



Newsletter

of the ASIAN CRYSTALLOGRAPHIC ASSOCIATION.

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President's Message

This is the second Newsletter for our Association. I am pleased to report that with most membership dues paid, the Association is now financially independent. This has been helped by a generous donation of 100,000 Yen from the Crystallographic Society of Japan. Professor T. Sakurai, the then-President of the CSJ, must be thanked for the continued support that he and his Society have given to our Association.

The news of crystallographic activities contained in this issue come from many different sources. It includes reports of events that missed the last newsletter but are still of interest to crystallographers in the region. The contents of these newsletters depend entirely on the information that has been sent in, or that has appeared in national newsletters. Any crystallographic news of the region sent to me will be included if space permits.

This issue does not contain the survey of the diffraction equipment promised in the last Newsletter. This will take much longer to compile than first expected. We have, however, provided where possible the most recent

memberships of the national crystallographic Societies. More details of the national executives and IUCr committees will be published as they come to hand.

The difficulty in obtaining complete details of crystallographic equipment in our region is not surprising. Most national associations do not have an inventory of equipment in their own country. Such information will, however, be very valuable to the future activities of the Association, both for the purposes of resource sharing and collaborative research. It will also provide us with a gauge of how crystallographic research facilities are progressing (or regressing!) in the region, and what the principal research directions are.

These are all important matters. The need for specialized research equipment is increasing, and the associated costs are very high. This can be better coordinated when we have a proper understanding of the current and future activities in the region. This will in many cases involve closer international collaboration since even the wealthiest nations will require outside support to justify such equipment. This has already been demonstrated by the activities of the Japanese Photon Factory which actively encourages

collaborative research ventures (this is discussed elsewhere in this newsletter).

In order that the survey of crystallographic facilities will be thorough, and therefore useful, a questionnaire will be sent to you by your ASCA council member. It has been kept as short and as simple as possible. Please fill it out and return it us promptly. I am well aware that completing questionnaires is a relatively irksome task, but keep in mind that it will provide us with information useful to us all. If the survey not comprehensive, it will be inaccurate and misleading, so please give it high priority.

In closing I wish to thank everyone that has sent in material for this edition of the newsletter. Communication will remain for the time being the main activity of ASCA. But, as the reports herein show, there are many crystallographic meetings going on in our region, and it seems only a matter of time before several of these will be combined for the first ASCA meeting. This will not happen, however, before the next IUCr Congress. Correspondents please keep in mind that the next ASCA Newsletter will be issued in January.

Syd Hall

Madras Data Base Workshop

A South Asian Workshop on "Data Storage, Retrieval and Dissemination in Science, with special reference to Chemical and Molecular Biosciences" was held in Madras, 18th-23rd January 1988. The workshop was organised by the NICRYS Centre of the Department of Crystallography and Biophysics, University of Madras, which is headed by Professor R. Srinivasan. The main focus in the meeting was on modern computerised data bases, particularly of the non-bibliographic hard data variety used in chemical and molecular biosciences. There were about 100 delegates mostly from India and the surrounding countries such as Bangladesh, Malaysia, Thailand, etc.

There were fifteen specialist speakers including from outside India, D. G. Watson (U.K.), G. W. A. Milne, R. Jenkins, S. Heller, F. Blattner, R. Feldman (U.S.), G. Bergerhoff, and R. Sievers (FRG). Groups from within India also presented results on the use of data bases, especially CSD operated by NICRYS at Madras. They were T. N. Guru Row, S. Krishnan, S. Ramakumar, C. Ramakrishnan, V. S. Jakkal, G. R. Desiraju, N. Yathindra, R. Srinivasan, A. S. Kolaskar, and J. Vijayalakshmi. The lectures were conducted mostly in the mornings, especially during the first half of the week. Demonstrations were held mainly in the afternoons and evenings.

Structural databases formed the major topic of the meeting. The Organic Crystal Structure (CSD), Inorganic Crystal Structural (ICSD), Powder Diffraction and the NBS-Crystal data bases were demonstrated. In addition to crystallographic data, mass spectroscopic data, the Beilstein Chemical data (both for use on PC's) were covered. Molecular graphic displays of both nucleic acids and proteins were demonstrated using a NEXUS 3000 graphics workstation. The nucleic acid sequence data

analysis using a PC/AT system with data on a CD-ROM (Optical disk) unit was a notable feature. Also considered was the development by NICRYS of the software for handling the CSD data using dBASEIII for PC/AT system.

News from Taiwan

In December last year crystallographers in Taiwan formed a study group under the Chemical Research Promotion Center, National Science Council. The group organizer is currently Dr. Ling-Kang Liu. The current directors of Chemical and Physical Research Promotion Centers are Prof. Yu Wang and Prof. Shih-Ling Chang, respectively. Both are crystallographers.

Since the formation of the study group, two crystallography symposiums have been organised. The first was held in Taipei on December 19 last year. The speakers were Dr. B. C. Wang from Pittsburgh and Dr. Andrew Wang from MIT. The second meeting was held in Shih-Men on March 19 of this year. The speakers were Dr. Ling-Kang Liu, and Prof. Peter Chieh. Prof. Chieh is currently on Sabbatical leave from Univ. of Waterloo, Canada and is a Visiting Professor in Tsin-Hwa University. The next annual meeting is to be held in Taipei on July 23.

The year 1987 proved to be an excellent one for crystallography in Taiwan. Two four-circle diffractometers were installed in Chemistry Departments, one CAD-4 and one Nicolet. In addition, three rotating anode generators were purchased by Physics Departments of several Universities; two Rigaku 12 kw/3000 cps and one Elliot 15 kw/6000 cps. These facilities included a powder diffractometer, a topographic camera, a Hubert four-circle goniometer and a small-angle scattering device.

Adelaide Computing School

In August last year an International School on Crystallographic Computing was held at the Flinders University of South Australia in Adelaide (the city to Bragg about!). It was held under the auspices of the International Union of Crystallography and the Society of Crystallographers in Australia. The School provided lectures and tutorials on the application of computing techniques for crystallographic studies. The Chairman of the Program Committee was Neil Isaacs and the Local Organizing Chairman was Max Taylor. The Hon. Barry Jones, Minister for Science, attended the dinner of the School and gave the opening address.

The School was attended by 85 scientists and senior post-graduate research students. There were 23 lecturers from the U.S.A., Canada, U.K., France, Netherlands, F.R.G., Italy, Israel, Switzerland, Czechoslovakia and New Zealand. The participants were from Australia (22), Brazil (1), Canada (6), Chile (1), China (1), Denmark (2), F.R.G. (6), France (2), India (8), Israel (1), Japan (4), N.Z. (1), Nigeria (1), South Africa (2), Sri Lanka (1), Sweden (1), Switzerland (1), Thailand (2), Netherland (2), U.K. (6), U.S.A. (13), and U.S.S.R. (1).

The emphasis of the School was in techniques for solving structures. These included direct, maximum entropy, anomalous dispersion and simulated annealing methods. The interpretation of structure analyses was considered graphically and statistically. Structures, from proteins through to small molecules and powders were covered. Other topics included diffractometry, electrostatic properties, methods of calculating electron wavefunctions and communication via electronic and computer networks. Participants were also instructed in the use of the Inorganic and Cambridge databases and in symbolic programming.

News from Japan

The Executive Office of the Crystallography Society of Japan (CSJ) is now located at: 3-32-5, Hongo, Bunkyo-ku, Tokyo 113, Hongo Heights 501, Phone: 03-815-8514, Fax: 03-815-8529.

The 1988 Executive of the CSJ is the President: Yukitomo Komura, Hiroshima University; the General Secretary: H. Hriuchi, Tokyo University; Treasurer: Yuji Ohashi, Ochanomizu University; Secretary for Foreign Affairs: Osami Nittono, Tokyo Institute of Technology;

Secretary for Annual Meetings: Tatzumo Ueki, Osaka University; Editor of the Journal CSJ: I. Ohsumi, PF, KEK; and Computing: Masaaki Ohmasa, Tsukuba University.

The Activity Reports of the Photon Factory of the National Laboratory for High Energy are available on request from the Technical Information Office, National Laboratory for High Energy Physics, Oho-machi, Tsukuba-shi, Ibaraki-ken 305, Japan. The easiest way for overseas users to work at the Photon Factory is to be come involved in a collaborative project with Japanese scientists. If you are interested in using facilities at the Photon Factory, it recommended that you contact a scientist at a Japanese University and arrange to become his or her host for the research project. A recent CSJ monograph has been published to tell overseas readers about the most recent techniques used in Japan's Photon Factory. It is "X-ray Instrumentation for the Photo Factory: Dynamic Analysis of Micro Structures in Matter" edited by S. Hosoya, Y. Iitaka and H. Hashizume (KEK Science Publishers/Tokyo, 1986).

The inauguration of Japanese Society of Synchrotron Radiation Research occurs next April, and the first President is Kazutake Kohra, a past Director of the Photo Factory.

Members of the CSJ who are currently members of IUCr Commissions are: Hitoshi Iwasaki (Journals, JAC); Tamaichi Ashida (Journals, Acta); S. Wakoh (Charge, Spin and Momentum Density); Hiroshi Komatsu (Crystal Growth, etc.); Hiroo Hashizume (Crystal Apparatus); Noritake Yasuoka (Cryst. Data); Hiroshi Iwasaki (Controlled Pres. Temp.); Michiyoshi Tanaka (Electron Diffraction); Masashi Iizumi (Neutron Diffraction); and Takamitsu Yamanaka (Powder Diffraction).

Meeting Diary

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| 28 Aug - 2 Sep 88 | European Crystallographic "ECM-11". <i>Vienna, Austria.</i> |
| 15 - 24 Sep 88 | IUCr Summerschool on Crystallographic Teaching. <i>Tianjin, China.</i> |
| 10 - 14 Oct 88 | Computational Methods & Chem. Design. <i>Elmau, FRG.</i> |
| Nov 88 | CSJ annual general meeting. <i>Osaka, Japan.</i> |
| 16 - 19 Feb 89 | SCA meeting "Crystal 16". <i>Lorne, Australia.</i> |
| 20 - 29 Aug 89 | European Crystallographic "ECM-12". <i>Moscow, USSR.</i> |

News from Australia

Here are some excerpts from the March '88 Newsletter of the Society of Crystallographers in Australia.

The current executive of the SCA is President : Peter Colman; Vice President: Neil Isaacs; Secretary: Geoff Williams; Treasurer: Colin Kennard; and Council: Bob Cheary, Jim Graham, Maureen Mackay, and Syd Hall (Past President).

A meeting of the SCA Council was held in Melbourne on the 25th February 1988. At the meeting a request was supported for \$2500 to assist Prof. Jack Dunitz to attend the SCA "Crystal 16" meeting being held at Lorne Victoria, February 16-19, 1989. Prof. Dunitz will be the first recipient of the "1987 Fellowship" set up with funds from the Perth IUCr Congress.

Congratulations to the SCA President (and ASCA Councillor) Peter Colman for winning the 1988 Lemberg Medal from the Australian Biochemical Society for his work on influenza viruses.

All those who have been welcomed to AINSE at Lucas Heights over the years by a smile from Bill Palmer, will be sad to hear of his impending retirement in August. From the many people who have worked and visited AINSE over the years, thanks and good luck Bill!

John Parise has resigned his position as lecturer in chemistry at the University of Sydney to take up a teaching and research position at the crystallographic lab. of the Department of Earth and Space Sciences, State University of New York at Stony Brook. We suspect some of the appeal of this new position is the proximity of the Brookhaven Synchrotron.

Neil Isaacs returned to Melbourne in March after spending six months with Dr. Guy Dobson at York. He was accompanied by his student Sandra Cowan. Steve Wilkins has escaped Melbourne's autumn by spending four months (from mid-March) at the Photon Factory, Tsukuba, Japan. Rod Hill, the SCA's past-Secretary, is taking nine months study leave in Germany at the Mineralogical Institute, University of Wuerzburg. Rod is on a Ludwig Leichhardt Fellowship with Prof. E. Tillmanns.

Syd Hall is also in Germany on 12 months leave at the Max-Planck-Institut für Kohlenforschung,

Mülheim/Ruhr. He is pursuing his usual XTAL activities, and will be attending the Vienna ECM and Elmau molecular modelling meetings.

Around October, David Stuart and Yvonne Jones from the Molecular Biophysics Laboratory, Oxford, will be visiting CSIRO Protein Chemistry and Materials Science (Melbourne) on Bicentennial Fellowship.

Bob Cheary is in Grenoble from July to October. He will work with Alan Hewitt at ILL and will then spend time at the Daresbury synchrotron until January '89.

Sadly, we note the death of two SCA members - Mr. Janis Fridrichsons and Dr. John Sanders. Janis, who retired from the Division of Chemical Physics, CSIRO, over twenty years ago, died in Canberra in July of last year. The death of John Sanders in December 1987 brought to a close a distinguished crystallographic career that spanned almost forty years.

Most readers will be aware that the First Ewald Prize for outstanding contributions to the science of crystallography was awarded by Theo Hahn, then-President of the IUCr, to John M. Cowley and Alex F. Moodie at the Opening Ceremony of the Perth IUCr Congress in August 1987. After the Congress, Theo Hahn passed through Sydney on his way back to Europe, and presented Hans Freeman with signed originals of the Ewald Prize citation to Alex Moodie and the Ewald Medal citation to Mrs. Ella Ewald. Hans has very kindly passed the Alex Moodie citation to the SCA for preservation in the archives, and the other citation will be framed for permanent display in the School of Chemistry at the University of Sydney. As Hans indicated, these are clearly collector's items which should be preserved, and it is the SCA's intention to frame the citation.

UNESCO Workshop in Malaysia

A Workshop on the Systematic Identification of Natural Products was held on Bangi, June 13-17, 1988. It was organised by the Department of Chemistry, University Kebangsaan Malaysia in cooperation with UNESCO, as an activity within the framework of the Regional Network for the Chemistry of Natural Products in Southeast Asia. The Chairman of the organizing committee was Dr. Ikram Said, and the Secretary was the Malaysian ASCA Councillor Dr. Abdul Hamid Othman. A report of this meeting will be published in the next Newsletter.

Tianjin IUCr Summer School

The IUCr is sponsoring a Summer School on Crystallographic Teaching at Tianjin Normal University, September 15 to 24, 1988. The school is jointly organized by the IUCr Commission on Crystallographic Teaching, the Chinese National Committee of Crystallography, Tianjin Normal University, and Peking University.

The Chairman of the Scientific Program Committee is Prof. Henk Schenk of the University of Amsterdam, and the Chairman of the Local Organisation Committee is Prof. Miao Fang-Ming of Tianjin Normal University. Prof. Shao Mei-Cheng of Peking University is Vice Chairman of both Committees.

The lecturers at the school are expected to include W. Clegg, T. Hahn, H. Schenk, C. Nordman, H. Hauptman, P. Main, Yao Jia-Xing, Fan Hai-Fu, P.T. Beurskens, D. Watkin, D. Schwarzenbach, A. Authier, I. D. Brown, J. P. Glusker, P. Murray Rust, R. Shirley, K. Davis, and R. Jenkins.

The school will be of eight days duration, with the mornings devoted to plenary lectures and the afternoons to working sessions. There will also be poster sessions. The working language will be English. Topics for the school span most aspects of crystallography, from measuring diffraction data to molecular modelling. Lectures on powder techniques will also be given. Registration forms and information are available from Associate Prof. Liu Xiao-Lan, Department of Chemistry, Tianjin Normal University, Tianjin, China.

Financial support for young crystallographers will be available from funds provided by the IUCr and the ICSU committee of COSTED. Crystallography students and postgraduates should apply to Prof. Liu Xiao-Lan. Preference will be given to those presenting posters.

News from India

The 14th National Seminar on Crystallography was held on 18-19 December last year at Gandhiji University, Kerala. Various aspects of crystallography was covered with emphasis on materials science. The meeting organized by Prof. M. A. Iyyachen of Gandhiji University.

The 15th National Seminar on Crystallography will be held at Banaras. For details about this meeting contact Prof. O. N. Srivastava,

Department of Physics, Banaras Hindu University, Varanasi 221005.

The Indian National Committee for IUCr currently consists of M. A. Viswamitra (Chairman), Indian Institute of Science, Bangalore; R. Chidambaram, Bhabha Atomic Research Centre; S. P. Sen Gupta, Indian Ass. for Cultivation of Science; M. Vijayan, Indian Institute of Science, Bangalore; E. Subramanian, University of Madras; G. R. Desiraju, University of Hyderabad; A. K. Singh, National Aeronautical Laboratory, Bangalore; O. N. Srivastava, Banaras Hindu University; and S. K. Sikka, Bhabha Atomic Research Centre.

The following have also been elected as members of the IUCr Commissions: M. Vijayan (Small Molecules; Biological Macromolecules); Krishan Lal (Crystal Growth); R. Srinivasan (Crystallographic Teaching); P. Krishna (Polymorphism, Quasi Crystals, etc.); and A. Sequeira (Neutron Diffraction).

As was reported briefly in the last Newsletter, the ASCA Vice President M. A. Viswamitra has been awarded the Third World Academy of Sciences (TWAS) Biology prize for his fundamental contributions to DNA structures. He received the Award at the TWAS Second General Conference (September, 1987) in Beijing, China. Prof. Viswamitra has also been awarded the 1988 Rameshwardas Birla National Award for his work on nucleoside co-enzymes and Drug-DNA studies. In addition he received the 1987 Bhatnagar Prize for his work.

New Society in Pakistan

Late last year the Pakistan crystallographers formed their own national association. Dr. Qurashi of the Pakistan Academy of Science reports on the new Crystallographic Society of Pakistan. The Executive of the CSP is the President: M. M. Qurashi; Vice-President: N. M. Butt, Pakistan Institute of Technology; the Secretary: S. S. H. Rizvi, P.C.S.I.R. Laboratories; and Treasurer: S. R. H. Baqri, Islamabad Natural History Museum. Local Secretaries are Khadim Hussain (Lahore); M. A. Qaiser (Peshawar); Ehsan H. Chauhan (Quetta); Saghir Ahmad (Karachi); and C. A. Majid (Islamabad). Committee Members are Zulfiqar Ahmed, University of Baluchistan; Niaz Ahsan, Pakistan Steels Mill Corporation; Asghri Maqsood, Quaid-e-Azam University; and Anwarul Haq, A. Q. K. Research Laboratories. Dr. Haq is on the ASCA council.

Names and Addresses of the 1988-1990 ASCA Council

Please contact one of the Council Members below if you have any enquires about the ASCA, or have any contributions for this Newsletter.

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