Society of Crystallographers

in

Australia

Newsletter No. 11

June 1985

Contents:

theory (maximum entropy), its relationship to traditional direct methods, and its application to the structure determination and refinement of macromolecules.

Dinner was followed by Vivian Cody (Medical Foundation of Buffalo, NY) with a superb presentation of her award-winning work on the relationship between molecular structure and the inhibitory potency of antifolate anticancer drugs. Explanations for the greater binding affinity of the antifolates with respect to their substrates focus on the modified pattern of hydrogen bond donor and acceptor interactions at the enzyme active site and a change in the electron density of the pyrimidine ring system.

David Rae (UNSW) began the final session of the School with an overview of the methodology, pitfalls, approximations, constraints and errors of least-squares refinement techniques, with particular emphasis on the RAELS code. Neil Isaacs (St Vincent's Inst Med Res) then gave up the Chair momentarily to present an excellent review lecture focussing on practical aspects of the refinement of macromolecules with real-space and constrained/restrained methods of analysis. Mitch Guss (U Sydney) then gave a very professional review of the properties of caligraphic (line-drawing) and rastor display devices, together with detailed descriptions of the capabilities and applications of the latest generation of graphics software systems, especially in the area of protein interaction modelling.

Crystal 15:

Approximately 20 additional crystallographers not registered for the Computing School arrived during the morning of May 14, resulting in a total attendance of about 100 for the Crystal Meeting. This must represent something of a record for an SCA conference held outside Victoria or NSW and is a testimony both to the organisational abilities of Max Taylor and to the many attractions of Adelaide and South Australia.

The meeting continued through Thursday evening, May 16, following the familiar format of specific-topic sessions opened by review lectures (7 in total), and continuing with a number of short oral presentations (20). Poster papers (35) were on display throughout the meeting in two locations in close proximity to the dining and lecture areas. Wednesday afternoon was left free for sightseeing and/or discussions, with the SCA Business Meeting at 4.30 and the Conference Dinner in the evening. Friday, May 17 was set aside for a post-conference tour of several wineries in the Southern Vales area.

The Crystal Meeting began with a session on protein crystallography and an up-date on the 'blue' copper-protein saga from Hans Freeman (U Sydney). Hans gave a fascinating step-by-step account of the progress that has been achieved on many fronts in understanding the properties and function of plastocyanin (obtained from the leaves of the poplar trees on the Sydney University Campus) and azurin since the solution of their crystal structures in 1978.

The evening session started with a presentation from Vivian Cody

on the use of computer graphics for the prediction of structure modifications necessary for the modulation of thyroid hormone metabolism and function. Her many hours spent on a graphics terminal were rewarded by the production of a superb colour film on the interaction between these hormones and their target protein binding site. In the last talk in this session, Ward Robinson (Univ of Canterbury, NZ) made us all think hard about recent disturbing changes in the attitudes and perceptions of Chemists and others on the merits of crystal structure analysis as a proper professional activity. This re-evaluation of chemical crystallography has been brought about by recent dramatic advances in instrumentation and software which have enabled structure solution to become an essentially automatic and very rapid process, able to be undertaken by non-specialists.

Dinner was followed by a joint meeting with the S.A. Branches of the RACI and the AIP, at which Wayne Hendrickson presented an address on the Mobility and Adaptability of Protein Structures. Cognizant of the many non-crystallographers in the audience, Wayne presented just the right mixture of background and specialist information to keep everyone enthralled. After this talk the audience adjourned to the dining area where a selection of South Australian wines was available for tasting while posters were examined.

Wednesday began with an excellent review of the Rietveld Method in Powder Diffraction by Chris Howard (AAEC, Lucas Heights). Chris traced the recent rapid developments in instrumentation and analysis techniques for neutron and X-ray data collected in both the fixed-wavelength and fixed-angle modes, and gave examples of its application to a wide range of materials science problems in laboratories around Australia. Other oral and poster presentations in the program, together with the high level of interest in Rietveld analysis shown by a large number of conferees not yet using the technique, were testimony to the resurgence in the use of powder diffraction data and the timeliness of Chris' review.

In the next session, devoted to the optimization of diffraction hard- and soft-ware, Ward Robinson again shocked us all (this is rapidly becoming a National trait of New Zealanders) by pointing out that data collection time and motor-wear savings of up to two-thirds can be achieved by the use of optimized tracking of the counter through reciprocal space.

The remainder of the afternoon was left free for discussions or visits to local scenery, but about 65 members and observers returned at 4.30 to attend the SCA Business Meeting. (Details of this meeting are summarized in a later section of the Newsletter). The Conference Dinner was held later that evening at the Brougham Restaurant in North Adelaide, overlooking the downtown area from a vantage point on the seventh storey of the Oberoi Hotel. This was an outstanding occasion which will be long-remembered by all those fortunate enough to attend. A highlight of the evening was a tribute to Sandy Mathieson delivered by Hans Freeman on behalf of all Australian Crystallographers to mark Sandy's imminent retirement from CSIRO.

The first session on Thursday was devoted to inorganic structural chemistry. It began with a presentation by Stephen Hyde (Physics, Monash Univ) on the Minimal Surface Description of Crystal Structures and Phase Transformations. This exciting new model in crystal chemistry allows apparently complicated interpenetrating structures to be simply understood in terms of periodic minimal surfaces separating the components. The model allows a rationalisation of ion conduction patterns, first and second order phase transformations and, possibly, the internal electric field of crystals.

The inorganic theme continued into the next session, with a lucid treatise on Electron Density, Electrostatic Potential and Lattice Energy by Ted Maslen (Crystallography Centre, UWA). In this review Ted pointed to the relative neglect of crystal energy, in favour of electron density, in the comparison of theory with diffraction experiment, and highlighted the importance of the promolecule (the assembly of overlapping but undeformed atoms centred on the nuclei) in calculations of binding energy.

The final session (again inorganic) commenced with a fascinating review by John Parise (Chemistry, NSWIT) of several new series of molecular sieves with the framework compositions AlPO4, GaPO4, and (Si,Al,P)2O4. These compounds have pore sizes just larger than a variety of commercially important organic molecules and are used in shape-selective, acid-catalysed processes such as alcohol dehydration, petroleum production and reforming, and xylene production. John's excellent computer graphics diagrams and complicated internal structural surfaces emphasized the strange parallels between this form of inorganic "molecule" design and the earlier protein/drug interaction studies described by the Organic/Protein Chemists earlier in the conference.

Rod Hill

On behalf of the membership of the SCA, Council would like to take this opportunity to congratulate the Organising Committee

Max Taylor (Chairman)
Neil Isaacs (Computing School)
Judge Bevan
Sally Birch
Sharon Lawton
Jury Mohyla
John Westphalen

on the outstanding success of both the Crystal Meeting and the Computing School, and to thank them for doing such a fine job for the Society.

A FEW MOMENTS CAPTURED FROM THE CRYSTAL 15 DINNER

Left to Right

Terry Sabine
Max Taylor

Maureen MacKay
Sandy Mathieson
Steve Wilkins

Ted Maslen (back)
Hans Freeman
Janice Snow
Terry Sabine
Mike Snow
Rosemary Taylor
Max Taylor

Sylvia Mair (side)
Vivian Cody
Syd Hall
Graham Gainsford

Bruce Poppleton
Meta Sterns
Bruce Hyde

Henry Scott
Henry Rossell
Syd Hall

Linda Welberry
Richard Welberry
Annas Rae
Ward Robinson
David Rae
Z-h Rao

NEWS FROM THE 1985 BUSINESS MEETING

Secretary's Report

The SCA Council met on four occasions in the period since the last Business Meeting held on August 31, 1983 at Morpeth, NSW; these occasions were 22/2/84, 27/6/84, 6/12/84, and 14/5/85. The major actions of Council arising from these meetings may be summarized as follows:

- Ballot papers for the amendments to the SCA Constitution required by the Articles of Incorporation were circulated to the membership. The amendments were ratified unanimously by the 48 members who returned the ballot papers and were duly included into the master copy of the Constitution.

- Arrangements were made for a meeting of delegates from countries in the South East Asian region during the Hamburg IUCr Congress. Minutes of this meeting were circulated to contact people in each of the countries and a draft Constitution was prepared. Copies of this draft were included in the registration papers of all Crystal 15 conferees for their delectation in advance of the 1985 Business Meeting.

- Nominations for new office bearers were received from the Nominations Committee and further nominations were called for in the Newsletter (see below for further details).

- Progress with the organisation of the IUCr Congress in Perth, its associated satellite meetings, and the Crystal 15/Computing School were monitored closely. The financial relationship between the Perth Organising Committee and the SCA was formalised in detail.

- The SCA gave its full support to the formation of an IUCr Commission on Small Molecules and offered the services of its Newsletter for the dissemination of relevant information.

- A subcommittee comprising Maureen MacKay and Frank Moore was formed to decide on a logo/letterhead for SCA correspondence and other material.

- The President of the SCA attended the Meeting of National Concern on Science and Technology on April 16, 1985 as the representative of the SCA.

- Four issues of the Newsletter were circulated to the membership.

- A total of 22 new members were welcomed to the Society.

Federation of Scientific & Technological Societies

Terry Sabine, in his capacity as the President of the SCA, attended a National Meeting of Concern on Science and Technology in Canberra on April 16, 1985. This meeting was attended by representatives of 68 Societies encompassing some 101,000 scientists and technologists. Three proposals were presented before the meeting:

- To set up a Federation of Scientific and Technological Societies

- To set up a Secretariat on Government Relations
  Cost ≈ $200,000 per year

- To set up a Secretariat Providing a Science and Technology Information Service
  Cost ≈ $200,000 per year

The formation of the Federation was enthusiastically supported at this meeting and an Interim Committee chaired by Prof T.F. Smith, President of the AIP, was set up. The tasks of this Interim Commitee are, in summary, to draft a constitution for the Federation and to investigate the cost of the Federation and Secretariats. The present costing suggests that each Society will be required to provide annual funding of between $5 and $20 per member to the Federation.

During the SCA Business Meeting in Adelaide, the membership was therefore asked whether it wished the SCA (i) to be part of a Federation of Scientific and Technological Societies, (ii) to support a continuing annual levy of an amount probably between $5 and $20 per member, and (iii) to support an immediate levy of between 50c and $1 to finance an Interim Committee. After considerable discussion, the Meeting resolved that the SCA "join in the interim work for the foundation of a Federation of Scientific and Technological Societies and, to help in funding this Federation, is willing to give $1 per member as an immediate levy".

Treasurer's Report

Maureen MacKay tabled her interim report on the financial status of the SCA, indicating that its assets were in the vicinity of $15,500. She informed the Meeting that an updated report would be circulated to the membership at the conclusion of the financial year.

The Meeting resolved that "in view of the probable future commitment of the SCA to the support of a Federation of Scientific and Technological Societies, and the need to provide a substantial backup to the financing of the Perth IUCr Congress, the SCA membership dues for a full member should be raised from $10 to $15".

Report on the 1987 Perth IUCr Congress

Ted Maslen presented a summary of the progress achieved with the organisation of the Perth IUCr Congress. In particular:

- The Social Program of the Congress is under the direction of Syd Hall.
- Andy Johnson's secretary has been appointed to help the Local Organising Committee.
- The first major item of expenditure will be the First Circular for the Congress, due to be released early in 1986.
- Three field trips have been proposed in response to requests from Mineralogists in the United States and Germany. Responses to these trips will be requested in the First Circular.
- Further details of the scientific program and accommodation arrangements will be available later in the year.
- Negotiations with Airlines are proceeding with care since the total attendance is likely to be dramatically affected by these arrangements.
- The WA Government has not yet been approached for support because of the impending State elections.

Hans Freeman reported on progress with the Program Committee's arrangements. In summary:

- The IUCr Executive has approved the membership of the Program Committee.
- All National Committees affiliated with the IUCr, and all IUCr Commissions, will be invited to submit suggestions for the Congress program.
- Arrangements will begin in earnest around the time of the next meeting of the Program Committee in Europe in July of 1986.

Satellite Meetings

Terry Sabine reported on the status of the organisation of the satellite meeting on Neutron Scattering. This meeting, and accommodation, will be at the NSWIT from August 5-8, 1987. Trevor Hicks and Terry Sabine are Chairpersons of the Program and Local Organising Committees, respectively.

Max Taylor reported on progress with the organisation of the Crystallographic Computing School associated with the Perth Congress. This meeting will be hosted by Flinders University from August 22-29, 1987, and will be funded partly by a grant of US$6000 from the IUCr. Neil Isaacs and Max Taylor will be the Program and Local Organising Committee Chairpersons, respectively. Computing facilities will be made available by Flinders University and PRIME Computers.

Brian O'Connor reported on progress with the organisation of the satellite meeting on X-ray Powder Diffractometry, to be held at York in WA on August 21 and 22, 1987. The Program and Local Organising Committee Chairpersons are Brian O'Connor and Jim Graham, respectively. The meeting will be divided into three broad areas: data acquisition, profile processing, and quantitative analysis. Industry support is expected to be in the vicinity of $5000. Hugo Rietveld will be the guest of honour.

Neutron Scattering Facilities in Australia

Chris Howard summarised the recent activities of ANBUG and the AAEC in relation to the refurbishment of HIFAR and its possible replacement by a new reactor. He indicated that certain of the existing experimental facilities on HIFAR (i.e., 4H1, 4H5B, and the triple-axis spectrometer) were being, or had been, upgraded with new detectors and/or computers, but the proposal to provide a cold source was almost certain to be rejected. The recent flurry of activity in relation to proposals for a new reactor were cut short by the Federal election in December of 1984. In view of the experience gained in this matter Chris recommended that current and potential users of HIFAR should have their cases for upgrading and/or replacement ready for a likely renewal of activity in the near future.

SE Asian Regional Crystallographic Association

The Constitution drafted for this Association by the SCA Council was included with the registration papers for the Crystal 15 Meeting. One amendment relating to the financing of the Association was carried by the Meeting. (The amended Constitution has now been circulated to all 18 delegates to the Association).

New Office Bearers

Since no additional nominations to the slate proposed by the Nominations Committee were received by the Secretary, an election was not required. The new list of Office Bearers is reproduced on page 2 of this Newsletter; they will hold office until the next Business Meeting of the SCA, which will be held during the 1987 Perth IUCr Congress.

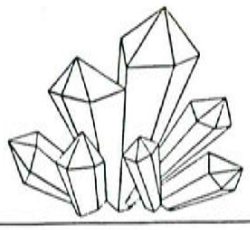
The Secretary would like to take this opportunity of thanking the members of the previous Nominations Committee, and in particular, Sylvia Mair and Joel Epstein, for giving very considerable thought and effort to producing a list of appropriate people to serve the Society for the next 27 months.

Next Crystal Meeting

In view of the considerable effort which will be required by a large number of SCA members in helping to organise the Perth IUCr Congress, the Meeting resolved not to hold another Crystal Meeting during the lead-up to the Congress. This will mean that Crystal 16 will not occur until 1988 at the earliest! The Editor invites comments and suggestions from the membership on this issue.

SCA LOGO/LETTERHEAD

Readers will remember that the SCA Council recently appointed a sub-committee comprising Maureen MacKay and Frank Moore to produce a suitable logo for use on SCA letterhead paper. Frank and Maureen worked hard on their task and came up with several possibilities which were displayed, along with variations on an entry from Bob Cheary, in the poster area during the Crystal Meeting in Adelaide. A total of 43 members voted for the logo of their choice on a 3,2,1 basis during the course of the Meeting and the three top scoring entries are as follows:

Entry	Score
 SOCIETY OF CRYSTALLOGRAPHERS IN AUSTRALIA	50
SOCIETY OF CRYSTALLOGRAPHERS IN AUSTRALIA	41
SOCIETY OF CRYSTALLOGRAPHERS IN AUSTRALIA	27

The top entry is therefore declared the winner and it will be adopted as our new logo/letterhead as soon as possible.

PERSONALIA / MISCELLANEOUS

Max Taylor of the School of Physical Sciences at Flinders University will be overseas for 6 months from 17th June, 1985. He will spend 3 months on long service leave in New Zealand and will then work with Dr J.P. Glusker for 3 months at the Institute of Cancer Research in Philadelphia, USA.

David Rae of the School of Chemistry at the University of NSW, and Trevor Hicks of the Department of Physics at Monash University, have both been appointed to Readerships in their respective Institutions.

Ted Maslen of IUCr 14th Congress fame has been given the rare honour of being appointed to the Executive of the IUCr. Ted is only the third Australian to be so honoured, the others being Sandy Mathieson and John Cowley.

Dudley Creagh of the Physics Department at the Royal Military Collge, Duntroon, has been appointed as Chairperson of the IUCr Commission on Apparatus.

Barbara (CSIRO Chemical Physics) and Gwant (Physics, Melbourne Univ) Moss have recently returned to Australia (via Tahiti) after 2 months in the USA; Barbara collecting neutron data at Brookhaven National Laboratory, New York, and Gwant finishing off some of his earlier work at the Medical Foundation of Buffalo.

Bill Sinclair has made a welcome return to Australia after several years working on cement technology at Oxford, UK. He has taken up a position at the Melbourne Research Laboratories of BHP to work on ceramics.

Prof Stephen Haggerty from the Dept of Geology, Amherst University, Massachusetts is currently working at the CSIRO Division of Mineral Chemistry with Ian Grey on some new high pressure members of the crichtonite mineral group. These new phases have been observed in diamond bearing kimberlites in Africa and have relevance to the mineralogy of the Earth's Mantle. Stephen will leave Mineral Chemistry at the end of July for a month or so with Prof Ted Ringwood at the RSES at ANU before returning to Amherst.

Steve Wilkins of the CSIRO Division of Chemical Physics will spend November of this year in Japan undertaking collaborative work with synchrotron radiation. Anyone with ideas for synchrotron projects is asked to contact Steve as soon as possible.

Readers should note that proposals for international scientific and technological collaboration can be sought under the various bilateral science and technology agreements administered by the Department of Science and Technology. These agreements are between Australia and Japan, the USA, Mexico, the Federal Republic of Germany, India and the People's Republic of China, with funding normally limited to economy class air fares and support for living costs for the collaborating scientists. Copies of the Australian guidelines containing details of application procedures are available from The Director, International Activities (Bilateral Science & Technology Agreements), Department of Science & Technology, PO Box 65, Belconnen, ACT 2616.

The Australian X-ray Analytical Association has recently been accepted as one of the 10 cooperating member organisations of the International Centre for Diffraction Data (JCPDS). Brian O'Connor (WAIT) has been appointed as the Australian representative to the ICDD. During the SCA Business Meeting in Adelaide Brian indicated that the AXAA has now formed a Users' Group for the JCPDS file and invited any interested SCA members to join. He also indicated that grants-in-aid are available from the ICDD for work on the powder diffraction data base. Please write to Brian at the School of Physics and Geosciences, WAIT, Kent Street, Bentley, WA 6102, for further information.

Dr A.C. McLaren is in the process of leaving the Department of Physics at Monash University to take up a position as Full Professor in the Research School of Earth Sciences at ANU.

Dr Stephen Weidle of the CRC Biomolecular Structure Unit, Institute of Cancer Research, Surry, UK, recently visited Melbourne and was a Plenary Lecturer at the 4th National Conference of the RACI Division of Medicinal and Agricultural Chemistry, Lorne, May 19-22.

Dr Vivian Cody, of the Medical Foundation at Buffalo, New York, has spent the last few weeks working with Maureen MacKay at La Trobe University and attended the Crystal Meeting in Adelaide, where she gave several lectures and films on protein/drug interactions. Vivian has been named as the recipient of a prestigious, national five-year Faculty Research Award for her study of the relationship between molecular structure and biological activity of drugs that inhibit tumor growth. The award is given by the US Cancer Society to scientists who have demonstrated the capacity to conduct meaningful cancer related research of their own design.

The lectures presented during the Crystallographic Computing School in Adelaide were of exceptionally high standard, as one might expect from such a distinguished array of Australian, New Zealand and United States Crystallographers. Syd Hall's talk on "Direct Methods: The Application of Structure Invariants", was exceptionally entertaining, liberally interspersed as it was with slides of Amsterdam by night (and one or two by day, probably taken by someone else). Knowing Syd, a better title to his talk may perhaps have been "The Application of numerous Methods for Invariably leading innocent visitors Directly towards a new drinking Structure".

NEW MEMBERS

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

Full:	Dr E. Bakshi	(St Vincent's Sch Medical Res)
	Mr K.D. Griffiths	(Res Sch Chem, ANU)
	Dr G.J. Gainsford	(DSIR, New Zealand)
	Dr S.E. Lawton	(Dept Chem, UBC, Canada)
	Dr M.B. Millikan	(Dept Chem, La Trobe Univ)
	Mr E.R.T. Tiekink	(Dept Chem, Univ Melbourne)
	Dr W.A. Wickramasinghe	(Res Sch Chem, ANU)

Student:	Ms J.M. Newnan	(Sch Chem, Univ Sydney)
	Miss T.M. Manning	(Sch Chem, Univ Sydney)
	Mr A. Linden	(Dept Chem, Univ Melbourne)
	Miss A.J. Edwards	(Dept Chem, Univ Melbourne)
	Mr I.S. Crick	(Dept Inorg Chem, Univ Melbourne)
	Miss J.M. Gulbis	(Dept Chem, La Trobe Univ)

We also announce, with regret, the resignation of Mr H.R. (Rick) Tietze, who has recently retired from the Dept of Chemistry at the University of Newcastle. Rick was, of course, the Chairman of the Local Organising Committee for the Crystal 14 Meeting at Morpeth in 1983.

OVERDUE SUBSCRIPTIONS

Maureen MacKay has indicated to the Editor that several members are in arrears with their SCA subscriptions. If this Newsletter is accompanied by a notice to this effect then please attend to your overdue subsciptions as soon as possible or you will be crossed off the membership list.

CRYSTALLOGRAPHY NEWS

From Physics Today / January 1985

Crystallography is the science that describes the geometrical structures and properties of crystals. A crystal is an arrangement of atoms in a solid which repeats regularly in three dimensions. This repetition causes the crystal to act as a diffraction grating for x rays, neutrons, or electrons. The diffraction patterns which result can be analyzed to reveal the structure of the crystal in atomic detail.

Crystallography and Dynamic Processes

The study of crystals using x rays and neutrons has provided much of the insight we have about matter at the molecular and atomic scale. Information about chemical structure (such as, which atoms are connected, how strong are the bonds, where is the electronic charge?), relative and absolute configuration (handedness, or the difference between one structure and its mirror image), conformation (molecular shape), and weaker forces between atoms and molecules (such as hydrogen bonds) can be routinely obtained from structure analysis of crystals that contain molecules.

All this information can be gleaned from a static representation of the crystal. There has been a steadily growing effort, however, to interpret the results from crystal structure determinations also in terms of dynamic processes. The fact that atomic motion affects how strongly a crystal scatters x rays was recognized by Peter Debye[1] long before practical x-ray crystallography came into being. In all determinations of crystal structure by modern methods one includes in the calculation a "temperature factor" for each atom (the Debye–Waller factor[2]) which allows for this thermal motion. In its simple isotropic form it has one parameter. A more sophisticated anisotropic form, with 6 parameters per atom, is also in very common use. The accurate geometrical structure of a crystal is generally obtained by a least-squares method ("refinement") which finds the best fit of a large number of parameters to an even larger set of scattering measurements. The thermal parameters which describe the motion are also determined, even if there is no particular interest in them. Many of the historical aspects of this subject have been summarized by Dunitz.[3]

The level of current interest in these dynamic processes is illustrated by the American Crystallographic Association (ACA) Symposium[4] entitled "Molecules in Motion" held as part of the 1984 ACA meeting in Kentucky. In one paper delivered at the meeting, entitled "From Crystal Statics Towards Molecular Dynamics," J. D. Dunitz of the Swiss Federal Institute of Technology, Zurich, reviewed two ways of getting indications of thermal motion from crystal structure determinations. One method uses the results for many crystal structures to find correlations which, for example, might indicate chemical reaction pathways. In the second method anisotropic vibration parameters (AVPs) are examined for indications of internal motion, such as torsion.

K. N. Trueblood of UCLA discussed the principles of thermal-motion analyses using a "Gaussian-ellipsoid" representation of the probability of atomic location, its application in the analysis of the motion of a molecule as a rigid body, and the modifications thereof to allow for flexible motion in the molecule. H. Schulz of the Max-Planck-Institute für Feskörperforschung in Stuttgart, West Germany, discussed the use of more complicated temperature factors in describing motion that is not harmonic and how an atom's energy state depends on position.

In "A New Spectroscopy for the Study of Molecular Motions in Crystals" C. J. Eckhardt of the University of Nebraska described piezomodulation spectroscopy of molecular crystals, in which changes in optical properties occur when a sonic vibration is imposed on a crystal. This permits the study of phenomena such as order–disorder phase transitions, which are sensitive to external stress.

Continuing the discussion of spectroscopy of the solid state, C. A. Fyfe of the University of Guelph in Ontario, Canada, reviewed the use of nuclear magnetic resonance (NMR) spectroscopy in studying molecular motions. A technique called "magic angle spinning" lets one get spectra from solids for which the resolution is similar to that for solutions. These spectra may yet reveal similarities between structure in solid and solution phases, and may also address the question of whether disorder is largely static ("frozen in") or dynamic (changing with time).

P. Murray-Rust of the GLAXO Group Research in the United Kingdom drew upon the very extensive file of the Cambridge Crystallographic Data Center to compare deformations of molecules in crystals and normal modes of vibration. For example, study of 18 steroid compounds, all con-

taining the same central structural unit, revealed that the distortions consisted of a smooth, concerted bending of this unit. It was further concluded that little energy was required to produce this bending.

Another session was devoted to theoretical studies and experimental results concerning dynamics in protein structures. These techniques are providing rich detail of the atomic motions in these very complicated structures and are giving a better understanding of how their shapes may change in biological processes.

This summary indicates the high level of current activity among crystallographers, spectroscopists, and theorists exchanging ideas and information about this subject.

John Stezowski, University of Stuttgart
David Templeton, University of California, Berkeley

1. P. Debye, Verh. Dtsch. Phys. Ges. 15, 738 (1913).
2. I. Waller, Z. Phys. 17, 398 (1923).
3. J. D. Dunitz, *X-ray Analysis and the Structure of Organic Molecules* (Cornell University, Ithaca, 1979).
4. J. J. Stezowski, ed., Trans. Am. Crystallogr. Assoc. (in preparation).

Diffraction by the Time-of-Flight Technique at Pulsed Neutron Sources

The recent development of accelerator-based pulsed neutron sources as an alternative to reactor sources has caused a renewed interest in time-of-flight neutron diffraction techniques. According to quantum mechanics, neutrons possess wave-like properties: neutrons can enter and be diffracted in a sample, revealing information about the sample's crystal structure.

At the Intense Pulsed Neutron Source (IPNS) at Argonne National Laboratory, 500-MeV protons from a synchrotron strike a metal target, creating short, intense bursts of neutrons with a broad range of energies. These energies can be measured by observing the time it takes the neutrons to traverse a known flight path.[1]

In the time-of-flight pulsed-source technique, high neutron energy resolution can be obtained through the use of long neutron flight paths, as long as 20 m.[2] Also, the pulse width from the source varies in such a way that resolution is constant over a wide range of wavelengths. These resolution characteristics have proven to be ideal for measuring residual stresses in bulk solids by studying the small shifts in a number of Bragg peaks appearing in the diffraction patterns.[3] The high resolution of "powder diffractometers" has also been used to study the crystal structures of solids which cannot be obtained as single crystals. Precise atom positions are determined by computer analysis of the diffraction pattern which, typically, contains hundreds or thousands of overlapped Bragg reflections. Analyses with over 100 variable parameters emerge with a precision comparable to that for single-crystal diffraction. This work is important in the study of a large number of technologically important materials, including ionic conductors, hydrogen storage compounds, superconductors, and catalysts.

Neutron diffraction studies of amorphous materials have also benefitted greatly from the pulsed-source, time-of-flight technique. The purpose of a diffraction measurement on an amorphous system is to construct a radial distribution function (rdf), that is, a function which expresses the atom density as a function of distance from a reference atom in the structure. The rdf becomes more accurate as the neutron wavelength becomes shorter or, equivalently, as the neutron energy increases. The pulsed sources produce neutrons at short wavelengths not available at reactors and make it possible to improve the spatial resolution of the rdf by a factor of three or more.

The resulting substantial improvement in the rdf for a number of amorphous systems has been nicely demonstrated at the Japanese pulsed source at the Tohoku University 300 MeV electron LINAC using a rather simple time-of-flight instrument and relatively low neutron fluxes.[4] Similar improvements have been observed for the study of liquids at Los Alamos National Laboratory WNR (Weapons Neutron Research) facility, which has been operated by borrowing a small fraction of the beam from the LAMPF accelerator.[5]

The time-of-flight diffraction instruments currently operating at pulsed neutron sources in the United States, Japan, and England are clearly successful and are demonstrating a number of unique capabilities. Within the next few years new facilities will begin operating at the Rutherford Laboratory in England and Los Alamos National Laboratory offering fluxes over 10 times that of Argonne's IPNS. Argonne is proposing a pulsed neutron source for the early 1990's with 200 times the IPNS flux. These future high fluxes promise to open up to neutron diffraction new research areas, such as the study of time-dependent phenomena, while permitting the use of higher resolution, smaller samples, and more extreme sample environments. Thus, advances in time-of-flight diffraction can be expected to be even more dramatic than those which have been seen in the last decade.

James D. Jorgensen, Argonne National Laboratory

1. Phys. Today 35, 19 (November 1982).
2. J. D. Jorgensen and F. J. Rotella, J. Appl. Crystallogr. 15, 27 (1982).
3. S. R. MacEwen, J. Faber, and A. P. L. Turner, Acta Metall. 31, 657 (1983).
4. M. Misawa, T. Fukunaga, K. Nihara, T. Hirai, and K. Suzuki, J. Non-Cryst. Solids 35, 313 (1979).
5. A. K. Soper and R. N. Silver, Phys. Rev. Lett. 49, 471 (1982).

FORTHCOMING MEETINGS

1985:

July 28 - Aug 3: Sagamore VIII - Conference on Charge, Spin and Momentum Densities, Sanga-Saby Conference Centre Sweden. Contact: Prof I. Olovsson, Inst Chemistry, Univ Uppsala, Box 531, S-751 21 Uppsala, Sweden.

July 29 - Aug 2: 2nd Int Synchrotron Radiation Instrumentation Conference, Stanford CA. Contact: K.M. Cantwell, SSRL Bin 69, PO Box 4349, Stanford, CA 94305, USA.

Aug 19-23: American Crystallographic Association Meeting, Stanford, CA. Contact: K.M. Cantwell, SSRL, Stanford Univ, PO Box 4349, Stanford, CA 94305, USA.

Aug 19-23: 5th International Congress on Quantum Chemistry, Montreal, Canada. Contact: Mr K. Charbonneau, Exec. Sec. 5th ICQC, National Research Council of Canada, Ottawa, Canada K1A 0R6.

Aug 19-24:	Int Conference on Neutron Scattering, Santa Fe, NM. Contact: Dr J. Eckert, Los Alamos Nat Lab, Mail Stop H805, Los Alamos, NM 87545, USA.
Aug 26-29:	Int Symp on Steric Aspects of Biomolecular Interactions, Sopron, Hungary. Contact: Prof A. Kalman, Central Res Inst Chemistry, Hung Acad Sci, H-1525 Budapest, POB 17, Hungary
Aug 26-30:	55th ANZAAS Congress, Melbourne, Vic. Contact: Executive Secretary, 55th ANZAAS Congress, Monash University, Clayton, Vic. 3168.
Aug 29-31:	Pre-meeting Workshop of ECM-9 on Direct Methods and their Application to Structures Showing Superstructure Effects, Turin, Italy. Contact: Dr R. Bohme, Inst Mineralogie der Ruhr-Universitat, Universtatstr 150, D-4630, Bochum, German Democratic Republic.
Sept 2-6:	Ninth European Crystallographic Meeting, Torino, Italy. Contact: Prof G. Ferraris, Dipartimento di Scienze della Terra, Univerita di Torino, Via S. Massimo, 22 I - 10123, Torino, Italy.
Sept 14-28:	Scottish Summer School in Physics 1985. Synchrotron Radiation Sources and their Applications, Aberdeen Univ, Scotland. Contact: Prof G.V. Marr, Dept Natural Philosophy, Aberdeen Univ, Aberdeen AB9 2UE, Scotland.
Oct 7-9:	4th Int Symp on Data Analysis and Informatics, Versailles, France. Contact: INRIA, Service des Relations Exterieures, Domaine de Voluceau Rocquencourt, BP 78153 Le Chesnay Cedex, France.
Nov 6:	Powder Diffraction Techniques, London, UK. Contact: Dr J.C. Halfpenny, Dept Applied Chem Sciences, Napier College, Colinton Road, Edinburgh EH10 5DT, Scotland.
Nov 19:	Systematics in Structural Chemistry, London, UK. Contact: Dr B. Beagley, Dept Chemistry, UMIST, PO Box 88, Manchester M60 1QD, England.
Dec 9-19	International Winter School on Direct Methods, Macromolecular Crystallography & Crystallographic Statistics, Madras, India. Contact: Dr S. Parthasarathy, Dept Crystallography & Biophysics, Univ of Madras, Guindy Campus, Madras-600 025, India.
1986:	
Feb 10-14:	6th Australasian Conference and Schools on X-ray Analysis, UNSW. Contact: Fred Scott, School of Metallurgy, Univ NSW, PO Box 1, Kensington, NSW 2033.
June 10-19:	Synchrotron Radiation for X-ray Crystallography (Summer School), Erice, Sicily. Contact: Prof L. Riva Di Sanseverino, Piaxxa 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 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 11-20: Int Summer School on Crystallographic Computing, Leipzig, GDR. Contact: Prof P. Paufler, Sektion Chemie der Karl-Marx-University, Liebigstr 18, 1710 Leipzig, German Dem Rep.

Aug 17-22: 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 31 - Sept 7: 11th Int Congress on Electron Microscopy, Kyoto, Japan. Contact: Congress Secretariat, XI ICEM, Dept Anatomy, Faculty of Medicine, Kyoto Univ, Konoecho Yoshida Sakyoku, Kyoto 606, Japan.

Oct 21-25: Int Symp on Molecular Structure, Chemical Reactivity and Biological Activity, Beijing, China. Contact: Dr Xu Xiao-Jie, Inst of Physical Chemistry, Peking Univ, Beijing, China.

Nov 19-26: 56th ANZAAS Congress, Sydney, NSW. Contact: Executive Officer, 56th ANZAAS Congress, GPO Box 873, Sydney, NSW 2001.

1987:

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.

Aug 12-20: 14th General Assembly and Congress of the IUCr, Perth, Western Australia. Contact: Dr E.N. Maslen, Crystallography Centre, Univ. of WA, Nedlands 6009, Western Australia.

Satellites: Neutron Scattering, Sydney, Aug 5-8. Contact: Trevor Hicks, Monash Univ.
X-ray Powder Diffractometry, Perth, Aug 21-22. Contact: Brian O'Connor, WAIT.
Crystallographic Computing, Adelaide, Aug 22-29. Contact: Max Taylor, Flinders Univ.
Solid State Properties of Minerals, Sydney, Aug 24-26. Contact: Prof D. Haneman, UNSW.