

Society of Crystallographers in Australia

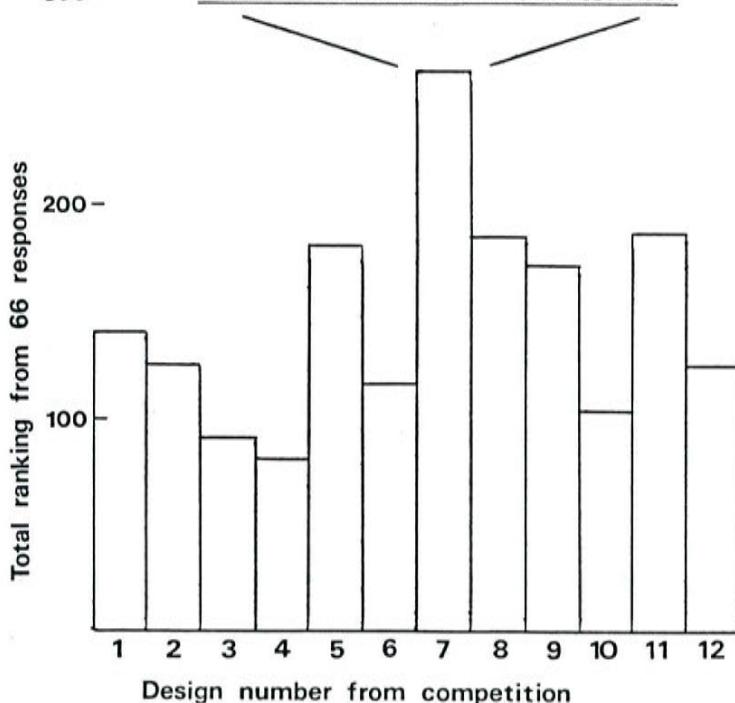
Newsletter No. 13

May 1986

CONTENTS

Office Bearers
Editorial Comment
Ballot Results:
 Constitution Amendment
 Logo Competition
Council Actions Since the Last
 Newsletter
Inaugural Newsletter to Asian
 Crystallographers
An Australian Experiment Station
 at the Photon Factory
Ewald Prize
J.D. Hanawalt Award

Summary of Responses to the
 IUCr Data Base Survey
JCPDS Australian User's Group
Crystallography News in 1985
As You Were
Personalia/Miscellaneous
Subscriptions for 1986
New Members
Situation Vacant
Scientific & Technological
 Exchange Programme
Forthcoming Meeting



- A copy of the inaugural Asian Crystallographic Association (ASCA) Newsletter has been circulated to all members, together with a copy of the first circular for the Perth IUCr Congress.
- Reminder letters have been sent to the 16 countries in the South-East Asian area that did not reply to the first request for comments on the draft constitution for ASCA.
- Discussions have been held with Prof Jimpei Harada during his recent trip to Australia regarding the quite extensive amendments proposed to the ASCA draft constitution by the Japanese Crystallographic Society.
- The Program Committee for the Perth Congress has been granted access to SCA funds for urgent secretarial assistance.
- The SCA Standing Committee on X-ray Diffraction, through its Chairperson, Stephen Wilkins, has spent a considerable amount of time preparing a case for direct Australian involvement in an experiment station at the Photon Factory in Japan (see below for further details). Peter Colman, during his term as Acting President of the SCA, sent a letter of support for these initiatives to the Dept of Science on behalf of the SCA membership.

- Hans Freeman, Chairperson of the National Committee for Crystallography of the Australian Academy of Science, has kept the SCA well informed of the activities of his Committee. These activities have included undertaking a survey on data base usage for the IUCr Data Commission, and collecting nominations for the Australian Ionising Radiation Advisory Council.
- The SCA has outlaid a further \$105 to maintain its membership in the Federation of Australian Scientific and Technological Societies (FASTS) through to June 30, 1986.
- Richard Welberry has accepted a nomination to join the FASTS Group 9 ad hoc Working Party reviewing the 1986/7 National Science Budget.

Editor's note: Copies of documents relating to the Constitution and Officers of FASTS (or, indeed, any other matter of interest) may be obtained from the SCA Secretary.

INAUGURAL NEWSLETTER TO ASIAN CRYSTALLOGRAPHERS

All members of the SCA should have recently received a copy of the inaugural Newsletter to Asian Crystallographers. This newsletter is a result of close collaboration between the Japanese and Australian Crystallographic Societies and represents the first formal activity of the Asian Crystallographic Association (ASCA). It is the fervent hope of these two Societies that the newsletter will become a powerful means for the dissemination of crystallographic information in the Asian region and that it will ultimately include contributions from all countries in the area.

Members of the SCA are encouraged to make contributions to the ASCA newsletter by submitting short articles on any of the following topics:

- (i) Activities of crystallographers, such as their changes of position, assumption of significant new duties, honours, etc;
- (ii) Exchange / scholarship programs;
- (iii) Proposed meetings, Congresses and Schools, etc;
- (iv) Correspondence and comments.

Please send these contributions either to Prof J. Harada, Department of Applied Physics, Nagoya University, Chikusa-ku, Nagoya, 464, Japan, or to Dr R.J. Hill, CSIRO Division of Mineral Chemistry, PO Box 124, Port Melbourne, 3207 Australia.

AN AUSTRALIAN EXPERIMENT STATION AT THE PHOTON FACTORY

As many of you are already aware, Stephen Wilkins has been heading a small, but very active group, the Australian Synchrotron Beam Users Group (ASBUG), which has as one of its objectives the establishment of an Australian experiment station on one of the 4 uncommitted synchrotron beam lines at the Photon Factory in Tsukuba, Japan. The initial proposal incorporates

EXAFS, powder diffraction and SAXS experimental rigs, these being the instruments most commonly cited in a recent ASBUG survey involving 45 interested groups representing 176 individual scientists in Australia and New Zealand. The cost for such a proposal has been estimated to be A\$650K in the first year (mainly capital costs), A\$240K in the second year, and about A\$180K in each subsequent year to cover the salary of a person on site at the PF and routine maintenance and upgrading. Although these costs seem high by Australian standards, they should be measured against the very high cost of constructing a facility on Australian soil and the loss of our high standing in the field of X-ray scattering research if access to a facility such as the PF is not achieved in the near future.

The proposal has been submitted to the ARGS and, in a preliminary form to the CSIRO. If the case for direct Australian involvement in the beam line at the PF can be shown to be of sufficient importance to Australian science and technology, then the experimental station may be designated a National Facility in much the same way as the Australian Telescope. This will only be achieved, however, if interested scientists mount a strong lobbying effort, drawing attention to those areas in which a synchrotron source could contribute to their research programs and any potential benefits to the National interest. A short letter of one or two paragraphs giving such details would greatly assist the cause and should be sent as soon as possible to (see over)

To speak of Australian physics would be meaningless, if what was implied was that the physics was in some way peculiar to Australia. The laws of physics are universal and the pursuit of their understanding is international. However, it is perfectly sensible to consider Australian physics in the sense of the research in physics that is undertaken by physicists in Australia.

Pure research may be conducted at a number of levels ranging from the truly innovative, breaking new ground, to the consolidating, filling-in-the-odd-corners. At all levels, advances in research techniques require continual upgrading of research equipment and facilities. The costs of establishing and maintaining the experimental facilities required for research at the forefront of physics are increasingly growing beyond the resources of a single country and international agreements to share costs are becoming more common. Such a trend towards sharing the expense of 'big science' has obvious advantages for the smaller and developing countries in that it provides access to facilities which allow the physicists in those countries to pursue their research at a level which would be otherwise unobtainable.

Where does Australia stand in regard to such international co-operation? Very much in the background, I would say. The bi-lateral science and technology agreements which exist between Australia and a number of countries only provide for the interchange of personnel. They do not guarantee access to scientific facilities and, to the best of my knowledge, there are no formal agreements that do.

Certainly, Australian scientists make good use of the facilities at CERN, ILL and no doubt many other laboratories, but this has been very much by trading on the

good will of the organisation involved. 'Suitcase' physics is one thing; but a reputation for 'hitch-hiking' is another. There is also the question of how much longer we can expect to continue to have free access to expensive facilities.

In its recent report on nuclear science and technology in Australia, ASTEC recommended that the Minister of Science should endeavour to secure access to overseas neutron beam and accelerator facilities, where possible by negotiation of reciprocal arrangements with Australian scientific facilities. Given the limited choice of scientific facilities unique enough in Australia to attract overseas interest, I can see little hope of any extensive trade-off arrangements of this sort.

An attractive and relatively inexpensive alternative is for Australia to respond to the various overtures that have been made to have an involvement in the construction of instrumentation. Such programmes would also require provision for the employment of a full-time resident scientist at the overseas laboratory. One such proposal for Australia to construct an instrument for use on a beam at the dedicated X-ray storage ring, the 'photon factory', at Tsukuba, Japan, is being actively pursued by Stephen Wilkins following his recent visit to the laboratory.

I believe it is essential for the future of Australian physics that formal agreements be established with overseas facilities. Without such arrangements it will only be a matter of time before we find we are no longer welcome and Australian physics is relegated to filling in the odd corners left by others.

T.F. Smith

From: The Australian Physicist, Vol 23, page 30, March, 1986,

Stephen Wilkins at the CSIRO Division of Chemical Physics, PO Box 160, Clayton, Victoria 3168.

A recent statement by Fred Smith (see above), in his capacity as President of the Australian Institute of Physics, eloquently sums up the need for a concerted effort to get this proposal off the ground. If you are at all interested in access to a synchrotron source without having to go begging on bended knees to the Americans or Europeans, then please give consideration (and then action) to the statements in Fred's article.

EWALD PRIZE

The International Union of Crystallography announces the establishment of the Ewald Prize for outstanding contributions to the science of crystallography. The name of the prize has been chosen with the kind consent of the late Paul Peter Ewald, to recognise Professor Ewald's significant contributions to the foundations of crystallography and to the founding of the International Union of Crystallography, especially his services as the President of the Provisional International Crystallographic Committee from 1946 to 1948, as the first Editor of the Union's publication Acta Crystallographica from 1948 to 1959, and as the President of the Union from 1960 to 1963.

The prize consists of a medal, a certificate and a financial award. It will be presented once every three years during the triennial International Congresses of Crystallography. The first prize will be presented during the XIV Congress at Perth, Australia, in 1987. This year will be the seventy-fifth anniversary of the discovery of X-ray diffraction in 1912.

Any scientist who has made contributions of exceptional distinction to the science of crystallography is eligible for the Ewald Prize, irrespective of nationality, age or experience. No restrictions are placed on the time or the means of publication of his or her contributions. The prize may be shared by several contributors to the same scientific achievement.

Nominations for the Ewald Prize are invited. They should be submitted in writing, accompanied by supporting documentation, to the Executive Secretary of the International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, United Kingdom. The closing date for nominations is 30 September 1986.

J.D. HANAWALT POWDER DIFFRACTION AWARD

The award is sponsored by the JCPDS - International Centre for Diffraction Data. It is to be presented every three years for an important, recent contribution to the field of powder diffraction. The award will consist of a certificate and \$1000. The awardee is expected to submit an abstract and present a paper on the work being recognized at the IUCr Satellite Meeting on X-Ray Powder Diffractometry, Perth, Western Australia, August 20-22, 1987. Travel expenses to the meeting will be provided.

The award was first presented in 1983 to Dr. Ludo Frevel at the Denver X-ray Conference. Work that is eligible for consideration for the second presentation of the award must have been published between 1 January 1980 and 31 August 1985. There are no restrictions as to age, experience, or nationality of the recipient.

The 1986 selection committee members are Walter Eysel (Universitat Heidelberg), Ben Post (Polytechnic Institute, NY), Brian O'Connor (Western Australian Institute of Technology), Catherine Foris (DuPont) and Camden Hubbard (U.S. National Bureau of Standards). The selection committee will welcome suggestions, nominations, and documentation of accomplishments for possible recipients through 30 April 1986 from any interested persons. These can be sent to any committee member or directly to the chairman C. R. Hubbard, A257 MATL, National Bureau of Standards, Gaithersburg, Maryland 20899, USA, (telex 894493).

Editor's note: Although the deadline has expired, I am sure that any truly outstanding nomination will still be considered.

SUMMARY OF RESPONSES TO THE IUCr DATA BASE SURVEY

SUMMARY OF RESPONSES

Question 1: Does anyone in your laboratory have experience in using one of the data bases (1) to (7)?

Cambridge Crystallographic Data File:	13	laboratories
Protein Data Bank:	3	"
Crystal Data (NBS):	1	"
Electron Density Data Banks:	1	"
Inorganic Crystal Structure Data Base	1	"
	—	—
	19	"
	—	—
By exchange of tapes:	10	"
By correspondence:	5	"
By telecommunications network:	4	"
	—	—
	19	"
	—	—

Question 2: Would it assist you to have more information than is currently available concerning
- the advantages of data bases?
- access to data bases?

- * There is a significant demand for more information concerning the advantages of data bases (9 of 16 respondents)
- * There is a strong demand for more information concerning access to data bases (16 of 17 respondents).

Question 3: Having regard to the technical facilities available to you, indicate the order of your preferences (among ways of gaining access to data bases).

- 1st preference: Interactive retrieval
 - for all data bases on a national network
 - for a single data base on an in-house facility.
- 2nd preference: Interactive retrieval
 - for all data bases on an international network.
- 3rd preference: Batch programs delivered with data
- 4th preference: Interactive retrieval
 - for all data bases on an in-house facility
- 5th preference: Individual in-house programs.

SURVEY FOR THE IUCr DATA COMMISSION

Question 3 (continued):

- * There is a genuine difference between the interests of laboratories which have need for only one data base and laboratories which require several data bases
- * The surprising first preference for a national, rather than an international, network may reflect a general lack of information concerning the procedures and costs involved in interacting with an international network.

Question 4: Is your institution connected to an international telecommunications network?

Yes: 11. No. 3. E:18.

Are you aware of specific financial problems in establishing a connection?

Hardware	Yes: 0.	No: 17.	E: 17
Telecomm. charges	Yes: 9.	No: 8.	E: 17
Data base charges	Yes: 11.	No: 6.	E: 17

- * Both telecommunication and data base charges are seen as significant deterrents against the use of data bases.

Question 5: For any one or more of the data bases (1) to (7) in which you have an interest, what type of access do you consider most appropriate in the Australian context?

Strong interest:	On-line access via national network
	On-line access via international network
Modest interest:	In-house implementation
	Publication in book form
Strong lack of interest:	Searches processed by national centre
	Searches processed by international centre

SUMMARY OF SUGGESTIONS FOR INCREASING NUMBER

OF DATA BASE USERS

Action Which Can Be Taken At International Level

1. Make access to data-bases via international networks easier
 - by improving the documentation
 - by making the software more user-friendly
 - by ensuring that search and retrieval can be performed without the necessity of local programs
2. Negotiate more favourable charges for international telecommunications when used for scientific data transfer.
3. Reduce charges for the use of the data bases
 - for academic users permanently, to encourage familiarisation by students
 - for other users during an introductory period
4. Increase awareness among non-crystallographers by advertising in non-crystallographic journals.

Action Which Can Be Taken At Local (e.g., Australian) Level

1. Familiarise crystallographers with the data-bases by publishing examples in local newsletters, (e.g., the Newsletter of the Society for Crystallographers in Australia).
2. Increase awareness among non-crystallographers by publishing examples in local scientific journals (e.g., 'Chemistry in Australia')
3. Conduct well-publicised workshops for chemists from industry, governmental laboratories and universities.
4. Train students in the use of data-bases as part of courses in Chemistry and Crystallography.
5. Form active users group.

RESPONDENTS WILLING TO ACT AS AUSTRALIAN

CONTACT FOR A DATA-BASE

(1) Cambridge C.D.F. ¹	Dr. G.A. Williams	Australian Radiation Laboratory Lower Plenty Road YALLAMBIE, VIC 3085 (03)-433-2211
(2) Crystal Data	Dr. R.J. Hill	CSIRO Division of Mineral Chemistry P.O. Box 124 PORT MELBOURNE, VIC 3207 (03)-647-0208
(3) Electron Density	Dr. E.N. Maslen	Crystallography Centre University of Western Australia NEDLANDS, WA 6009 (09)-380-2727
(4) Inorganic C.S.D.	Dr. R.J. Hill	[see above]
	Dr. B.P. Hoskins	Department of Inorganic Chemistry University of Melbourne PARKVILLE, VIC 3052 (03)-341-6471
	Dr. G.A. Williams	[see above]
	Mr. C. Dean	Department of Physical and Inorganic Chemistry University of Adelaide GPO Box 498 ADELAIDE, SA 5001 (08)-228-5712
(5) Metals		
(6) Powder Data File ²	Dr. R.J. Hill	[see above]
	Dr. B. O'Connor	School of Physics and Geosciences Wester Australian Institute of Technology BENTLEY, WA 6076 (09)-350-7539
(7) Protein Data Bank ³		

Footnotes: ¹ Cambridge Crystallographic Data File is already distributed by CSIRO Central Information Section (Director: Dr. C. Garrow), PO Box 89, EAST MELBOURNE, VIC. 3002. Ph: (03)-418-7333. TX: AA 30236

² Dr. B. O'Connor represents the Australian X-ray Analytical Association on the International Centre for Diffraction Data.

³ Users purchase the Protein Data Bank tapes either directly from Brookhaven National Laboratory or indirectly via the CSIRO Central Information Section (see footnote 1).

The biggest news in crystallography in 1985 was the award of the Nobel Prize to Jerome Karle of the Naval Research Laboratory in Washington, D.C., and Herbert Hauptman of the Medical Foundation of Buffalo. They shared the prize for their revolutionary development, about 30 years ago, of direct methods for the crystal structure determination of chemicals, drugs, hormones, and antibiotics. Their work plays a major role in allowing the structure determination of the tens of thousands of structures contained in the Cambridge Structural Database (see the article below). Both men are still active today in efforts to apply similar techniques to the determination of protein structures, a research area that may undergo a revolution (also described in an article below) in the next decade.

X-ray crystallographic data are playing an ever expanding role in molecular biophysics and pharmacology. Primary factors responsible for this growth include rapidly developing technologies, the feasibility of macromolecular engineering, and the continued growth of structural databases. The increased availability of synchrotron radiation sources and area detectors will be producing more and better intensity data on proteins.

Larger computers and more powerful mathematical techniques to automate the process of structure solution will lead to an exponential increase in our knowledge of protein and macromolecule structure. Advances in computer graphics will allow more rapid analysis and digestion of this information so that new insights into the structural basis for all biological processes will pave the way for the design of drugs and macromolecules to rectify metabolic flaws and combat disease.

William Dux, Medical Foundation of Buffalo

In the past 25 years the time required to determine the crystal structure of an average organic molecule has accelerated from years to days. This accounts for the presence of 45,000 structures in the Cambridge Structural Database. This avalanche of reliable data on molecular structure has contributed immeasurably to our understanding of the properties of atoms and molecules. We have reliable sources from which to predict characteristic bond lengths, valence angles, and nonbonding contacts for almost all atoms of practical interest.

Although the speed with which the crystal structures of proteins are determined has also been accelerated, an average protein structure determination still takes 2–3 years. The limiting factors in this process are preparation of suitable crystals doped with heavy atoms needed to permit structure determination, the availability of sufficient supply of stable single crystals for a data collection process that often requires months, if not years, and computing power capable of refining thousands of observed data.

As a result of recent technological advances many of these drawbacks of protein structure analyses are about to disappear and in the next few years it may be possible to

complete x-ray structure determination within 4 to 6 months of the time that single crystals of the native protein are prepared. The data collection process is being accelerated by the use of synchrotron radiation sources¹ and area detectors. Because synchrotron radiation is hundreds of times more intense than normal x-ray radiation, smaller crystals and much shorter exposure times can be used to obtain intensity data that often exceeds the data resolution possible from normal sources. By using film techniques a full set of intensity data on a native crystal of a 40,000 molecular weight protein can be collected in less than a week using just a few crystals. The thousands of diffraction intensities gathered on dozens of films using a synchrotron source must be read on a microdensitometer and merged into an internally consistent set of relative intensities. This process takes far longer than the actual data collection. However, sophisticated software to accomplish this task is gaining wide distribution and the availability of more powerful computers indicate that this barrier is also about to tumble.² Area detectors are multiwire electrical devices that will further accelerate the pace of protein data collection.³ Area detectors allow the simultaneous collection of hundreds of intensities in a digital form, thereby eliminating the time consuming step of film reading.

Advances in the area of methods of structure determination will also contribute to this explosion. The determination of a crystal structure depends upon determining the phases of a significant number of the observed intensities. It has been clearly demonstrated that the intensities contain information about their phases and techniques for extracting phase information from the intensities have been developed over the past 30 years. Because of the phenomenal success of these techniques they have become the method of choice in solving small molecule structures. Now it would appear that some of the strength of these techniques can be applied to protein studies so that semi-automated solution of the phase problem using data from just one heavy atom derivative in combination with the native data,⁴ data sensitive to anomalous scatters in the native protein,^{5–7} and/or data gathered from tunable wavelength sources⁸ can be expected to contribute to much faster determination of protein structures and the elimination of the need for many heavy atom derivatives.

The challenge of protein crystal structure analysis that has proven least vulnerable to attack is the initial step, that of growing diffraction quality single crystals. Protein and small peptide growth has generally been considered a branch of witchcraft rather than science. As other aspects of protein crystallography become more routine, investigators are turning their attention to developing reliable procedures for protein crystal growth. Topics addressed at the first International Conference on Protein Crystal Growth at Stanford in August of 1985 included crystallization under microgravity environment, measurement of concentration gradients, effects of polyethylene glycol, and high salt concentration on crystallization, and the mapping of solution properties during crystal growth. Experiments involving the growth of protein crystals aboard Spacelab 2 in the summer of 1985 generated a debate about the merits of such experiments.⁹ Charles Bugg of the University of Alabama, one of the pro-

ponents of the experiments suggested that crystal growth without gravitational effects and convection currents had the advantage of permitting crystals to remain suspended in a homogeneous medium during growth.

William Dux

1. T. J. Greenhough and J. R. Helliwell, *Prog. Biophys. Mol. Biol.* **41**, 67 (1983).
2. *Chem. Eng. News* August 12, 1985.
3. S. C. Harrison, *Nature* **309**, 405 (1984).
4. H. Hauptman, *Acta Crystallogr. Sect. A* **38**, 289 (1982).
5. W. A. Hendrickson and M. M. Terrell, *Nature* **290**, 107 (1981).
6. H. Hauptman, *Acta Crystallogr. Sect. A* **38**, 632 (1982).
7. W. Furey, B. C. Wang, A. H. Robbins, L. L. Clancy, and C. D. Stout, *Structure Determination of Cd. Zn Metallothionein at 2.3 Å Resolution*, *ACM Meeting Abstract A-42*, Stamford, CA, August, 1985.
8. J. Karle, *Acta Crystallogr. Sect. A* **40**, 366 (1984).
9. *Science* **239**, 370 (1985).

Crystallographic Databases and Molecular Biophysics

The Cambridge Structural Database and the Brookhaven Protein Data Bank are primary resources for molecular biologists, pharmacologists, and medicinal chemists. The Brookhaven Protein Data Bank¹ contains atomic coordinates for 237 protein structures determined by x-ray crystallographic techniques. These data provide accurate information on the molecular architecture of the active sites of numerous enzymes and other proteins of physiological importance (see Fig. 1). Systematic analysis of the data have been used to elucidate basic patterns in tertiary structure of proteins. These patterns have been useful in tracing molecular evolution and in developing guidelines for predicting the three-dimensional structure of proteins on the basis of their amino acid sequence. The frequency with which different amino acid residues have been observed to occur in α -helical segments of proteins has long been one of the most reliable guides to predicting protein conformation. Recently a careful examination of the β turns in the protein structure in the data bank revealed a new correlation, an unexpected relationship between the twist of the hairpin turn and the twist of the β sheet formed by the turn.² Two distinct classes of β turns could be identified and a strong correlation between the identity of the amino acid residues at the turn and the type of β turn generated was detected.

The Cambridge Structural Database (CSD)³ contains precise, accurate, and detailed information on the molecular structures of over 45,000 organic and organo-metallic compounds including drugs, natural products, and chemicals. Over 5000 new structures are added each year. Computer software developed at Cambridge, England allows the database to be searched by molecular name, connectivity, or bibliography. Fragment searches allow one to retrieve all structures having a specific fragment. The variation in molecular geometries of the fragment can be analyzed so that the effect of substitution upon its stereochemistry and atomic properties can be determined.⁴ Through such analysis it has been possible to demonstrate that specific types of bond lengths and angles seldom deviate from characteristic values and

that when they do the intramolecular source of variation can be readily identified. These types of data are useful guides to the development of empirical force field and molecular mechanics programs of ever increasing sophistication. These programs can in turn be used to predict the shape, stability, and properties of new candidates for synthesis and biological testing.

Recently, Murray-Rust and Raftery analyzed the Cartesian coordinates of 48 tripeptide fragments from the CSD to classify the molecules into groups and analyze the variation of geometry in the groups.⁵ Through their analysis they were able to elaborate upon and refine a previously proposed classification scheme. The results of this type of analysis can

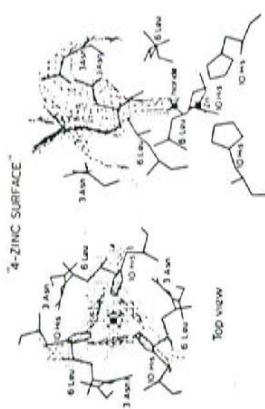


FIG. 1. Graphitrix analysis illustrates the inaccessibility of the Zn ion at the bottom of the narrow channel that accounts for the slow dissolving property of this therapeutically useful slow dissolving insulin [G. D. Smith et al., *Proc. Natl. Acad. Sci. U. S. A.* **81**, 7093 (1984)].

be used to guide the synthesis of synthetic peptide hormones which would have desired overall shapes, to permit more reliable prediction of protein folding, and to predict the influence of amino acid variation on protein binding or active site characteristics.

William Dux

1. For further information contact Thomas Koetzle, Brookhaven National Laboratory, Building 555, Upton, NY 11973.
2. B. L. Sibanda and J. M. Thornton, *Nature* **316**, 170 (1985).
3. For further information contact W. L. Duzak, Medical Foundation of Buffalo, 73 High Street, Buffalo, NY 14203.
4. F. H. Allen, O. Kennard, and R. Taylor, *Acc. Chem. Res.* **16**, 146 (1983).
5. P. Murray-Rust and J. Raftery, *J. Mol. Graph.* **3**, 50 (1985).

Molecular Structure and Engineering

Most biological processes are controlled by specific molecular interactions. In a great many cases the binding of a small molecule (drug or hormone) to a macromolecule (protein or nucleic acid) is a controlling factor in the process. In most cases the drug or hormone involved in the biological process has been isolated, purified, and identified and very often precise information on the three-dimensional

mination reveals that the repressor interacts with the DNA just as the models had predicted and produces very little deformation of the B-DNA structure. In contrast, the restriction enzyme DNA complex revealed distortions in the helical structure that are likely to be correlated with the functioning of the enzyme.

Making extensive use of the most recent technological advances, Michael Rossman and co-workers at Purdue University, Indiana and the University of Wisconsin have determined the structure of the human cold virus HrV14.⁶ The 800,000 intensity data needed for the study were collected using the Cornell University High Energy Synchrotron Source and the structure determination and refinement were completed using a Cyber 205 supercomputer. The structure was found to be strikingly similar to known icosahedral plant RNA viruses. Immunogenic regions on the virus identified by biochemical studies conducted by Roland Ruckert at the University of Wisconsin were observed to reside on external protrusions of the icosahedron, a large cleft on each face is proposed as the host cell receptor binding site. Armed with detailed knowledge of the surface geometry new kinds of antiviral drugs may be designed to treat colds.

The crystallographic structure determination of a second mammalian virus, the polo virus was reported by a group from the Research Institute of the Scripps Clinic.⁷ Describing the significance of these x-ray determinations of virus structures David Baltimore of the Winthead Institute in Cambridge, Massachusetts said: "These) beautiful pictures will forevermore be the basis of thinking about how viruses are assembled, how they are held together, and how they are taken apart to infect cells."⁸

The prominent role played by hydrogen bonding in the determination of stereospecificity was elegantly demonstrated in a study conducted by a group at the Imperial College of London⁹ that involved protein engineering of tyrosyl-tRNA synthetase. By systematically altering the amino acids in the active site of the enzyme the strength and importance of the hydrogen bonds that determine the substrate specificity was clearly demonstrated. One of the remarkable and unexpected findings of this study was that a hydrogen bond involving a side chain with a net charge is stronger by a factor of 6 than a hydrogen bond to an uncharged side chain. Thus, the substrate affinity can be readily increased or decreased by altering the residues in the active site accordingly.

Evidence for the importance of hydrogen bonding in another class of proteins came from the x-ray analysis of a sulfate binding protein from *Salmonella typhimurium*.³ This is one of a family of proteins which act as initial receptors for active transport systems.

Other milestones in structural elucidation of the past year include the x-ray structure determination of the first complex of a DNA repressor protein with the DNA sequence that it recognizes, the first mammalian virus structure, and the structure of the octamer histone core of the nucleosome.

Regulatory proteins turn genes on and off by binding to specific DNA sequences. The crystal structures of a number of the uncomplexed regulatory proteins have been determined since 1981 and models for the binding of the protein to B-DNA were postulated and simulated using computer graphics. In 1984, John Rosenberg of the University of Pittsburgh School of Medicine reported the 3 Å resolution determination of the structure of a complex of the restriction enzyme EcoRI with its target DNA sequence.⁴ Restriction enzymes bind to the DNA, just as the regulatory proteins do, but the enzymes cut the DNA instead of activating or repressing it. Anderson, Ptashne, and Harrison from Harvard have now reported the x-ray study of a complex of the repressor protein of coliphage 434 and the 14-base pair DNA sequence that the protein recognizes.⁵ The structure deter-

structure is available from x-ray analysis. In favorable cases the protein target of the drug or hormone has also been purified and crystallized but more often than not the protein or nucleic acid target has not been isolated and fully characterized. The target proteins include transport and binding proteins, receptors, and enzymes that control specific metabolism or growth related processes.

If the crystal structure of the macromolecular target with the drug or hormone in the active site can be determined the molecular details of the interaction revealed can guide the synthesis of new drugs having specific properties. One can alter the strength and duration of the substrate-protein interactions by chemical modification of either the drug or the macromolecule.

Dihydrofolate reductase is an enzyme essential to the synthesis of DNA. Because the blockade of this enzyme results in cell death, inhibition of the enzyme is useful for cancer chemotherapy and the development of more potent and specific blockers of the enzyme is of great interest. The crystal structures of dihydrofolate reductase from four sources have been determined as complexes with enzyme cofactors and inhibitors. These results provide information concerning the backbone conformation, spatial arrangement of the residue side chains, and a description of the inhibitor binding site.¹

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Other milestones in structural elucidation of the past year include the x-ray structure determination of the first complex of a DNA repressor protein with the DNA sequence that it recognizes, the first mammalian virus structure, and the structure of the octamer histone core of the nucleosome.

Regulatory proteins turn genes on and off by binding to specific DNA sequences. The crystal structures of a number of the uncomplexed regulatory proteins have been determined since 1981 and models for the binding of the protein to B-DNA were postulated and simulated using computer graphics. In 1984, John Rosenberg of the University of Pittsburgh School of Medicine reported the 3 Å resolution determination of the structure of a complex of the restriction enzyme EcoRI with its target DNA sequence.⁴ Restriction enzymes bind to the DNA, just as the regulatory proteins do, but the enzymes cut the DNA instead of activating or repressing it. Anderson, Ptashne, and Harrison from Harvard have now reported the x-ray study of a complex of the repressor protein of coliphage 434 and the 14-base pair DNA sequence that the protein recognizes.⁵ The structure deter-

From: Physics Today, January 1986, p. S23-26

JCPDS AUSTRALIAN USER'S GROUP

Since 1984, the Australian X-ray Analytical Association (AXAA) has been a cooperating organization of the JCPDS, that is, one whose members have a continuing interest in the JCPDS and are willing to further its purposes.

Brian O'Connor (WAIT) is the official AXAA representative on the JCPDS Technical Committee, but Australia has gained another voice on this committee by default since Larry Calvert (formerly of the National Research Council of Canada) now resides in Victoria. Both regularly attend the twice-yearly JCPDS Technical Committee meetings, so that if there are any questions and/or problems related to JCPDS products, either Brian or Larry are well placed to draw attention to these matters.

A JCPDS Australian User's Group has now been formed, under the umbrella of the AXAA, with 19 members as at 24 February, 1986. The objectives of the User's Group are:

- (a) to improve communications between JCPDS and Australian users;
- (b) to resolve difficulties experienced by Australian users;
- (c) to encourage Australian users to contribute to the development of JCPDS services;
- (d) to increase knowledge of the use and applications of JCPDS data and products in Australia; and
- (e) to update the JCPDS mailing list for Australian users.

William Dux

1. B. Mathews, J. Biol. Chem. 260, 392 (1985).
2. A. R. Fersht, J. P. Shi, J. K. Knill-Jones, D. M. Lowe, A. J. Wilkerson, D. M. Blow, P. Brick, P. Carter, M. U. Y. Waye, and G. Winter, Nature 314, 235 (1985).
3. J. W. Plaugrath and F. A. Quinchio, Nature 314, 257 (1985).
4. C. A. Frederick *et al.*, Nature 309, 327 (1984).
5. J. E. Anderson, M. Ptashne, and S. C. Harrison, Nature 316, 596 (1985).
6. J. P. Griffith *et al.*, Nature 317, 145 (1985).
7. J. M. Hoyle, M. Chow, and D. J. Filman, Science 239, 1358 (1985).
8. D. Baltimore, Science 239, 1366 (1985).
9. T. J. Richmond, J. T. Finch, B. Rashish, D. Rhodes, and A. Klug, Nature 311, 532 (1984).
10. R. W. Burlingame *et al.*, Science 238, 546 (1985).

The committee is: Dick Coyle - Convenor
Alan Drummond - Hon Secretary
Brian O'Connor - AXAA & JCPDS representative
Larry Calvert - AXAA & JCPDS representative

Further information can be obtained from Alan Drummond, SEC
Herman Research Lab, Howard St, Richmond, 3121, tel. 03 4202593.

AS YOU WERE

The Editor has not exactly been overwhelmed by responses to his numerous calls for old photographs of Australian crystallographers at work and play. However, over the past year or so a small number of members have, after considerable prodding, very generously dug out some of their precious memorabilia and have allowed them to be copied and incorporated into the slowly expanding SCA Archive File.

Four examples of the contents of this file are reproduced below for your delectation; the originals are, of course, of a much higher quality than is apparent in the photocopies. Please, if you have any photographs of this kind buried somewhere, get them out and send them to the Editor right now. You can be assured that they will be very carefully photographed and then returned to you immediately. This is an increasingly urgent matter since some of the photographs in the SCA's possession are already of sufficient vintage to make the assignment of an accurate date and location virtually impossible. The details relating to the photographs reproduced below are, however, reasonably well known:

1. Crystallographers at ANZAAS meeting, Brisbane, June 1961.
(L to R) John E.W.L. Smith (MSc student, Sydney)
Janet and Max Taylor (PhD student, Sydney)
Hans Charles Freeman
Ann and Gordon Robinson (Post Doc, Sydney)
John Cowley (Physics, Melbourne)
2. CSIRO Division of Mineral Chemistry, June 1968.
(L to R) Malcolm Fraser (Minister of Science)
Ivan Newnham (Chief of Division)
Dave Wadsley
3. CRYSTAL 9 Dinner at the Edelweiss Restaurant, Heidelberg,
Victoria, February 15, 1973.
(L to R) Jack McConnell, Nan Dawson, Nev Stephenson,
Mike Snow, . . . , Doug Lloyd, Beth Wunderlich,
Barry Dawson, Jeff Wunderlich
4. Lunch in Stephans-Platz, Hamburg, during the I.U.Cr.
Congress, August, 1984.
(L to R, standing) Joanne Hodge, Bob Cheary, Gary McIntyre,
?, ?, Mogens Lehmann, Sax Mason, Alan Hewat
(clockwise, seated) Sandy Mathieson, Hans Freeman, Sylvia
Mair, Sharman Hill, . . . , Peter Colman, Lois
Mathieson

1



2



3



4



A Call for Papers for

Powder Diffraction

- *New Product Announcements* This section will include details of recently introduced instruments, accessories and related devices.

Diagram call-outs must permit reduction by the printer and the author's judgement is required to estimate the necessary reductions to be used. The type in the final published diagram should be 2 to 3 mm high.

Full Length Manuscripts

Languages
Full length manuscripts will be accepted in English, French or German and may be sent directly to the Editor-in-Chief, or via the Managing Editor or to any member of the Editorial Advisory Board.

Referee Review

Full length manuscripts which are submitted to *Powder Diffraction* are sent to Referees (usually two) before they are accepted for publication. If, in the opinion of either the Referees and/or the Editor-in-Chief, the paper is considered to be more suitable for publication in *The Journal of Applied Crystallography* or in *Acta Crystallographica*, the author will be given the option to offer the paper in its original form to the recommended journal. A similar reciprocal agreement has been established with the editors of these two journals with regard to papers they may consider more suitable for *Powder Diffraction*.

Manuscript Length

An individual manuscript will typically be no longer than 6000 words (a column of "solid" text in *Powder Diffraction* is approximately 540 9-character words). If the author feels that a paper should be of greater length than this, consultation must be made with the Editor-in-Chief or the Managing Editor to determine the possibility of presenting the paper in convenient sub-sections to be published over the course of two or more issues of *Powder Diffraction*.

Each manuscript will begin with a 100 to 200 word Abstract suitable for reproduction by abstracting services.

Manuscript Presentation to the Editor
Double space typing, one side to a page, ~25mm margins. Three copies of the entire manuscript are to be submitted; a fourth copy is to be retained by the author.

Author(s) name and address (sufficient for correspondence) must be included. (Unless otherwise instructed, all correspondence from the Editors of *Powder Diffraction* will be sent to the first named author.)

Diagrams
Diagrams, curves, schematics, etc. should be well drawn in ink or presented in the form of good quality photographic reproductions. Diagrams should not be mounted, but sent with sufficient protective and stiffening material to prevent bending by postal handling.

Short Communications

The 'short communication', which may be submitted to Editor-in-Chief, or to the Managing Editor will be between 500 and 1500 words long and will describe typically, for example, experimental techniques, sample preparation, instrument modification and other such data which do not justify the publication of a full length manuscript.

Short communications are not intended to be used for interim reports of work in progress, except that such accounts may be accepted where they concern long range projects, i.e., those whose completion may not reasonably be expected within a period of eighteen months.

The following represent two typical types of short communications:

a) *Computer Programs*. This short communication will describe the purpose, strategy, computer language, machine requirements, input requirements and the type of results obtained.

(Computer Programs will be referred to in the normal way.)

b) *Laboratory Notes*. These are typically brief descriptions (wherein further detail may be obtained from the author) of special devices, equipment modifications, techniques for accomplishing certain common tasks, etc. A schematic drawing of a device is generally preferred to a photograph. The notes should be written so that the first sentence forms an abstract of the entire Note.

Departments

This section includes various contributions not included in the above and should be submitted to the Departments Editor.

• *JCPDS News*. Items of interest currently in progress at the International Centre for Diffraction Data, including reports from the various sub-committees and working groups.

• *Letters to the Editor* (to be sent to the Managing Editor only). These letters may deal with non-technical aspects of crystallography, its role, its propagation, the proper function of its Societies, etc. Also, the letters may contain technical observations that would be usefully brought to wide attention.

Meeting Report

• *Crystallographers* This category is intended to be a collection of short paragraphs dealing with the activities of crystallographers, such as their changes of position, promotions, assumptions of significant new duties, honors etc. Obituaries will also be presented in this section.

• *Upcoming Meetings and Short Courses* This category will include details of meetings of scientific societies, congresses, summer schools, etc. of interest to crystallographers.

Powder Data

Submission of powder data of well characterized materials are encouraged and the author is urged to submit full experimental details along with the experimental data. It is strongly recommended that the author submit powder diffraction information in the format recommended in *Powder Diffraction Notes for Authors*. Typically the author will be asked to offer the powder data to the International Centre for Diffraction Data for inclusion in the Powder Diffraction File.

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PERSONALIA / MISCELLANEOUS

Crystallographers the World over will be saddened to hear of the death of Martin J. Buerger on February 25, 1986. Martin Buerger will be long remembered by all who knew him as a warm, generous and good-natured man. His name and his scientific contributions will survive as long as crystallography survives.

Frank Moore has resigned from the Australian Institute of Nuclear Science and Engineering, effective January 27, 1986. No-one is too sure exactly what he is now doing, but rumour has it that he is Directing the Stanwell Park Amateur Theatre in their quest to win the 1986 Bawdy Song Competition. Apparently he has seconded Bill Palmer to administer the coloraturas Joan Watson, June Brownjohn and Joan Smith, with Lindsay Davis on percussion, Margaret Elcombe solo on the triple-axis keyboard, Chris Howard in fine shape on French Horn, Clyde Bock, Jeff White and Ian Middleton engineering their merry way on first, second and third violins, respectively, and Bob Knott keeping a low (angle) profile, as usual.

Frank was, of course, born in New Zealand some time ago. He obtained an MSc from Auckland University in 1959 for work on organometallic zinc complexes, spent a year in the Army, and lectured at a Teacher's Training College for a short time before heading off to Harwell to take up a position as a Research Assistant. In 1963 he obtained a Medical Research Council Associateship at Oxford and was awarded a DPhil for work in chemical crystallography in 1967. He then returned to Australia to take up a position with AINSE and has remained there ever since. Whatever his new interests are, we all wish Frank the best of good fortune and happiness and hope that he keeps in touch.

And speaking of AINSE and the ASTO/AAEC, a tremendous amount of activity has been going on behind the scenes over the past couple of years in a desperate attempt to maintain (and hopefully improve) the neutron beams from HIFAR. Scientific research has had to take a back seat on several occasions as lengthy submissions go back and forward between Lucas Heights and Canberra. The ASTEC report was, thank goodness, very favourable to neutron scattering and we can only hope that the Government heeds its recommendations. However, its not over yet and another round of negotiations has begun on nuts-and-bolts issues (hang in there Chris). Hopefully, there will be something concrete to report in the next newsletter.

Professor Makoto Sakata of the Dept of Applied Physics at Nagoya University, Japan, will be spending about 8 weeks at the CSIRO Division of Chemical Physics from May to June. He will be working primarily with Australia's new Envoy to Japan and self-appointed resident expert on Japanese/Australian international relations, one Stephen William Wilkins.

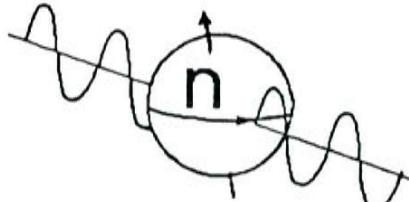
As an addendum to the article on the Photon Factory above, members interested in securing regular access to neutron sources can also play a part in gaining scientific fruits for Australia by taking every opportunity to lobby Government about the many

advantages of formalising access to the spallation neutron source (SNS) at the Rutherford Laboratory, and to the steady-state source at the ILL. The possibility of direct Australian involvement at these institutions has arisen from the proposed cutback in British support for the Anglo Australian Telescope, and the resultant suggestion that Australia might agree to trade off its additional contribution to the AAT if it was granted formal access rights at the SNS and ILL. Your attention to this matter is strongly encouraged.

The 3rd AINSE Neutron Scattering Conference will be held at Lucas Heights on the 6th and 7th of November, 1986. The conference will consist of a series of invited review papers, together with shorter oral or poster papers on any aspect of neutron scattering research. A special session will be scheduled to give attention to Industrial Applications of Neutron Scattering. For further information, please contact Mrs J. Watson, Conference Secretary, AINSE, Private Mail Bag, PO Sutherland, NSW 2232.

A satellite meeting on X-ray Powder Diffractometry will be held in association with the 14th Congress and General Assembly of the International Union of Crystallography in Freemantle, Western Australia from August 20 to 22. The meeting will consist of a symposium on automated data acquisition and analytical procedures in industry with special reference to data acquisition, automated profile processing and quantitative studies of materials, including Rietveld methods. A copy of the first circular can be obtained from: Dr E.H. Nickel, Division of Minerals & Geochemistry, CSIRO, Private Bag, PO Wembley, W.A., Australia 6014.

With all the problems Council has had in deciding on a logo for the Society, it was with some envy that we witnessed the rapid and painless way in which the organizers of the Neutron Scattering Satellite Meeting selected and implemented their rather nice logo, shown opposite:



Anyone trying to contact Bernard Hoskins at Melbourne University this year can save time by calling him at the CSIRO Division of Mineral Chemistry. Bernard is spending most of 1986 working with Ian Grey on the crystal structures and chemistry of compounds associated with the recovery of NaOH from the "black liquors" used during paper pulp manufacture.

Who was it that said CSIRO could not collaborate with Industry to save its life? For the information of all those sceptics outside CSIRO, in Industry, and in Government, close collaboration was in evidence in all its magnificent glory at a recent dinner party held in honour of Jimpei Harada at a certain newly renovated house in Blackburn, Victoria: one BHP and two CSIRO scientists were observed to take only 19.5 minutes to reassemble a Rubic's cube from a one metre long plastic loop-chain. A stunned Alec Moodie was heard to mutter after the event that the feat was a product of "pure naked intellect".

SCA SUBSCRIPTIONS FOR 1986

Members who have not paid their SCA subscriptions for 1986 are reminded that they are now long overdue. For the benefit of these tardy members a part of Rule 1, Section 2 of the SCA Constitution is quoted as follows:

".... Members whose subscriptions are not paid will be kept on the membership list for one year. Members still in arrears at the end of the year will be dropped from the membership list."

Thenceforth, no more horrible requests for payment of overdue subscriptions, but....no more notices of meetings, no more pictures of colleagues, no more competitions, no more crystallographic news from around the world, no more Asian Crystallographic Association newsletters. You'll be on your own, because none of the financial members will let you have their newsletter to read!

NEW MEMBERS

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

Full:	Mr Z.H. Rao	St Vincent's Sch Med Res, Vic
	Dr H. Wagenfeld	Applied Phys, RMIT, Vic
	Mr W.E.B. Shepard	Chemistry, Univ Auckland, NZ

The resignations of the following are noted with regret:

Dr L.M. Hogan	Univ Queensland, Qld
Mr J.H. Auld	ARL, Vic

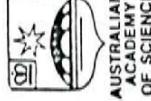
SITUATION VACANT

Postdoctoral Position - Electron Density and Chemical Bonding

A Research Associateship is available for research on the relationship between electron density and chemical bonding. Diffraction equipment and computing facilities are available. A background in crystallography and/or theoretical chemistry is necessary. Interest in improving techniques for achieving accuracy in single crystal diffraction measurements would be helpful.

Contact Dr E.N. Maslen, Director, Crystallography Centre, University of Western Australia, Nedlands, WA 6009

AUSTRALIAN ACADEMIES
AND
ROYAL SOCIETY



AUSTRALIAN ACADEMY OF SCIENCE
SCIENTIFIC AND TECHNOLOGICAL EXCHANGE PROGRAMME

APPLY NOW FOR 1987 EXCHANGE VISITS:

The Australian Academy of Science and the Australian Academy of Technological Sciences signed a Memorandum of Understanding with The Royal Society in 1985. The objective of the Memorandum is to foster cooperation in the natural and technological sciences (and such other fields as fall within their responsibilities) between Australia and the United Kingdom.

To meet this objective the two Australian Academies operate an exchange programme, which is funded by the Australian Department of Science. Scientists and technologists who are Australian residents and who are of at least post-doctoral or comparable status may apply to participate in the programme.

Applicants should propose a specific activity or a joint research project which has been developed in consultation with a host scientist in the United Kingdom.

Proposals will be assessed on their scientific and/or technological merit. The host scientist or institution in the United Kingdom must be appropriate to the objective of the proposal, and the length of the visit must be suitable for conducting the proposed research. Finally, the expected outcome of the visit should be of value to Australian science.

Visits may be long-term (six months or more) for extended research or short-term (not less than two weeks). Support will not be given when the primary purpose of a visit is to attend a conference.

Successful applicants will receive from the Academies a grant-in-aid which will cover the cost of a return excursion air fare to the United Kingdom and contribute to his or her living and travel costs within the United Kingdom. The contribution towards living costs will not normally exceed full allowance for a period of six weeks. Participants staying longer than six weeks will be expected to supplement their allowance from other sources.

Participants are responsible for any medical or hospital costs incurred during their visit. They are also responsible for all costs associated with visits by accompanying family members.

Participants must organize their itinerary in conjunction with their host scientist and make their own travel arrangements.

Application forms are available from:

International Exchanges Officer
Australian Academy of Science
GPO Box 783
Canberra, ACT 2601
Telephone: (062) 47-3966

The deadline for applications is 1 September preceding the calendar year for which support is sought.

FORTHCOMING MEETINGS

1986:

June 10-19:

Synchrotron Radiation for X-ray Crystallography (Summer School), Erice, Sicily. Contact: Prof L. Riva Di Sanseverino, Piazza Porta San Donato 1, 40127 Bologna, Italy.

June 22-27:

American Crystallographic Association Meeting, Hamilton, Ontario. Contact: Dr I.D. Brown, Inst Materials Research, McMaster Univ, 1280 Main St West, Hamilton, Ontario L8S 4M1, Canada. July 8-11:

Int Symp on Molecules, Clusters and Networks in the Solid State, Birmingham. Contact: Dr J.F. Gibson, Royal Soc Chem, Burlington House, London, W1V ORN, UK.

July 13-18:

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.

Aug 1-4:

Organic Crystal Chem Symp, Rydzyna Castle, Poland. Contact: Dr Z. Kaluski, Inst Chem, Adam Mickiewicz Univ, Grunwaldzka 6, 60-780, Poznan, Poland.

Aug 4-9:

10th European Cryst Meeting (ECM-10), Wroclaw, Poland. Contact: Dr K. Kubiaik, Inst for Low Temp and Structure Res, Plac Katedralny 1, 50-950 Wroclaw, Poland.

Aug 10-14:

12th Conf on Applied Cryst, Cieszyn, Poland. Contact: Dr E. Lagiewka, Uniwersytet Slaski, Inst Fizyki i Chemicznej Metali, ul Bankowa 12, 40-007 Katowice, Poland.

Int Summer School on Crystallographic Computing, Leipzig, GDR. Contact: Prof P. Paufler, Sektion Chemie der Karl-Marx-University,

Liebigstr 18, 07110 Leipzig, German Dem Rep. 7th Int Zeolite Conference, Tokyo, Japan. Contact: Hiro-O Tominaga (7 IZC), Dept Synthetic Chemistry, Faculty of Engineering, Univ Tokyo, Hongo, Bunkyo-Ku, Tokyo 113, Japan.

Aug 17-22:

Participants must organize their itinerary in conjunction with their host scientist and make their own travel arrangements.

Aug 31 - Sept 7: 11th Int Congress on Electron Microscopy, XI ICEM, Dept Anatomy, Faculty of Medicine, Kyoto Univ, Konoecho Yoshida Sakkyoku, Kyoto 606, Japan.

- Sept 9-10: Symp on 3D Structure and Drug Design, Tokyo.
Contact: Prof Y. Iitaka, Univ Tokyo, Faculty of Pharm Sciences, Bunkyo-ku, Tokyo, Japan.
- Sept 15-19: Int Symp on Molecular Structure: Chem Reactivity and Biological Activity, Beijing. Contact: Dr Xu Xiao-Jie, Inst Physical Chem, Peking Univ, Beijing, China.
- Oct 20-26: Computational Chem in Molecular Design: Molecular Modelling and Computer Graphics, Garmisch, Germany. Contact: J.J. Stezowski, Inst Organische Chemie, Biochemie und Isotop, Univ Stuttgart, Pfaffenw 55 D-7000 Stuttgart 80, Fed Rep Germany. 1988
- Nov 6-7: 3rd AINSE Neutron Scattering Conference, Lucas Heights, NSW. Contact: Mrs J. Watson, Conference Secretary, AINSE, PMB, PO Sutherland, NSW 2232.
- 1987:
- Jan 26-30: 56th ANZAAS Congress "Science in a Changing Society", Palmerston North, New Zealand.
Contact: Dr M. Baxter, Massey Univ, Palmerston North, New Zealand.
- Feb: 15th Australian Spectroscopy Conf. Contact: Conf Sectretariat, Aust Acad Science, GPO Box 783, Canberra, ACT 2600.
- Apr 7-9: BCA Spring Meeting, Heriot-Watt Univ, Edinburgh, UK. Contact: Dr J.C. Halfpenny, Dept Chemistry, Napier College, Colinton Rd, Edinburgh EH10 5DT, UK.
- July 13-16: Conf on Small Angle Scattering and Related Methods, Praha, Czechoslovakia. Contact: Dr J. Baldrian, Praha, Czechoslovakia.
- Aug 12-19: World Congress of Theoretical Organic Chemists, Budapest, Hungary. Contact: E.A. Lang, Hungarian Chemical Society, H-1061 Budapest, Anker koz 1, Hungary.
- Aug 12-20: 14th General Assembly and Congress of the IUCr, University of Western Australia, Perth, Western Australia. Contact: Dr E.N. Maslen, Crystallography Centre, Univ. of WA, Nedlands 6009, Western Australia.
- Satellites:
- Validity of Structures from Electron Microscopy, Melbourne, Aug 7-9. Contact: Dr J.V. Sanders, CSIRO Mat Sci. Locked Bag 33, Clayton 3168 Australia.
 - Neutron Scattering, Sydney, Aug 8-10. Contact: Prof T.M. Sabine, NSW Inst Tech, PO Box 123, Sydney 2007 Australia

Aug 30 - June 7: Crystallography of Molecular Biology (Summer School), Erice, Italy. Contact: Prof L. Riva Di San Severino, Piazza Porta San Donato 1, 40127 Bologna, Italy.

- X-ray Powder Diffractometry, Perth, Aug 20-22.
Contact: Dr B.H. O'Connor, School of Physics & Geosciences, WA Inst Tech, Perth 6102 Australia
- School on Crystallographic Computing, Adelaide, Aug 22-29. Contact: Dr M.R. Taylor, School of Physical Sciences, Flinders Univ Adelaide 5042 Australia
- Accuracy in Structure Factor Measurements, Melbourne, Aug 23-26. Contact: Dr S.W. Wilkins, CSIRO Chem Phys, PO Box 160, Clayton 3168 Australia

These are the times that try Men's souls.
The Summer Soldier and the Sunshine Patriot will in this crisis, shrink from the service of his country. But he that stands now, deserves the love and thanks of Man and Woman. Tyranny, like Hell, is not easily conquered, yet we have this consolation with us, that the harder the conflict, the more glorious the triumph. What we obtain too cheap, we esteem too lightly, 'tis dearness only that gives everything its value.

Tom Paine

