb89* SCA general meeting. Melbourne.
- Aug89* ECC annual meeting. Moscow.
- Aug89* ICCG-9 Conf. Crystal Growth Sendai.