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Henk Schenk

Teaching and life go along hand in hand. No singing birds, no language, no science, no society without teaching. Here in Erice, where I'm writing this letter, the older generations teach advanced crystallography to the younger ones - in formal sessions but, perhaps more importantly, also informally and by example. The other day David Sayre recalled a little movie I showed in the 'participant slide show' of the meeting in 1978: three-year-old kids learning to ice skate by example. Falling hundreds of times and standing up again, supported by parents. The kids take all that trouble just because they want to skate like the other people. By working hard, watching and copying they make very rapid progress. David told another nice story: his wife Anne observed from the window of her workroom how swans learn to fly. One day the parents decide it's time for the kids to fly. So father leads them to the starting line and shows them how to do it: he moves his wings up and down whilst running on the surface of the water - and off he goes. Then the kids try. But in the beginning they just end up under the water, comforted by mother swan. Then one day they come free from the water for the first time and are so surprised that they forget to keep their wings moving and fall down again. But soon the whole family flies in a nice order.

Why these stories? Well, if we want to skate with future generations, if we want children to fly, we have to teach them! These days it seems that Science is losing its attraction to Society, resulting, in reduced numbers of students. If we want to turn this round, we must go out, find the kids and teach. The younger the age group we aim at the more likely we reach the next generation of scientists.

Long ago Betty Wood wrote a small monograph for primary school teachers to help them to teach children about the world of crystals. It is very good that this book is available again, as an IUCr Teaching Pamphlet, but it is in English only. Because it should reach school teachers all over the world, we need volunteers to translate it into as many languages as possible.

But I think more is needed. If we want children to be science minded we have to work on their education. School curricula are based on what the community wants future generations to know; this usually leads to curricula with little time allocated to science. So we should teach them the fun and beauty of our subjects through the web, in as many languages as possible. Ideally we should have a range of subjects providing many hours of pleasure for all ages. But I think we should start with the primary school children of age 10 to 12, who could be the crystallographers of 2015. The material should be so eye- and interest-catching that even adults should be taken by it. Therefore I'm inviting all of you to provide input, so that we can build an attractive web site for schoolkids! Send your suggestions, offers, material to cw@iucr.org or to my lab address. I hope your reactions are numerous!

Henk Schenk
schenk@chem.uva.nl



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If you would like to see a copy of the IUCr Newsletter in your college or university library, send the address to the Newsletter office so that we can add it to our mailing list.

Dear Bill,

I hate to wake you from your well deserved slumbers by writing a 'Letter to the Editor', but the gremlin Editor modified the Glasgow IUCr Congress report on 'Cryo Preservation and Decay', resulting in a printed statement directly opposite in meaning to the one I intended. As submitted, the report on G. Bunick's talk read: 'Where cryo cooling has not reproduced room temperature mosaicity, crystals may be....'. This was edited to 'If cryo cooling has reduced room temperature mosaicity, crystals may be...'. If only we could reduce crystal mosaicity by cryo cooling! Unfortunately cooling often increases the mosaicity, and I have never heard of a case where the mosaicity at cryotemperatures is less than the room temperature value.

Elsbeth Garman, U. of Oxford, UK

Dear Bill,

I photographed this plaque at North Terrace, Adelaide, a major road going past the Railway Station, the Parliament, The Museum, the Art Gallery, the cricket ground, the University and of course the Casino. There were a whole collection of plaques in the footpath (sidewalk). And right next to one listing the achievements of Don Bradman, the most famous cricketer of all time (a regular Babe Ruth), was this to the Braggs (note: even in Australia we have things in alphabetical order). As you are aware WH was a Professor of Physics at Adelaide early last century, and WL was actually born in Adelaide. While I was doing my Ph.D. in about 1959, WL returned and was feted by my University (NSWUT at the time). I thought this image might be good for the ACA Newsletter.

Colin Kennard, retired, formerly U. of Queensland, Australia



Dear Bill

When I read the report the Jürg Waser had died, I immediately phoned Judy Schomaker. She immediately phoned Pludi Waser, in La Jolla, who reported that Jürg is just fine. ????

Dick Marsh

Dear Bill,

The editor's report on p. 4 of the current issue of the *IUCr Newsletter* reports my demise. Not so!! I think that I am still good for at least another 10 years. I am curious about where you got this info. A correction would be appreciated.

Jürg Waser

Dear Dr. Waser,

I owe you an apology for what is without doubt my greatest editorial error yet. I am delighted to learn that I was wrong and to hear that you are alive and well and living in La Jolla. I must have misunderstood my highly placed source. I accept sole responsibility for this grievous mistake and hope you will forgive me.

Bill

Dear Bill,

Could you please let me have, if you know, an address of a company which makes crystal structures models of simple inorganic substances - such as NaCl, CsCl, Rutile, etc. These are for teaching degree students in college. Contact K. Venkatesan at ockven@orgchem.iisc.ernet.edu.

K. Venkatesan

Dear Bill,

Bill Streib and I are planning to retire in the next few years. We have *Acta Cryst*, the first 17 volumes bound, then the remaining volumes through 36 not bound. We also have duplicates of several of the basic x-ray crystallography text books, such as Buerger's books. We were wondering if you have any suggestions for the use of these books. We hate to see them go to the recycling place. We would be grateful for any suggestions you might have. Thank you.

Kirsten Folting Streib

Dear Kirsten,

Thank you for offering your volumes of *Acta Cryst*. It should be possible to find them a home where crystallographers need them. There may be places in South America, Africa and the Pacific Islands that could make good use of them. The ACA covered shipping costs to send Ben Post's set to Cuba. We will announce availability in the ACA and IUCr Newsletters and websites. Other crystallographic books would probably also be appreciated. Please don't send crystallographic related books for recycling until we try to locate potential recipients.

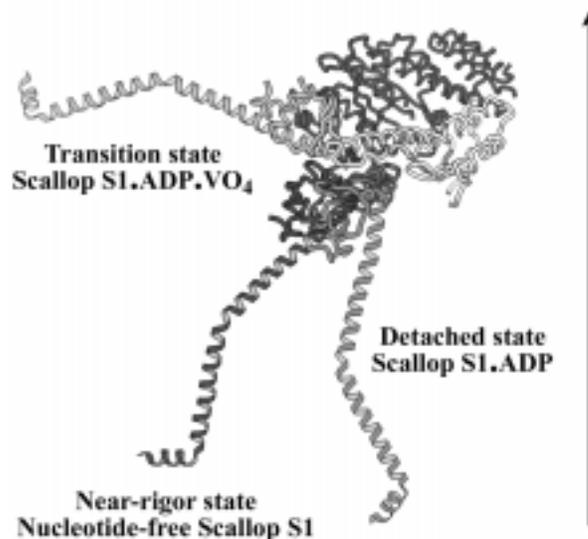
Bill



This issue contains reports for all of the microsymbiosia on High Pressure Crystallography from the Glasgow IUCr Congress. The reports were collected and edited by Commission Chair Richard Nelmes. Richard organized the High Pressure sessions at the IUCr Congresses in Seattle and Glasgow with great care from the planning process right through execution and preparation of final reports setting a standard that other commission chairs may want to emulate.

In February 2000 Carolyn Cohen received the Elizabeth Roberts Cole Award from the Biophysical Society for her significant contributions to the understanding of the structural basis for the biological activity of proteins involved in motility. In her address Carolyn made some cogent observations concerning the disparity between traditional hypothesis-based exploration of the structural basis for molecular function and “new wave” structural genomics. Carolyn agreed to have her remarks printed in this issue of the IUCr Newsletter. When I attended Anne Houdusse’s talk at the Glasgow IUCr meeting on Scallop S1.ADP, one of the myosin structures that Carolyn and Anne have analyzed together (in collaboration with Andrew Szent-Gyorgyi), I requested a copy of one of her illustrations for use on a newsletter cover. Patricia Coley took Anne’s beautiful illustration and developed the cover for this issue.

The cover has a number of possible interpretations. The Cohen/Houdusse structures upon which it is based exemplifies the value of studying the same molecule under different conditions to under-



Scallop myosin subfragment 1 in three different conformational states (adapted from Houdusse, A., Szent-Gyorgyi, A.G., and Cohen, C.) (submitted for publication).

stand its capabilities and correlate changes with molecular function. The replication of many copies of the structure on the cover alludes to the evolution of families of proteins. The march of the molecules can be seen as robotic movement of molecular lemmings. It suggests the mind-numbing prospect of structure for the sake of structure with biochemists and crystallographers potentially so overwhelmed with new structural information that they haven’t the time or ability to think about the meaning or functions of structures in any significant and thoughtful way.

I have been gathering material related to the role of crystallography in the genome project for over two years. On pages 18-20, we have reprinted Carolyn Cohen’s remarks, along with my observations and those of others on the challenge of structural genomics.



“Where is Colonel Sanders when you really need him” cries Carol Brock at the Glasgow Reception.

Triplet-Phase Measurements Using a 2D Detector

Acta Cryst. A56 (2000), 268–279, *Acta Cryst. A56* (2000), 264–267, *Acta Cryst. A56* (2000), 280–283



Unlike ordinary two-beam diffraction experiments performed for intensity measurements, three-beam experiments are also sensitive to the phase difference (triplet phase) of the three structure factors involved. Already during the late 1940s, a suitable experiment based on *Renninger* Ψ -scans was proposed. In the mid-1970s, the first three-beam interference profiles were observed, and since the end of the 1980s, one practical application has been the determination of the absolute structure of low Z ($Z \leq 8$) compounds. From the beginning of the 1990s, three-beam interference effects have been observed from crystals of small proteins, whose structures can in principle be solved by this method.

Up to that time, nearly all experiments were based on the *Renninger* Ψ -scan technique, which requires the alignment of a primary reciprocal lattice vector \mathbf{H} with its diffraction position and an accurate rotation about \mathbf{H} to excite a second reflection \mathbf{G} . During such a three-beam experiment, two wavefields are propagated in the direction \mathbf{k}_H of the first reflection \mathbf{H} . These are the direct wave due to \mathbf{H} and the twice-scattered *Umweg* wave due to \mathbf{G} , which is rescattered by $\mathbf{H}-\mathbf{G}$. This leads to characteristic intensity changes in the \mathbf{k}_H direction that depend on the phase difference between the two wavefields $\Delta\Phi_{tot} = \Phi_3 + \Delta\Phi(\Psi)$ with the triplet phase $\Phi_3 = \phi_G + \phi_{H-G} - \phi_H$ and the resonance phase shift $\Delta\Phi(\Psi)$ of the \mathbf{G} reflection as it passes through the Ewald sphere. The advantage of this procedure is the possibility to optimize experimental conditions for each three-beam case individually, resulting in a quite small phase error ($\approx 20^\circ$). However, the method is slow compared with an intensity data collection using area detectors because only one triplet phase at a time can be determined.

To tackle this problem, Shen *et al.* propose an experimental procedure [“Triplet-phase measurements using reference-beam X-ray diffraction”, *Acta Cryst. A56* (2000), 268–279] that enables the use of a 2D detector (either an image plate or a CCD). This technique should speed up the measurement of triplet phases considerably. Hereby, a strong reflection \mathbf{G} aligned to a rotation axis ϕ is rocked through its diffraction position stepwise by a second rotation (say θ) perpendicular to the ϕ axis (Fig. 1). For each step in θ an oscillation image about ϕ over the same angular range is recorded. The intensity of each reflection \mathbf{H}_i recorded on the detector results now again from the interference of the direct wave due to \mathbf{H}_i and a twice-scattered *Umweg* wave due to \mathbf{G} and $\mathbf{H}_i-\mathbf{G}$ as explained above. The series of intensities recorded for each reflection \mathbf{H}_i as a function of the rocking angle θ

of the strong reflection \mathbf{G} contains in principle the same information as a standard Ψ -scan interference profile. However, using a 2D detector a large number (≥ 1300) of interferences can be measured in a short time in one series. The intensity changes due to the three-beam interaction are in the range of $\pm 2\%$ for a crystal of tetragonal lysozyme (Fig. 2). In the example shown, the almost symmetric increase and decrease due to the constructive and destructive interference, respectively, of a three-beam interference with a triplet phase close to $\pm 90^\circ$ is clearly visible. Because the wavefield of the strong reflection can be considered as a sort of reference wave that interferes via the reciprocal lattice vectors $\mathbf{H}_i-\mathbf{G}$ with all directly excited reflections \mathbf{H}_i , the authors named this technique ‘reference-beam X-ray diffraction’. The geometry and wavelength cannot be optimized for many three-beam cases simultaneously; therefore, the phase information obtained is less accurate compared with the standard Ψ -scan technique, for example because of overlap of neighbouring three-beam interference profiles. The authors report a mean triplet-phase error of 54° after rejection of about 60% of the measurements by suitable criteria derived from the fit of the experimental intensity profiles. However, the significantly larger number of phases that can be determined in a given time might easily counterbalance this larger phase error. The authors report further that this method can also be applied to quasicrystals.

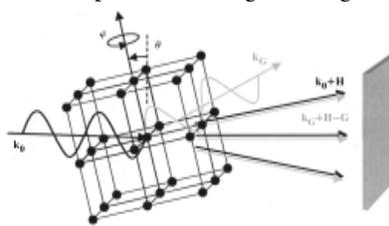


Figure 1. Reference-beam diffraction in Bragg-inclined geometry, where two sets of diffraction patterns (black and grey) interfere and generate a phase-sensitive diffraction image on an area detector.

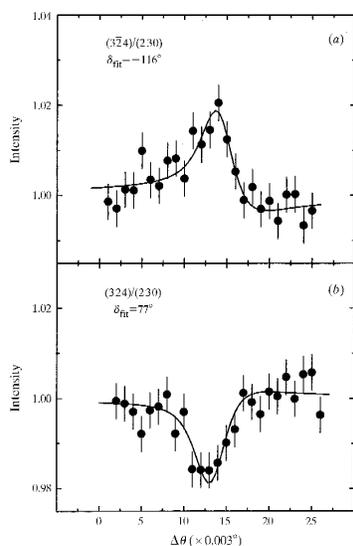


Figure 2. Reference-beam diffraction profiles of a Friedel pair on lysozyme, (a) $\mathbf{H} = (324)$, $\mathbf{G} = (230)$, and (b) $\mathbf{H} = (324)$, $\mathbf{G} = (230)$, recorded in inverse reference-beam measurements.

The authors report a mean triplet-phase error of 54° after rejection of about 60% of the measurements by suitable criteria derived from the fit of the experimental intensity profiles. However, the significantly larger number of phases that can be determined in a given time might easily counterbalance this larger phase error. The authors report further that this method can also be applied to quasicrystals. In a second contribution [“Enantiomorph determination using inverse reference-beam diffraction images”, *Acta Cryst. A56* (2000), 264–267], the same authors were able to show that the statistical significance achieved is sufficient for the determination of the absolute structure.

An important topic in this context — the utilization of the measured triplet phases in a structure solution procedure — is discussed in a third communication [“*Shake-and-Bake* applications using simulated reference-beam data for crambin”, *Acta Cryst. A56* (2000), 280–283]. Direct-methods programs like *Shake-and-Bake* that combine reciprocal space methods with real-space peak-picking techniques have already demonstrated several times that they are able to solve even the structure of small proteins *ab initio* if high-resolution intensity data ($\approx 1.2 \text{ \AA}$ and better) are available. Additional experimental phase information might help these programs to also work with intensity data of significantly poorer resolution. The proposed reference-beam technique provides for a single series of images triplet phases that all contain one reflection \mathbf{G} and phase information from an almost two-dimensional slab in reciprocal space. In this contribution, the authors used simulated data for the small protein crambin to investigate the important question of how many phases or series of reference-beam phase sets at what accuracy

are needed to boost direct methods significantly. They discovered that they could find a set of reasonably good trial phases for all resolutions (3 Å and better) of the available intensity data provided one series of triplet invariants is available by the method discussed above with a phase error of less than 40°. This phase error is less than what seems to be available by the experiment but reasonably

close for promising further developments. If more than one series of reference-beam phases are available, slightly higher phase errors can be tolerated, almost matching today's experimental achievements.

Thus the future of experimental phase determination would be very promising if the crystals could be persuaded to always crystallize with a mosaicity low enough for three-beam interference experiments.

Edgar Weckert, HASYLAB at DESY, Germany

Crystallography Journals Online

<http://journals.iucr.org/>

Crystal Structure Prediction

Acta Cryst. B56 (2000), in proof



The ability to reliably predict some function or physical property of a system based on prior information and computational calculation has long been the goal of many scientists as it reduces the need for expensive resource and time-consuming experimentation. Of particular interest over the past decade has been the potential to reliably predict crystal structures of molecular compounds. Crystal structure prediction is of considerable interest to those working in industries that process molecular materials, for example pharmaceuticals or pigments, where an outbreak of polymorphism can wreak havoc with the physical properties of the desired final form. To those scientists observing the field from the sidelines, the progress of the technique has been difficult to follow with claims of outrageous successes on compounds that are “too sensitive” to mention, only leading the technique further into urban mythology. It is with this background in mind that the recent paper by Lommerse, Motherwell, Ammon, Dunitz, Gavezzotti, Hofmann, Leusen, Mooij, Price, Schweizer, Schmidt, van Eijck, Verwer & Williams [“A Test of Crystal Structure Prediction of Small Organic Molecules”, *Acta Cryst.* B56 (2000), in proof], testing the ability of 11 established research groups in the field of crystal structure prediction to correctly predict the structures of three different molecular compounds of varying complexity, is particularly timely. It also gives the reader a sense of what is and what is not achievable. The paper reports the results of a blind test of the major methodologies for *ab initio* crystal structure prediction that were presented at a collaborative workshop held in May 1999 at the Cambridge Crystallographic Data Centre (UK).

Three compounds of differing complexity (I, II, III) were selected by an independent referee from a set of 20 unpublished molecular structures. All three structures were restricted to a maximum size of 30 atoms including hydrogen and had to belong to a relatively common space group with one single molecule in the asymmetric unit. The three levels of complexity were defined as:

- 1) a small rigid molecule with less than 20 light atoms (C, H, N, O)
- 2) as 1) but containing some less common elements
- 3) a molecule with a small amount of conformational flexibility.

The participants were also invited to determine the unpublished structure of propane as an added extra. Compound I has two polymorphs, but this information was not provided to participants. They were allowed to submit a maximum of three predictions per compound and asked to give reasons and a degree of confidence for their selection. The paper provides a short overview of the processes involved in crystal structure prediction discussing both the lattice minimization and the statistical methods. This is followed by more detailed descriptions of the individual methodologies representing the principal computer programs used by the research groups themselves.

The results of the study were revealing in that no one program provided consistently reliable results; however, seven proposed structures were close to an experimental one and as such were classified as correct. Four of the seven correct structures were predictions for structure I in the first level of complexity; however, for this polymorphic structure only the unstable form in all cases was correctly predicted. One structure was correctly predicted for II and III and one for propane. The methods that gave accurate predictions all came from the lattice energy minimization procedures and not the statistical methods.

From these results it is clear that the technique is still very much in its early stages although I have no doubt that it will mature in time to yield meaningful information about systems that are not tractable by experimental methods. The answer to the question raised by Gavezzotti in 1994 in the review “Are Crystal Structures Predictable?” [*Acc. Chem. Res.* 27 (1994), 309–314] has certainly moved on from the categorical “No” to “Maybe sometimes”.

Christopher Frampton
Roche Discovery, Welwyn, UK

I

II

III

High Pressure 1999

This year marked the end of the first triennium of the Commission on High Pressure. The Commission's principal activity is to organize symposia and workshops to keep the high-pressure crystallography community abreast of a rapidly developing field, and build links to other related areas of high-pressure science. A large effort was put into organising the Commission's six microsymbiosia and an Open Commission Meeting (OCM) at the Glasgow Congress. Commission member A Katrusiak served on the Congress Programme Committee. All other members and consultants acted as microsymbiosia Chairs or Co-chairs, and two members (W.F. Kuhs and D. Häusermann) presented keynote lectures.

The microsymbiosia covered high-pressure structures and phase transitions, structures and techniques at extreme pressures and temperatures, physical properties and novel materials under high pressure, high-pressure data acquisition and analysis, high-pressure studies of biological and other soft matter, and new frontiers in high-pressure crystallography. These sessions attracted audiences ranging from 65 for the most specialised to 150 for the wide appeal of geoplanetary science at extremes of pressure and temperature. The OCM focused on laboratory-based high-pressure crystallography, including non-diffraction techniques, and the keynote lectures provided overviews of research into water structure in ices and clathrates, the latest developments in crystallography in extreme conditions of pressure and temperature, and what can now be achieved by *ab initio* molecular dynamics. In all, there were 45 invited lectures, and 65 poster presentations. It added up to a rich and stimulating programme – effectively a substantial international workshop embedded in the Congress programme – that attracted considerable numbers of new participants from the wider field of high-pressure science. A similar format had proved successful at the Seattle Congress, and some 30% more participants (over 100) were attracted to Glasgow. Some of this increase came from the inclusion of a session on biological and other soft matter – an important and successful development of the range of the Commission's activities over the past three years. Short poster orals – three-minute summaries of the highlights of related presentations in the poster sessions – were introduced to link the posters to the oral sessions and general discussion. This innovation was welcomed by the participants. To recognise the contribution of the posters to the overall programme, the Commission funded prizes for the best. First Prize went to Dominique Gourdain (Paris VI U., France) for her high P-T studies of KNbO_3 , and Second Prizes went



Speakers in the Structures and Techniques at Extreme Pressures and Temperatures session in Glasgow. (left to right) Dave Mao, Guillaume Fiquet, Anil Singh, David Price, Russell Hemley, Raymond Jeanloz, Guido Chiarotti (at the back).

to Maki Okube (Osaka U., Japan) for her novel EXAFS determinations of anharmonic effective pair potentials, and to Olga Degtyareva (Paderborn U., Germany) for her studies of binary lanthanide alloy's. The Commission is concerned to encourage and assist the participation of young scientists in its meetings, 30-40 were in attendance and two were given funding assistance by the Commission. The success of the programme owed much to members and consultants of the Commission, and other session Chairs and Co-chairs (M. I. McMahon, M. Kunz and R. Winter). *Detailed reports on all the microsymbiosia and the OCM have been posted on the Commission's website.*

Among the items of Commission business discussed were the report on the 1998 workshop at Argonne, USA, and its final accounts; future workshops and schools; links to the ICDD (C T Prewitt in attendance); membership of the Commission for 1999-2002; a planned directory of high-pressure crystallographers; and further development of the Commission's web site to include a comprehensive listing of future high-pressure meetings, and information on central facilities for high-pressure crystallography and how to access them. The assistance of J S Loveday with the directory and the web site listings was gratefully noted. Following the recommendation of the Executive Committee (EC), all the members and consultants for 1996-1999 were elected by the General Assembly to serve for the next triennium. The EC also agreed to the Commission's recommendation that M Kunz (ETH, Zurich) and J Tse (NRC, Ottawa) be appointed as consultants for the next triennium.

It was agreed that the Commission would organise workshops at Spring-8, Japan, in 2000, with member O Shimomura as the local organiser, and at Saclay, France, in 2001, with member I N Goncharenko as the local organiser. The Commission will seek for the Jerusalem Congress in 2002 a programme and format broadly similar to Glasgow. Commission member A Katrusiak reported on plans now well in place for a School on High Pressure Crystallography to be held at Erice, Italy, from May 27 to June 8 in 2003.

The programme and planning at the Glasgow Congress made significant steps in the Commission's development, and launched a second triennium with work to be done but much to look forward to.

R.J. Nelmes, Chairman

Crystal Materials in Tunisia

The IUCr Commission on Crystal Growth and Characterisation of Materials is organising an International School on Growth of Materials for Energy Production and Energy-Saving Applications. The School will be held November 19-26, 2000 in Monastir (Tunisia) on the Tunisian coast, which is accessible directly *via* its international airport or by rail and motorway from Tunis. The School will be co-chaired by R. Fornari (CNR-MASPEC Inst., Italy) and H. Maaref (Fac. of Sciences, Monastir) and will include lectures by international experts on general crystal growth principles, crystal growth techniques, growth and characterisation of semiconductors for solar cell fabrication, superconductors for energy storage, wide bandgap semiconductors for white light production, small bandgap semiconductors for thermoelectric applications, soft magnetic materials and more.

Contact H. Maaref, Physics Dept., Fac. of Sciences, Monastir, Tunisia, E-mail: Hassen.Maaref@fsm.rnu.tn, www.semiconductors.co.uk/skanes-gemes.htm

Roberto Fornari

International Tables, Volume C, Second Edition

The publication, in June, 1999, of the second edition of Volume C of the *International Tables for Crystallography* was a major milestone in a project that has been under way for nearly 20 years. This volume, subtitled *Mathematical, Physical, and Chemical Tables*, was originally conceived of as a consolidation and revision of the materials in Volumes II, III, and IV of the previous series of the *International Tables*, but it was evident almost at the beginning that a useful volume would have to include extensive new material. When the first edition, edited by A.J.C. Wilson, was published in 1992, it contained a lot of outdated information. For example, the table of the wavelengths of the X-ray emission lines and absorption edges was a photocopy of the table that was published in Volume III, which appeared in 1962, and which in turn contained information dating back to the 1930s. Professor Wilson's death in 1995 left the task of preparing a second edition that would fill all of the gaps unfinished, and the Executive Committee appointed me to the editorship to complete it.



During the time when material for the first edition was being assembled, the revolution in the technology of publication had not reached the point where word-processor files could be reliably imported into typesetting programs, so that, although authors were invited to supply machine readable files, and many of them did, the volume ultimately had to be typeset by hand. One unfortunate result was that there were no useful files that could be used for the second edition, and disappointingly few of the authors had retained any of their original files. Those chapters and sections that were unchanged or needed only minor corrections had to be typeset by hand all over again. On the other hand, many authors were able to supply files of numerical data, all of the new or extensively revised text was provided in some machine-readable form, and importation of these files into the typesetters' system was generally successful. One way or another, all of the second edition of Volume C now exists in electronic form, which will make future reprints, corrections, and revision much easier and less expensive.

Of the chapters in the first edition that were carried over from the earlier series, only one, an editorial condensation by A.

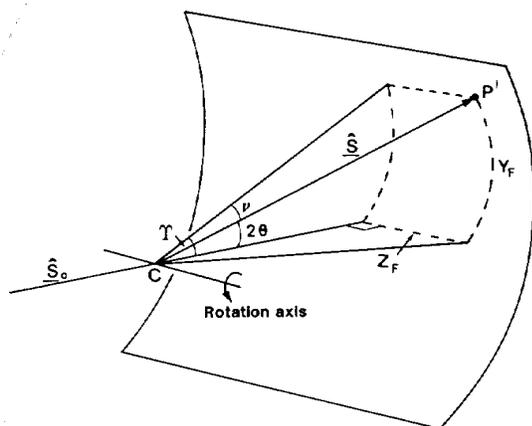
J.C. Wilson of the chapter on measurement of refractive index by E.S. Larsen and R. Meyerowitz, remains. There are completely new chapters on neutron diffraction topography by M. Schlenker and J. Baruchel and on neutron reflectometry by G.S. Smith and C.F. Majkrzak. Other replaced or extensively revised chapters and sections include an updated section on X-ray wavelengths by R.D. Deslattes, E.J. Kessler, Jr., P. Indelicato, and E. Lindroth, sections on filters and monochromators, for X-rays by D.C. Creagh and for neutrons by I. S. Anderson and O. Scharpf, and chapters on crystal growth, mounting, and orientation by P.F. Lindley. A major effort was made to include the current state of the art in all aspects of experimental crystallography.

For additional information, including ordering information and a table of contents, see the IUCr home page at <http://www.iucr.org>.

Edward Prince

An editor should be respected, even feared, maybe even disliked, by his contributors. His job is to dock their prolixities, unify their styles, and force them to conform to a consistent and clearly defined vision of the work in hand. It is no job for a democrat.

*D. Jones, U. Newcastle upon Tyne
in a book review in Nature*



Geometrical principles of recording the pattern on a cylindrical detector.



(see also Volume 7, No. 4 and Volume 8, No. 1)

The High Pressure Program from Glasgow

Structures and Phase Transitions

This was the first of six high-pressure sessions at the Glasgow Congress. S. Hull (ISIS Facility, UK) opened the proceedings with a lucid account of his high-pressure high-temperature studies of binary halides. These simple materials exhibit surprisingly complex behaviour, with transitions from cubic NaCl to CsCl structures progressing through a number of other lower-symmetry intermediates. The complex behaviour exhibited by simple materials was re-emphasised by U. Schwarz (MPI, Dresden, Germany), who described recent diffraction studies of Cs, Si and Rb. These reveal that the long-uncertain structures of Cs-V, Si-VI and Rb-VI are orthorhombic with a new structure type. However, although the crystallographic structures are the same in each case, the calculated electron densities are different. The next three invited talks focused on molecular systems. N. Hamaya (Ochanomizu U., Japan) described studies of AX_4 structures at SPring-8. A new re-crystallised phase of SnI_4 existing at 7 GPa and 500 K was studied using anomalous dispersion techniques to determine the structure. The results were consistent with a disordered cubic structure. An amorphous phase of GeI_4 was also reported above 30 GPa. The breakdown in the molecular structure of CO_2 at high-pressure to form a polymer was described by C-S. Yoo (Lawrence Livermore Nat. Lab., USA). This polymeric form, which may act as a frequency-doubler, has a bulk modulus very similar to that of cubic-BN. Unfortunately, it is not recoverable at ambient conditions. The ability of pressure to create new materials was the subject of a talk by S. Tsuneyuki (Tokyo U., Japan) who described calculations aimed at identifying new high-pressure structures. Calculations of a new phase of SnI_4 above 61 GPa described by Hamaya suggest it is a substitutional solid solution of Sn and atomic iodine. In the final talk of the session, J.B. Parise (SUNY, Stony Brook, USA) reviewed the large number of current (and conflicting) diffraction, transport and magnetic studies of FeS. A clear picture is beginning to emerge from conflicting results that probably arise from slight changes in sample homogeneity and composition. The session included three short oral summaries of poster presentations on studies of ice-VI and ice-VII using single-crystal neutron diffraction (M. Guthrie, Edinburgh U., UK); complex structures of lanthanide (La-Pr-Ce) alloys (O. Degtyareva, Paderborn U., Germany); and calculations of the high-pressure phases of PON, which is isoelectronic with SiO_2 (D. Klug, NRC Ottawa, Canada).

M. I. McMahon, Co-chair



Speakers in High Pressure Structures and Phase Transitions session. (left to right) U. Schwarz, N. Hamaya, S. Hull, C-S Yoo, J.B. Parise and O. Shimomura (session chair).

Extreme Pressures and Temperatures

This session highlighted recent advances in structural studies of materials up to megabar (>100 GPa) pressures and at temperatures from cryogenic conditions to thousands of degrees. The motivation for many of these studies is the need to understand from both experiment and theory the behaviour of materials that comprise the deep interiors of the planets. R. Jeanloz (UC Berkeley, USA) provided a brief overview of geophysical problems and the importance of phase transitions for understanding the deep Earth. He then focused on recent diamond-anvil x-ray diffraction studies of whole rock samples subjected to high pressure-temperature conditions of the lower mantle, and reported evidence for a new silicate perovskite phase. H. K. Mao (Carnegie Institution, Washington) described the wide range of high-P/T techniques now available. Examples include radial diffraction for elasticity studies and phonon density of states measurements, such as those made on Fe which has been recently measured to Earth core pressures (i.e. to above 140 GPa). The new elasticity techniques were explored in more detail by A. K. Singh (Bangalore, India), who described additional applications. G.D. Price (University College London, UK) complemented these experimental talks with the results of *ab initio* calculations on both the solid and liquid phase of iron under core conditions (to 363 GPa). Solid phase stability, vibrational dynamics, and phase diagrams, including melting curves, were found to be in excellent agreement with the most accurate experimental data. G. Fiquet (ENS Lyon, France) presented the results of x-ray diffraction experiments on magnesite ($MgCO_3$) and diamond samples of different isotopic composition. Magnesite was found to undergo a transition above 80 GPa to an altogether new phase, and the diamond study showed very small isotope effects, in contrast to previous claims. Finally, G. L. Chiarotti (Trieste, Italy) reported theoretical investigations of the fate of methane, water, and ammonia at extreme conditions by *ab initio* constant-pressure molecular dynamics simulations. The results included predictions of high pressure-temperature superionic phases of H_2O and NH_3 , metallization of liquid water and ammonia, and the condensation of methane to form heavier hydrocarbons, with important consequences for Neptune and Uranus. The session also included four poster orals on single-crystal x-ray diffraction studies to 30 GPa that reveal significant changes in crystal chemistry of Fe under pressure (L. Zhang, Marburg U., Germany); compressibility studies of refractory materials, including evidence that Co_6W_6C may be even more incompressible (and possibly harder) than diamond (N.A. Dubrovinskaia, Uppsala U., Sweden); *in situ* x-ray diffraction of the graphite-to-diamond transition indicating that the transition can occur without melting of the catalyst and that solid $MgCO_3$ can be an important solid catalyst (W. Utsumi, SPring8, Japan); and, finally, x-ray studies of oxygen that suggest the material remains molecular in its metallic state above 100 GPa (G. Weck, CEA, Paris, France).

R. J. Hemley, Chair

Physical Properties and Novel Materials

This session covered a variety of topics at the boundary between traditional crystallography and others fields of condensed matter science: magnetism and superconductivity under very high pres-

tures, unusual properties of carbon-based materials, and the theory of simple elements and compounds. J. Akimitsu (Aoyama-Gakuin U., Japan) presented high-pressure studies of superconductivity and magnetism in spin-ladder compounds having peculiar structural and electronic properties. M. M. Abd-Elmeguid (Cologne U., Germany) described Moessbauer results on pressure-induced magnetic order in Yb-based heavy-fermion compounds. Could somebody measure superconducting properties at pressures as high as 1 Mbar and temperatures as low as 0.1 K? An example of such study was given in an exciting talk by K. Amaya (Osaka U., Japan). J.-M. Mignot (LLB, Saclay, France) emphasized recent progress in precise neutron diffraction measurements under pressure, and the potential of this technique for studies of mixed-valence compounds. D.E. Sklovsky (Moscow State U., Russia) introduced high-pressure studies of recently discovered nanoscale materials, and discussed abnormal elasticity of carbon nanotubes. Pressures of a few thousand Mbar are only a dream for experimentalists, but someone hearing the talk of J. Tse (NRC Ottawa, Canada) on structural principles of simple elements and compounds would be pleased to see that theoreticians are already actively working in this pressure range. The poster oral presentations of K. Ohwada (Tokyo U., Japan) on a spin-Peierls transition in vanadates, of M. M. Abd-Elmeguid (as above) on *f* and *d* magnetism in Eu-Co compounds, and of D. Chasseau (CNRS, Bordeaux, France) on molecular systems under high pressures enlarged the programme of the session and stimulated further discussions.

I. N. Goncharenko, Chair

Data Acquisition and Analysis

Crystallography at high-pressure is inherently hampered by a degradation of the data quality due to the high-pressure environment. This session was dedicated to pushing the experimental limits to higher pressures and temperatures, optimizing the data quality under the given constraints, and the development of data analysis tools to extract a maximum of information out of the data available. L. Dubrovinsky (Uppsala U., Sweden) reported on the construction of an externally heatable pressure cell, which allows the generation of temperatures up to 1200 K in combination with pressures in the megabar range. With this cell and in-house facilities, several crystallographic experiments at mantle conditions were completed. Y. Zhao summarized the work of his group (at LANSCE, USA) in developing a heatable large-volume cell, which is compatible with neutron experiments. A first version based on the Paris-Edinburgh design is able to achieve simultaneously pressures of 10 GPa and temperatures around 1500 K. A new model is in development that will allow cryogenic and combined P-T experiments in the 30 GPa / 2000 K range. The latest developments for high-pressure data analysis were shown by S. Belmonte and R. Papoular. S. Belmonte (Edinburgh U., UK) presented his ground-breaking work in exploiting texture due to preferred orientation in diamond-anvil cells (DAC's) to extract additional structural information from a powder pattern. R. Papoular (LLB, Saclay, France) impressively demonstrated the potential and limitations of Maximum Entropy methods if applied to locate proton positions from a DAC-powder data set. A combination of data acquisition and data analysis was given in the talk of M. Mezouar (ESRF, France). He showed the latest experimental development of the ESRF high-pressure group towards obtaining very clean time-resolved powder patterns from a Paris-Edinburgh cell, allowing kinetic studies of phase transitions and



High pressure studies can be serious business. Front row. (left to right) I. Goncharenko (chair), Y. Fujii (co-chair), and J. Akimitsu; Back row: M. Abd-Elmeguid, J.-M. Mignot.

reactions. This was complemented by the presentation of the latest developments of *FIT2D*, which permits automatic processing of the large amount of powder data generated during such time-resolved studies. The session was spiced up by three excellent poster oral presentations. Y. Barrans (CNRS, Bordeaux, France) introduced the development of a DAC optimized for the use with a cryostat. J. Parise (SUNY, Stony Brook, USA) illustrated his presentation of the CHiPR large volume/IP set-up with a state-of-the-art movie presentation, and R. Angel (Bayreuth, Germany) – co-authoring with L. Finger – gave us the latest news about the development of the 4-circle diffractometer control software *SINGLE*.

M. Kunz, Chair

Biological and Other Soft Matter

The session was divided into two parts, separated by the partial solar eclipse. The first part was devoted to discussion of pressure effects on polymers. K. Mortensen (Riso, Denmark) discussed neutron diffraction studies on polymer and copolymer blends, systems sufficiently understood theoretically that specific predictions of the effects of pressure can be made and tested. H. King (Exxon R. & E., USA) summarized the historically important role of pressure in understanding the structure of crystalline and amorphous polyolefins, major commodity materials produced in huge volumes. King also discussed recent experiments on water-soluble polymers which shed light on the roles of the van der Waals and hydrogen bonding energies in determining the pressure behavior. Talks on the effects of pressure on biological materials followed the eclipse. R. Templer (Imperial College, UK) described x-ray studies on the effects of pressure on lyotropic liquid crystals made of biomembrane lipids. These are some of the most pressure sensitive condensed matter systems known and exhibit large changes in phase structure with changes of only a few hundred atmospheres of pressure. The final three talks were devoted to pressure effects on proteins. G. Hummer (Los Alamos National Lab., USA) described theoretical work aimed at understanding why proteins unfold when pressure is applied. The central theme is that the unfolding results from the increased proclivity of water molecules to intercalate into the protein, as opposed to the more conventional wisdom that pressure promotes a proclivity for the polypeptide strands to disperse into the bulk water. Thus, water under pressure acts as a kind of plasticising agent. An important prediction of the work is that the radius of gyration of a pressure-denatured protein would be smaller than that of a thermally denatured protein. C. Royer (Centre de Biochimie Structurale, Montpellier, France) reviewed the substantial progress now being made in experimental studies of the folding and unfold-

ing process – both its nature and its kinetics – and showed that radius of gyration measurements of pressure-unfolded staphylococcal nuclease support Hummer's predictions. P. Urayama (Cornell University, USA) noted that there is little understanding of the structural basis of the many effects of pressure on proteins because there have been so few crystallographic studies of proteins under pressure. He described a technique that allows high-resolution crystallography to be performed on proteins which have been frozen into a high-pressure state. Short poster oral presentations were given by W.C.K. Poon (Edinburgh U., UK) on agarose gelation and R. Winter (Dortmund U., Germany) on lipid high-pressure phase behavior. The microsposium served to illustrate both the richness of effects of modest pressures on biological and other soft condensed matter and the need to understand the structural basis of these effects.

Roland Winter & Sol M. Gruner, Chairs

New Frontiers in High Pressure Crystallography

This session focused on experimental, computational and conceptual breakthroughs. M.I. McMahon (Edinburgh U., UK) described promising techniques for obtaining data from one or more single crystals grown *in situ* in diamond-anvil cells for high-pressure phases previously studied only by powder methods. This allows much more detailed structural information to be obtained – as he illustrated with single-crystal studies of InSb, cerium and barium. I.N. Goncharenko (LLB, Saclay, France and Kurchatov Inst., Moscow, Russia) presented recent magnetic neutron diffraction in the 50 GPa pressure range – well above previous limits. Using a combination of sapphire and diamond opposed-anvil devices, and neutron focusing optics, magnetic structures and phase transitions in the 50 GPa pressure range, and temperatures down to 1.5 K, are being studied in systems such as simple binary compounds of Eu and Gd. K. Knorr (Kiel U., Germany) discussed the pressure dependence of disorder in KPF_6 and computer simulation of the reconstructed densities using a flexible evolutionary algorithm. With F. Mädler, he found two pathways for the reorientation of KPF_6 at high pressure which together fully explain the shape of the electron density found experimentally. A. Fitch (ESRF, France) described software tools developed in collaboration with A.P. Hammersley and T. Günzel for more flexible data-processing, including automation of the *FIT2D* package that integrates 2-D images to 1-D profiles to allow routine treatment of hundreds of images for time-resolved *in situ* studies. The program "CINDEX" facilitates interactive indexing of 2-theta scans providing a stream-lined interface to a number of standard indexing algorithms. H.F. Grünsteudel (ESRF, France) discussed the advantages of a third-generation light source for studying the Mössbauer effect at high pressure. He explained how the diamond-anvil cell technique is especially suited, and how the next steps will involve

the simultaneous heating and pressurizing of samples. Complementary posters from the group described instrumentation used at the ESRF to carry out these experiments and some results on ^{119}Sn . K. Hämäläinen (Helsinki U., Finland) presented the final invited talk on the exciting prospects for inelastic X-ray scattering under high pressure – a unique tool to probe electronic ground state properties of materials. He described successful experiments that confirm the possibility of studying fine structures related to the Fermi surface topology in materials such as sodium at high pressure. Some other interesting developments were outlined in short poster orals – by I.D. Brown (McMaster U., Canada) on using the bond-valence model to simulate the effects of high pressure on structures by increasing ionic charges; by Jay D. Bass (Illinois U., USA) on extending the P-T range of Brillouin scattering as a complementary technique to diffraction in studying mineral equations of state; by M. Okube (Osaka U., Japan) on a novel use of EXAFS to make direct determinations of anharmonic effective pair potentials; and by D.P. Kozlenko (Frank Lab., Dubna, Russia) on joint elastic and inelastic neutron scattering studies of ammonium halides under high pressure.

John Parise, Chair

Open Commission Meeting on Laboratory-based High-Pressure Crystallography

The Commission on High Pressure organized this meeting to focus on laboratory-based high-pressure science and techniques, and bring experts together with crystallographers keen to learn about the possibilities, limitations and essential equipment for starting or extending their laboratory-based activities. 3rd generation synchrotron sources have taken high-pressure crystallography into realms which before were inaccessible, and the question arises as to whether there is still relevant research to be done with in-house facilities. This meeting demonstrated that there is, not only in traditional single-crystal diffraction but also in powder diffraction, in extreme P and T regimes, and through application of non-diffraction techniques. D. R. Allan (Edinburgh U., UK) and R. Angel (Bayreuth U., Germany) summarized state-of-the-art single-crystal methods. David Allan demonstrated the determination of hydrogen locations with an off-the-shelf diffractometer, and Ross Angel focused on the optimization of a diffractometer to obtain highly accurate cell parameters for equation-of-state measurements. J. Haines (CNRS, Meudon, France) explained the experimental set-up his group is using for powder diffraction with a standard sealed-tube source, and showed that such facilities are by no means limited to carrying out preparation for synchrotron experiments, but can support substantial leading-edge high-pressure research. L. Dubrovinsky (Uppsala U., Sweden) introduced the X-ray set-up of the Uppsala group, consisting of a rotating-anode generator and a SMART CCD-detector. With this very effective combination, experiments across the P-T range of the lower mantle are performed successfully in-house. An extended tea-break sponsored by Diacell Products, was followed by three talks focusing on non-diffraction techniques. J. D. Bass (Illinois U., USA) gave a lucid presentation of a basic set-up for high-pressure Brillouin scattering, and showed how it could be used as a powerful technique for determining sound velocities in minerals. M. Abd-Elmeguid (Cologne U., Germany) presented an overview of the essentials of high-pressure Moessbauer techniques, and clearly defined the limits of what can be done with such an experiment. The meeting ended with an overview by K. Amaya (Osaka U., Japan) of the impressive techniques developed by his group to measure electric and magnetic properties of materials in the megabar range.

M. Kunz, Chair



Happy faces from the Soft Matter crowd. Left to right: (Back row) K. Mortensen, R. Winter (chair), H. King, S. Gruner (co-chair) (front row) P. Urayama, C. Royer

European Crystallographic Society

<http://www.ba.cnr.it/eca>

Agenda items for the ECA Council meeting in Nancy, August, 2000 include elections for members of the Executive Committee and selection of future meeting sites. Nominations for Executive Committee members and meeting sites are invited. 250 registered Individual Members require election of two Councillors at Large.

Paul Beurskens, Secretary ECA, ptb@sci.kun.nl



British Crystallographic Assn

<http://gordon.cryst.bbk.ac.uk/BCA/index.html>

Honorary Members

Arnold Beevers, Bill Cochran, Bob Evans, Bruce Forsyth, Ron Jenkins, Aaron Klug, Helen Megaw, Max Perutz, John E. Walker, and Terry Willis.

ACA American Crystallographic Assn

<http://www.hwi.buffalo.edu/ACA/>

The 1999 ACA Transactions, Volume 34, *Two Decades of Synchrotron Radiation Research* is now available. Contact the ACA office (aca@hwi.buffalo.edu) or visit the website.

Int'l X-Ray Analysis Society (IXAS)

A new type of scientific society focused on the use of X-rays, neutrons, and electrons in materials characterization has been established. This fully electronic non-profit society will have free, open membership to the world's community of X-ray analysts requiring only that they have access to the World Wide Web. The purpose of the Society is to serve professionals working in the field of materials analysis by: (a) fostering interaction among materials scientists, chemists, physicists, geologists, and others engaged in the use of X-rays and other radiations, including neutrons and electrons, for materials analysis; (b) sponsoring meetings of interest to those in the field of materials analysis; and (c) disseminating information of interest to the materials analysis community.

The Society will provide e-discussion groups, a job clearing-house, future meetings bulletin, analysis problems bulletin board, newsletter e-mailed, X-ray analysis meetings proceedings and abstracts on web, free fully electronic journal JXA on the web, data committee: XRF fundamental parameters on the web.

An international steering committee met at the seventh European Powder Diffraction Conference in Barcelona on May 20, 2000 and completed the formal establishment of IXAS. R.L. Snyder will serve as the first president.

The founding sponsor of IXAS is the ICDD, which provided the funds to the Denver Conference Organizing Committee to establish the International Steering Committee. Eric Mittemeijer as a representative to the IXAS council and the IUCr's Commission on Powder Diffraction has also agreed to name a representative to council. The first version of the IXAS website is available at www.ixs.org.



ECA Council Members (left to right) P. Beurskens, (Secretary), F. Allen, P. Paufler, M. Carrondo, C. Giacobozzo (President), J. Bernstein (Vice President), and S. Harkema.

Society Officers

Crystallographic Society of Japan

<http://www.soc.nacsis.ac.jp/crsj/index-e.html>

President: Fujiko Iwasaki
 General Secretary: A. Takenaka
 Treasurer: S. Ohba
 Committee Chairmen:
 Meeting and School of Crystallography: Y. Kai
 International Communication: M. Takata
 Data Base and Information: Y. Satow
 Journal of the CSJ: Satoshi Sasaki

Professor Iwasaki is the first woman President to be elected by the CSJ.

Polish Academy of Sciences

http://kom_kryst.int.pan.wroc.pl/

President: K. Lukaszewicz
 Vice-President: J. Lipkowski
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Polish Synchrotron Radiation Society

<http://zeus.ifpan.edu.pl/PTPS/>

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<http://www.sca.asn.au>

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 Councillors: J. Martin
 S.W. Willkins
 G.B. Jameson
 Past-President: M.R. Taylor
 ANCCr Representative: J.W. White

Crystallography in...

Australia

Biomolecular Research Institute

Protein structure analysis at Parkville dates back to the 1950s, with Bruce Fraser and Tom MacRae using X-rays and, later, Peter Tulloch using electron diffraction to study natural fibers. The laboratory took a new direction in 1978 when Peter Colman brought some of the first crystals of influenza neuraminidase to what was then the CSIRO Div. of Protein Chemistry. By 1983, the structure of neuraminidase had been solved, and the possibility of using the neuraminidase structure to develop antiviral compounds was suggested. Biota Holdings was floated in 1985 to support the development of neuraminidase inhibitors in conjunction with the Victorian College of Pharmacy. Other structure work in the 80's included electron and X-ray crystallography of neuraminidase-Fab complexes by Peter Tulloch and Bill Tulip, single crystal studies of a plant virus and structure determination of a seed storage protein by Mike Lawrence.



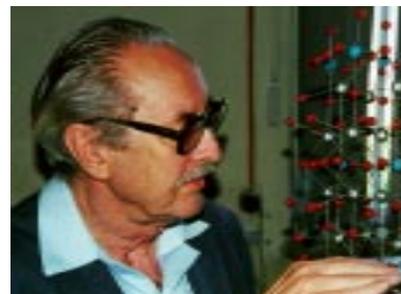
In 1990, the Biomolecular Research Institute was formed with Peter Colman as Director, combining virology, biochemistry and organic chemistry to providing an integrated approach to structure-based drug design. The focus of the work is on proteins of medical interest, viral and bacterial pathogens, growth factors, antibodies, carbohydrate processing enzymes and engineering protein thermostability. Having an emphasis both on basic research and on its application, a number of projects have now been taken through to the stage of drug design and synthesis. A thermostable enzyme has also been produced for the brewing industry.

Tom Garrett, SCA Newsletter No 43, November 1999

Russia

Institute of Crystallography, Moscow

The X-ray laboratory was established by Academician Professor N.V. Belov in 1943. The current focus of the laboratory is upon correlations between crystal structure and physical properties of materials. X-ray diffraction is being used to determine structures ranging from minerals to biologically active molecules. Temperature studies and investigations under pressure illuminate phase transition mechanism at the atomic level. Structural studies of modulated phases, the anomalous behavior of the thermal vibrations, chemical bonding in crystal and second-order phase transitions are being pursued. Recent results include:



1. Studies of T1 and Y-high-temperature superconductors below and above the superconducting phase transition.

2. Investigations of Na⁺ and Li⁺ solid electrolytes in their superionic phase transition.

3. Studies of non-linear optical materials of the KTiOPO₄ family and modification of their superionic, and ferroelectric properties.

4. Studies of (M²⁺_{1-x}R³⁺_x)F_{2+x} solid solutions and the structural basis for their high ionic F1- conductivity.

5. Studies of crystals possessing special physical properties – including La₃Ga₃SiO₁₄, (Ba,Sr)Nb₂O₇, LiNbO₃, and K(H,D)PO₄.

Three Doctors of Sciences, seven Candidates of Sciences, a staff of skilled engineers-designers work in the laboratory, which has four 4-circle single crystal diffractometers.

V.I. Simonov, Head of X-Ray Laboratory, simonov@rsa.crystal.msk.su

Switzerland

The Swiss Society of Crystallography (<http://www-sphys.unil.ch/sgk/index.html>) has issued an illustrated brochure presenting a complete description of crystallographic activities in Switzerland. The aim of the brochure is to show the importance, relevance and diversity of the field of crystallography for the scientific community and to attract undergraduate or graduate students to the field.

The 10 chapters of the brochure cover:

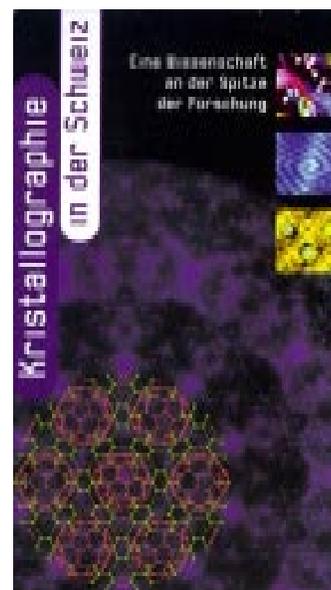
- Structures of macromolecules in the pharmaceutical industries and universities;
- Aperiodic crystalline structures – Quasicrystals, incommensurate and composite materials and their properties;
- Zeolites, semiconductors or metal hydrides of practical industrial importance;
- Services for structural analysis - Recent developments in area detector technology and powerful new sources of radiation have created new horizons for crystallography;
- Dynamical properties of structures;
- Neutron and synchrotron sources;
- Crystal synthesis – Designing new materials with specific properties;
- Crystallography in earth sciences - the formation of the earth and the study of minerals;
- Crystal physics – Relations between structures and physical properties and the development of new technologies.

Each topic includes a list of Swiss groups working in the field including their web site addresses. For the moment, only a German version of this brochure is available. A French version is currently planned.

(Editor's Note: It is a beautifully illustrated brochure that could be a model for other countries and crystallographic societies)

To request a copy, contact: Prof. Volker Gramlich, Lab. of Crystallography, ETH Zentrum, 8092 Zurich, Switzerland;

Fax: 41 1 632 1133, e-mail: v.gramlich@kristall.erdw.ethz.ch



Crystallography and Proteomics

The sequencing of the genomes of over two dozen species including the human has opened up research opportunities on a grander scale than has ever been possible before. It is clear that we know very little about the functions of more than 50% of the gene products whose existence is predicted by the sequences being determined with mind numbing rapidity. Many proposals have been made concerning the best way to codify, analyze and use this information. There is general agreement that it is worthwhile to determine what all of the gene products do, how they do it and how we can control these processes. Potential economic and health benefits arising from this new knowledge have generated heated debate and high anxiety over many aspects of the process including the possibility that by patenting genes, the medical industrial complex could hold the world hostage. The exorbitant investment required to determine what all of these gene products do has led to an equally divisive debate about which techniques (x-ray crystallography, NMR spectroscopy, mass spectroscopy, computer modeling, and computational methods) will be most effective, economical and efficient in providing the answers.

It has been proposed that sequence analysis software will make it possible to catalog all protein structures into a finite number of families that have a common fold, that structure prediction programs can be used to predict the three dimensional shapes of the various folds, and that predicted shapes will permit accurate prediction of function. There is ample evidence to suggest that this scenario, while appealing, is greatly over simplified. We know that large families of proteins can have equivalent folds without so much as one fully conserved amino acid, that proteins having the same fold can have entirely different functions, and that many proteins have a number of significantly different forms that may be functionally important.

X-ray crystallographers have participated in the development of schemes for rapid throughput determination of a core of structures expected to map out the full range of folds. Ironically the macromolecules about which the least is currently known, integral membrane proteins, are being excluded from most proposals for high throughput structure determination because they present challenges that are incompatible with current technology and its facile automation.

Ironically, X-ray structures that provide

atomic level resolution seem to be considered *passé*. If a crystal diffracts to better the 3Å resolution, the structure of the molecule crystallized appears to be ineligible for publication in *Science*, *Nature* or other journals that define what is currently fashionable in science.

The following are some quotations from recent articles addressing the topic of structural proteomics and beyond that capture some of the range and flavor of this important debate.

The speed of acquiring data is now exceeding our ability to comprehend it and put it into the proper biological context. T. Hesman, *Science News*, 157, April 29, 2000

The fact gathering tendency is apparent not just in structural genomics, but also in functional genomics (to identify the role of each gene in the genome) and proteomics (with similar aim for each protein in the cell or organism). Evidently, there are enough facts to keep biologists busy gathering them for decades. **So when will they have time to think?** *Nature* 403, Jan. 27, 2000

The US National Inst of General Medical Sciences (NIGMS) will launch a structural genomics initiative. After an initial five-year pilot stage, the NIGMS programme aims to generate 10,000 structures from as many protein families as possible. Some groups intend to characterize every protein structure within small organisms such as the bacterium *Mycoplasma genitalium*, while others may try to obtain as many structures as possible involved in a single cellular process, such as cell division. Paul Smaglik, *Nature* 403, Feb 17, 2000

So far, 4,473 species of bacteria in 905 genera have been validly described, of these, just 29 species in 21 genera have been fully sequenced. The assumption that we now have an essentially complete knowledge of microbial metabolism, and need only skim new genomes to compare to existing ones, risks missing the novelty that has been, and will continue to be, present in each new microbial genome. Julian Parkhill, *Nature Biotechnol.* 18, May 18, 2000

Only 265-350 of the 480 protein-coding genes of *M. genitalium* (which has the smallest known genome of self-replicating organisms) including 100 genes of unknown function, are essential for growth under laboratory conditions. *Nature Biotechnol.* 17, 207, 1999

Combinatorial chemistry has caused a great cultural change- the redefining of the scientific method itself. For hundreds, if not thousands, of years, scientists have been taught to execute experiments one at a time with very careful control of parameters. Combinatorial chemistry and high throughput methods in general suggest that this fundamental concept can be successfully challenged and expanded. Peter E. Cohen, *C&EN*, May 15, 2000 *Who needs careful control when there is money to be made?*

Molecular analysis is clearly required to understand higher levels of biological organization, but the converse is also true: the biology of the molecules of life can only be understood in the context of functioning cells and organisms. F.C. Kafatos, *Science* 287, Feb 25, 2000

Pharmacogenomics requires an understanding of the apparent genetic 'disorder' in any organisms genome, of genotype-phenotype mapping, of gene-gene interactions, of intraspecific genetic variability, and of self-organizational processes, rather than endless lists of DNA bases. Sol Hadden, *Nature* 404, April 6, 2000

Features of the very same system depend on the scale of observation. This precludes the extrapolation of knowledge at one level to higher levels where the "complexity" increases. Understanding why this is so, and determining how to formalize the problem of emergent features and multiscale description is one of the goals of the science of complex systems. Sui Huang, *Nature Biotechnol.*, 18, May 18, 2000

Cambridge Healthtech Institutes Beyond Genome 2000 Conference, June 19-23, 2000 covers Bioinformatics and Genome Research, focusing on the computational advances necessary to comprehend the vast amount of information gathered through the Human Genome Project, Silico Biology that explores tools being developed to translate raw data into workable models that will provide guidance for target selection, and Proteomics, which will provide in depth coverage of recent developments in the field of high throughput protein expression analysis and its impact on diagnostic and therapeutic product development (from a meeting announcement). *And all in five days!*

Seeing and Knowing in Structural Biology



Carolyn Cohen, Prof. of Biology at Brandeis U., gave a talk with the title "Seeing and Knowing in Structural Biology" at the 2000 Biophysical Society meeting in New Orleans. Her thesis in this paper was that "seeing an image... often poses an enigma, and the solution of that enigma allows seeing to become knowing." Dr. Cohen cited a number of examples from her own work and that of others, especially in the field of motility. One problem in this area is the ambiguity involved in assigning biochemical states in the contractile cycle for the three conformations of the myosin molecule which have been determined crystallographically. We quote here the coda of the talk, since we believe it expresses well one point of view toward current approaches to Structure/Function studies.

"...In my final remarks, I want to emphasize how we are, in fact, only at the threshold of knowing how the motor machine splits ATP to produce contraction. Of course, in order to explore what I shall call "conformational space" for myosins, we need a thorough crystallographic study of a wide variety of isoforms to visualize the possible structural steps in the contractile cycle. Lee Sweeney's recent imaginative prediction about the polarity of myosin VI ... is a beautiful example of a new structure that will test and clarify our current thinking about the working of the myosin machine.¹ ...[And] Yanagida's recent single molecule experiments. ... point to the need for a coordination of all of our current techniques in molecular biology, biophysics, and biochemistry to test and interpret functional models. Without a broad scientific culture, it seems unlikely that we can interpret an image correctly - or test our interpretations.

All of the work I've described today has followed the traditional path of "determining the structures of proteins known to be biologically important."² And to someone like myself, the rate at which such structures are being generated seems very great. But, as many of you know, there are also plans to create so-called "fast throughput" centers for protein crystallography to speed up this process, "as in an assembly line." And to generate, as well, a more comprehensive family of protein folds deduced by computer modeling from the great number of sequences now becoming available. There is the notion here that, with or without the aid of supercomputers like the IBM Blue Gene, these computational efforts will yield useful global structures for these proteins. On this logic, the next step - the one I've spoken of this morning - seems to some not to be a great hurdle:

that is to proceed from either a detailed (or real) protein structure or from a global (or virtual) structure to an understanding of both its function and how it accomplishes this function. Some aspects of these enterprises may well turn out to be stimulating and useful - and some may be entertaining, as well. Certainly, the new conceptual and computational approaches, such as the use of phylogenetic profiles by Eisenberg and colleagues³ which discover functional links between different proteins, will be immensely revealing.

But I maintain my conviction that an understanding of functions will come - as it always has - from the creative insight of a few individuals. And that their understanding will be both inspired and constrained by the evidence for this solution. It is also plain that in many cases a detailed solution for one structure will disclose the ways in which other - more or less closely related structures - operate. I think that this route for discovery in science - this passage from seeing to knowing - has a great tradition whose lessons we should remember...or learn again."

References:

- [1] Wells, A.L., Lin, A.W., Chen, L., Safer, D., Cain, S.M., Hasson, T., Carragher, B.O., Milligan, R.A., Sweeney, H.L. Myosin VI is an actin-based motor that moves backward. *Nature* **401**, 505-8 (Sept. 30, 1999).
- [2] Thomas Steitz, cited in Wadman, M. U.S. plans giant effort on protein structure, *Nature* **400**, 494 (Aug. 15, 1999).
- [3] Eisenberg, D., et al. A combined algorithm for genome-wide prediction of protein function. *Nature* **402**, 83-86 (Nov. 4, 1999).

Structural Genomics



Crystallography is poised to play a critical role in research to determine the biochemical functions of proteins encoded by human, animal, insect, and bacterial genes. Since the function of a gene product is tightly coupled to its three-dimensional structure, determining the structure, or its folding pattern can provide insight into its biochemical function. The human genome alone is estimated to have >80,000 genes. The current estimate of genes that encode products with 'known' biochemical and biological functions varies from approximately 30-60% depending on the organism. An examination of the Brookhaven Protein Data Bank reveals a smaller number of new folds are discovered each year. Many proteins are composed of two or more folding domains. Some folds are found among proteins from all three kingdoms: bacteria, archaea and eukarya. It is postulated that there are a finite number of folds making up a 'fold basis set'. Several studies revealed that only about 20-35% of open reading frames of known genomic sequences are represented in the current protein structure base. Gene products of

unknown function having no sequence similarity with protein of known function and membrane-bound proteins constitute a major portion of the unknown folds. Assuming that the PDB collection presently represents about one third of all protein folds, 700-10,000 new folds need to be experimentally discovered. The structure determination of gene products by crystallographic and NMR methods will need to be coordinated internationally. Development, optimization and automation are needed for large scale cloning and expression of chosen genes, and high throughput purification of the genes products. Also needed are high throughput crystallization screening method and automation of X-ray diffraction data acquisition. Synchrotron radiation is essential not only for the highest quality data acquisition and throughput of data but also for working with microcrystals and for structure determination using the multiple wavelength anomalous diffraction (MAD). There is a clear and compelling role for crystallography in providing a foundation for functional genomics, which is the ultimate objective of sequencing the entire genome of an organism.

Soug-Hou Kim, condensed from *Nature Structural Biology*, Aug 1998

More Proteomics...omics...omics...omics...omics

In one of the first examples of the role of crystallography in the new age of proteomics, Sung-Hou Kim and company, [*Nature Structural Biology* 6, 691-696 (1999)], determined the three dimensional structure of the protein of unknown function from a gene in the sequence of the genome for *Methanococcus jannaschii*. Half of the predicted gene products of *M. jannaschii* are unknown. Kim's determination of the structure has a new fold, part of which is homologous to a nuclear binding protein. The structure suggested biochemical analysis that indicated Mj0226 is a novel nucleotide triphosphatase that hydrolyzes non-standard nucleotides but not standard nucleotides in the presence of Mg²⁺ or Mn²⁺ ions. The gene products has sequence homology with predicted gene products in six other species including man, fungus, bacteria and worms. (*Welcome to the brave new world.* - ed.)

Genome Scoreboard. Genomes OnLine Database tracks the status of over 250 genomes – from Salmonella bacteria to the just-completed human chromosome 21. The links-packed site, which also includes viruses, phages, and organelles, recently found a new home with a company, but will remain free. (igweb.integratedgenomics.com/GOLD)
Science, Vol. 288, June 9, 2000

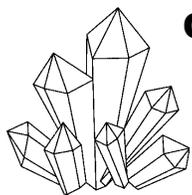
Proteins: Structure, Function and Genetics has inaugurated a new short format of Structure Notes designed to provide brief accounts of X-ray crystal structures that contain “too little new information to be worthy of publication as a full-length article”. (*What do you expect from robots?* ed.)

Show Me the Money. Structural GenomiX, a San Diego company that specializes in high throughput x-ray crystallography, completed a second round venture financing that netted \$32 million. The company will use the money to continue building a database for analyzing protein structures in drug and compound discovery. The 3-D protein structures the company generates are useful in target validation, rational drug design, pesticide discovery, and industrial catalysis.

Drug Design and Development, May 2000

So Simple, A Child Can Do It! “The crystallography laboratory that you collaborate with produced crystals of your protein weeks ago. They collected X-ray diffraction data and plugged it into their workstation-based molecular-modeling system, coming up with a three-dimensional structure of your protein showing where the component amino acids were located and how they associated with a metallic cofactor at the proteins center.” Holly Ahern, *The Scientist Newspaper* (*Batteries not included*, ed.)

Reality Check? In an article entitled “Protein Crystallography Pinpoints Drug Candidates” (*Drug Discovery and Development*, April 2000, p26, www.dddmag.com) it's encouraging to read that “there is nothing simple or straightforward about macromolecular crystallography”. J. Becker, of Merck, and a member of the Industrial Macromolecular Crystallography Assn Collaborative Access Team (twelve pharmaceutical and chemical companies) claims that diffraction analysis lets you see how drugs actually interact with targets. The article summarizes the various steps in macromolecular crystallography and is illustrated with pictures of instruments, molecules and Andy Howard (wearing a smile that could sell used cars).



Crystal XXI

A student's view from Australia

I particularly liked the fact that there were no simultaneous sessions at the Crystal XXI, the 1999 annual meeting of the Society of Crystallographers in Australia (SCA). There was never a dilemma concerning which talk to go to at the expense of missing something else just as interesting. The unofficial name "The Bush Crystallographers" evokes all of the feelings I experienced from meeting this closely knit group of Australian and New Zealand crystallographers.

It is hard to say which presentations stood out as being the most interesting. I was fascinated by Cameron Kepert's talk on *Desorption in Microporous Molecular Framework Materials* for the crystal structure content, elucidation of physical properties from experiment and the beautiful models used to represent these structures. It was spellbinding to watch Mark Spackman's *Pictorial Representation of Intermolecular Interactions in Crystals*. Visual representations are powerful tools in understanding and interpreting interactions as well as communicating them in a most attractive form.

The combination of techniques described in some of the talks, was of particular interest. Ian Grey's presentation on *Combining Electron Microscopy with Powder X-ray and Neutron Diffraction to Solve and Refine Complex Oxide Structures* was very emphatic on this point. Fascinating too was Steve Wilkins' presentation on *Quan-*

titative Phase Contrast Imaging using both Laboratory and Synchrotron Sources of X-rays because it exposed techniques in X-ray imaging that yield an enormous amount of information lost in conventional methods. I enjoyed the 1987 Lecture, *Crystallography with Electrons - From the House of the Dead* by Douglas Dorset and Peter Colman's *From Crystallography to Collins Street*, striking titles for two very different, very absorbing lectures.

Discussions with delegates concerning my work helped me see it in a broader context and clarify and define areas of future work. Such an intense pooling of ideas at conferences like this, is a tremendous eye-opener, especially in the awareness of complementary techniques. The environment at this conference could not have been more conducive to leisurely discussions and the generation, exchange and absorption of ideas. I would like to thank Philips Analytical for providing a student prize and all the sponsors for supporting this wonderful meeting.

Philip Nakashima, U. of Western Australia, from the *SCA Newsletter*

First Belgian Crystallography Symposium

More than 140 scientists took part in the First Belgian Crystallography Symposium (BCS-1), Oct. 28, 1999 in Brussels to promote interdisciplinary contacts between Belgian scientists who use diffraction and microscopy techniques in condensed matter chemistry and physics, material sciences, earth sciences and life sciences. Plenary lectures included *From small to large in crystallography* (J. Kroon, Utrecht), *Modern aspects of powder crystallography* (D. Louër, Rennes) and *Electron microscopy techniques for structure analysis* (D. Schryvers, Antwerp). There were 54 posters grouped in five sections, Techniques and Methods, Physical Crystallography and interfaces in, and organic - small organic molecule, and macromolecular Chemical Crystallography.

The Belgian National Committee for Crystallography plans a symposium at biennial intervals. The meeting was sponsored by both Royal Academies of Belgium for Science and the Arts, and the firms Bruker, EFG, MarResearch, Nonius, and Philips.

Luc Van Meervelt



Organizers and speakers at the First Belgian Crystallography Symposium BCS-1 (left to right) Luc Van Meervelt, Jean-Paul Declercq, Harry Reynaers, Geoffrey King, Jan Kroon, Dominique Schryvers, Daniel Louer.

Leadbetter Retires

Alan Leadbetter, Professor of Physical Chemistry, U. of Exeter, earned international reputation for his research in the thermodynamic properties of solids, the structures and dynamics of glasses, order disorder transitions and molecular rotations in crystals, and the structures and molecular dynamics of liquid crystals. As Associate Director, Head of Science Dept. and Head of Neutron Div. at the Rutherford Lab he oversaw the completion, commissioning and internationalization of the world's most powerful pulsed neutron source, ISIS. As Director of Daresbury Lab he helped to establish SRS as a leading X-ray synchrotron research facility. He retired from his position as British Director-Adjoint and Director of Science at the Inst. Laue Langevin in Grenoble in August, 1999. Over sixty colleagues gathered to honor him in October at a meeting organized by the Neutron Scattering Group of the Inst. of Physics and the Faraday Div. of the Royal Society of Chemistry, entitled *Science, Facilities and Facilitating Science*, that provided an overview of the current international status of research fields as diverse as physical chemistry, neutron scattering, synchrotron studies, and nuclear and particle physics.

Alan Leadbetter with Colin Carlile.

Bob Cywinski, (from *BCA Crystallography News*, Dec. 1999)



The Hungarian Chemical Society

Alajos Kálmán, who was a member of the Executive Committee of the IUCr from 1984-1990 and served as its Vice-President 1990-1993, was elected President of the Hungarian Chemical Society (MKE).

The Hungarian Chemical Society (MKE) was founded by 50 chemists in 1907 to serve the interests of Hungarian chemists. Their program was centered on promoting the development of chemical science and chemical industry.

The objective of MKE is to raise the professional level of its members, promote their public activity, recognize their work, and promote technical, economic and social development in Hungary.

The Society organizes scientific, technical and economic lectures, meetings, and exhibitions, organizes radio and TV programs in subjects related to the chemical industry, and publishes *The Hungarian Journal of Chemistry*, *Hungarian Chemical Journal* and *Chemical Papers for Secondary School*. MKE has created four annual awards.

Alajos Kalman

Congratulations to...

American Assn for the Advancement of Science Fellows:

Joel Bernstein (Ben-Gurion U., Beer-Sheva, Isreal), Michael G. Rossmann (Purdue U., Purdue, IN, USA), and Jenny P. Glusker (Fox Chase Cancer Center, Philadelphia, PA, USA).



Robin D. Rogers (U. of Alabama, Tuscaloosa) has been appointed editor of the American Chemical Society's new Journal *Crystal Growth & Design*. Primary topics will include crystal growth of inorganic, organic, and biological substances; prediction and control of crystal structure; crystal engineering; and industrial applications.

Protein Society Awards 2000:

Brian Matthews (U. of Oregon) received the Moore and Stein Award; Stephen Benkovic (Pennsylvania State U.) received the Christian Anfinsen Award; David Eisenberg (U. of California, Los Angeles) received the Amgen Lecture Award.

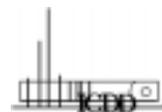
First European Crystallography Prize

The European Crystallographic Assn will award the first European Crystallography Prize to Ada Yonath of the Weizmann Inst. of Science Rehovoth, Israel and the Max-Planck Research Unit for Ribosomal Research, DESY, Hamburg, Germany. Yonath is being recognized for her pioneering achievements in structural studies on the ribosome, the universal cellular organelle on which protein biosynthesis takes place.

The European Crystallography Prize, which includes a monetary award as well as a certificate of recognition, will be presented at the upcoming 19th European Crystallography Meeting to be held in Nancy, France, August 25-31.

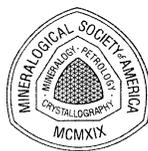
Professor Yonath was born in Jerusalem and received her Ph.D. under the direction of Prof. Wolfie Traub at the Weizmann Institute, where she is the incumbent of the Martin A. Kimmel Chair in Structural Biology and Head of the Kimmelman Center for Biomolecular Assemblies. Her pioneering work over many years in pursuit of the ribosome structure which she has orchestrated on an international scale, has been concentrated in Europe, with a significant portion of her activity centered at the Max-Planck Research Unit in Hamburg, which she also heads.

Members of the European Crystallography Prize Committee, appointed by the Executive Committee of the European Crystallographic Assn, are M. Hursthouse (UK), N. Isaacs (UK), J. Kroon (The Netherlands), C. Mealli (Italy), and E. Mittermeijer (Germany). The Committee was chaired by J. Bernstein (Israel). The Prize is sponsored by Bruker Analytical X-ray, STOE & CIE GmbH, and Philips Analytical B.V.



ICDD 2000 Officers and Directors

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Structural Mineralogy

The Mineralogical Society of America (MSA) has 1938 members of whom 488 express interest in crystallography/crystal chemistry. The MSA publishes a newsletter (*The Lattice*), and a new electronic journal - Geological Materials Research online at <http://gmr.minsocam.org/>, and a popular review series, *Reviews in Mineralogy* (R.M). A recent volume on the series *Ultrahigh-Pressure Mineralogy* was edited by Russell Hemley and David Mao. In collaboration with the Geochemical Society, the R.M. has become RMG (Reviews of Mineralogy and Geochemistry). New publications in the MSA Monograph series include *N.L. Bowen and Crystallization Differentiation* by Davis Young, *Methods of Optical Crystallography* by D. Bloss a special issue of the MSA journal (American Mineralogists on mineral physics will honor Charles Prewitt). <http://www.minsocam.org/>

Why Publish in *Acta Cryst*?

ISSN 0021-8897 Volume 56 Part 1 January 2000	Acta Crystallographica Section A Foundations of Crystallography Editor: André Authier
ISSN 0021-8897 Volume 56 Part 1 February 2000	Acta Crystallographica Section B Structural Science Editor: Frank Allen
ISSN 0021-8897 Volume 56 Part 1 January 2000	Acta Crystallographica Section C Crystal Structure Communications Editor: George Ferguson
ISSN 0021-8897 Volume 56 Part 2 February 2000	Acta Crystallographica Section D Biological Crystallography Editor: Jenny P. Glusker

The journals of the IUCr are under active scrutiny all the time to improve such things as publication times, standards, quality and saleability. The latter is particularly important because 70% of the International Union's income is derived from the sale of the journals. If the journals do not produce the goods the Union will fail.

To keep subscription numbers up, the journals need more and high quality manuscripts. I encourage SCA members to consider publishing more of their research in these foremost international journals. There are six journals to choose from, the four *Acta Crystallographica* sections plus the *Journal of Applied Crystallography* and the *Journal of Synchrotron Radiation*. In my view, it is usually best if small molecule structures are published along with the chemistry to which they are related in a chemistry journal, but if that

is not possible, then *Acta Crystallographica C* is an excellent vehicle. *Acta Crystallographica B* (Structural Science) is a premier journal for publishing structural chemistry across the whole range, and considering the strength of structural science and materials science in Australia and New Zealand, the number of papers from this region seems too low.

Acta Cryst. D (Biological Crystallography) is the top rated crystallographic journal for citations in macromolecular crystallography. There is currently a move to produce a purely electronic, cif-based, journal for rapid publication of small molecule structures.

Max Taylor, Past President of the Soc. of Crystallographers in Australia *SCA Newsletter*, Nov. 1999

Sustainable Sciences Institute

Sustainable Science Inst. is a non-profit organization that develops scientific capacity to address public health needs worldwide.

With the help of interested colleagues at the U. of California, Berkeley, the President of the Board of SSI, Eva Harris, began organizing a series of in-country workshops to teach scientists in developing countries the theory and practice of molecular biology techniques - such as the polymerase chain reaction (PCR) - that could be appropriately applied to local infectious disease problems. These efforts evolved into the Applied Molecular Biology/ Appropriate Technology Transfer (AMB/ATT) Program, and eventually, the SSI.

In 1999 the SSI was founded, initiated a Small Grants Program, co-sponsored a technology transfer workshop in Guatemala, and established a volunteer network. Year 2000 goals include: a hepatitis C conference in Egypt, the launch of online interactive material aid and consultant databases, and funding 10 infectious disease research projects initiated by investigators in developing countries.

The website (www.ssilink.org) contains information about SSI's history, ethical principles, programs, collaborators, and a comprehensive list of online scientific resources.

From the SSI Newsletter

Y3K bug

Virtual-reality innovator Jaron Lanier, Columbia U. Prof. David Sulzer, and conceptual illustrator Lisa Haney submitted an entry to a New York Times Magazine contest for designing a time capsule to reach earth's inhabitants in the year 3000. Their entry was to have notes, the contents of every 1999 issue of The New York Times Magazine converted from the two digit binary to the four-character genetic code, and spliced into the introns of cockroaches. Then, through a rigorous breeding program, the cockroaches of New York City would be transformed into scurrying little time capsules, copulating madly, and certainly giving earth's inhabitants of the future at least one product of biotechnology that is guaranteed to survive. *Nature Biotechnology Vol 18, Jan. 2000*

AACG and Space Flight

The American Assn for Crystal Growth (AACG) has had two members in space, NASA scientist Roger Crouch in July 1997 (Roger brought the AACG banner and a packet of membership cards on the journey) and Lodewijk van den Berg in April 1985 (the membership card for 1999 with the NASA space shuttle logo).

T. Gentile

Rigaku Acquires Osmic

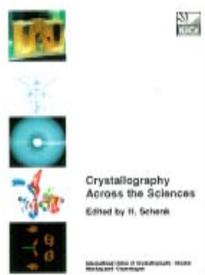
Rigaku/USA, Inc. Danvers, Massachusetts announced that they have completed the acquisition of Osmic, Inc., a leading producer of x-ray optics. Osmic has long been a critical supplier of X-ray optics to Rigaku and other X-ray instrument manufacturing companies.

Largest Crystal?

The world's largest fast-growth crystal, weighing in at 701 pounds, has been grown by researchers at the US Dept of Energy's Lawrence Livermore National Laboratory.

The pyramid-shaped KDP (potassium dihydrogen phosphate) crystal measures approximately 26 inches by 21 inches by 23 inches high. It was grown in a record 52 days using a special rapid-growth technique developed in Russia and advanced at Lawrence Livermore by Nataalia Zaitseva and Ruth Hawley-Fedder.

Crystallography Across the Sciences, A Teaching Tool?



The primary role of a teacher is to provide the student with the knowledge base upon which to develop his or her own initiatives. Students taking basic crystallography may have very different backgrounds and interests; solid state physics, material science, crystal chemistry, biochemistry, biology, etc. It is often difficult for these students to find adequate introductory literature to supplement a general course in crystallography. **Crystallography Across the Sciences** (IUCr-Chester, Munksgaard-Copenhagen, 1998) is very useful in this respect. The book form of a Special Issue in *Acta Crystallographica* (Vol A54 (1998), 687-955) with H. Schenk as Guest Editor contains 26 articles with a total of 51 authors. The book covers a broad range from fundamental diffraction physics to applications in biology, chemistry, physics and material science.

Six papers cover material of general interest to the crystallographic community while the remaining 20 review the state-of-the art in specific areas. Students in crystallography courses from the undergraduate to Ph.D.-level will find useful material in this book.

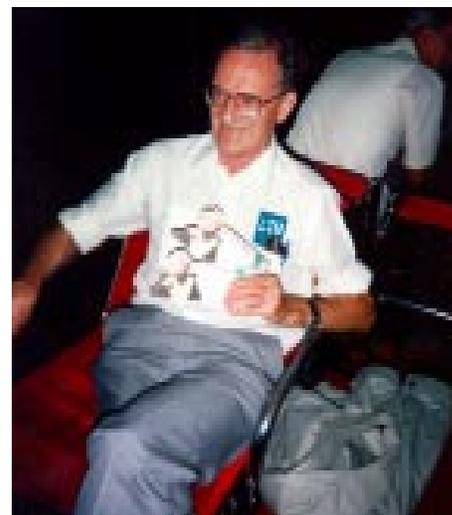
Two articles, "Aspects of the of the History of the International Union of Crystallography" and "The Teaching of Crystallography: a Historical Survey" includes material useful for any teacher who wants to give some perspectives on a crystallography course. Chapters entitled "The Development, Status and Scientific Impact of Crystallographic Databases"; "Data Languages and Dictionaries for Crystallography"; and "Symmetry in Crystallography" can be directly used as course material once the student has had some experience of symmetry; the chapter on "Diffraction Physics" is probably most useful in advanced courses.

The five chapters in the biology-biochemistry field cover structures ranging from simple salts to viruses, proteins involved in muscle contraction, time-resolved crystallography, membrane protein, and the ribosome. The six chapters concerning frontiers in the chemistry-materials science field cover phase transformations in smart materials, inclusion complexes, host-guest interactions, hydrogen bonding networks, real-time *in situ* chemical reactions, structure correlation, superconducting materials, and supramolecular structures.

Nine articles concerned with methods development are crystal growth, charge-density analysis, synchrotron, electron, and neutron crystallography, X-ray crystallography of surfaces and interfaces, X-ray optics, N-beam diffraction, and advances in powder diffraction analysis.

Crystallography Across the Sciences has been used as a teaching tool at the undergraduate and graduate level. In one course, each student selected an article for thorough study and presentation to their fellow students. This has proven to be a very rewarding and successful approach. I recommend the book as a teaching tool with a reasonable price.

Ake Oskarsson, Lund U., Sweden



Geoffrey King scalping Madonna tickets in the Singapore Airport on the way to the IUCr meeting in Australia, 1987.

Over a Century and a Half of Science Classics from Ox Bow Press (oxbow@gte.net):

The Optical Principles of the Diffraction of X-rays, R.W. James, 1948.

Collected Papers, Peter J. Debye, 1954.

Hampton

Abraham Clearfield: A Biography. The first issue of the Journal of Molecular Structure for 1998 was dedicated to Abraham Clearfield on the occasion of his 70th birthday, in recognition of his scientific contributions and his dedication to the welfare and training of a wide spectrum of students.



The volume contains an impressive collection of papers by his former Masters and Ph.D. students and post docs.

George Jeffrey (1915-2000)

George Alan Jeffrey was born in Cardiff in 1915 and received a B.S.C. in 1936, a Ph.D. in 1939 and a D.Sc. in 1953 at the University of Birmingham. He then moved to the University of Pittsburgh to teach Physical Chemistry. There, George Jeffrey created the Crystallography Laboratory, which in 1969 became the first Department of Crystallography in the USA. He was its Chairman until 1985 and Professor Emeritus until his death on February 13th.

At the beginning of his long research career in Pittsburgh, Jeffrey studied the structures of clathrates, discovering a surprising variety of different forms derived from the dodecahedron; later, he began a systematic structural study of carbohydrates, first by X-ray diffraction and later also by neutron diffraction. In both areas he became one of the world's leading authorities on the subject. These studies led him to question the classical formulation of hydrogen bonding and to spend many years reviewing and organizing all the data and knowledge concerning this type of chemical interaction in a great variety of compounds, from aminoacids to nucleotides, barbiturates, from purines and pyrimidines to carbohydrates and, more recently, in proteins. In his many lectures and papers on this subject he contributed significantly to the advancement of Science, implementing new concepts and definitions, which he summed up in the book he wrote with Wolfram Sanger on "Hydrogen Bonding in Biological Structures", published by Springer-Verlag in 1991.

Over the last years of his career, Jeff became increasingly interested in structural studies of very high precision, correlating low temperature neutron diffraction studies with *ab initio* calculations and electron density studies, and the study of liquid crystals and inclusion compounds. His scientific career is well documented in more than 300 papers, reviews and books.

The enormous creativity, energy and enthusiasm of George Jeffrey was also devoted to the benefit of the scientific community. Jeff contributed to the establishment of the American Crystallographic Association, of which he was President in 1963, the Program Chairman for the Eighth General Assembly and Congress of the International Union of Crystallography in 1969. He was also Co-Editor of *Acta Crystallographica* between 1973-1984. His many awards included the Pittsburgh award (1978), the Claude S. Hudson award (1980), the Alexander von Humboldt Senior U.S. Scientist Award (1983-84), the ACA Buerger award (1988) and the David Harker Award at the Annual Meeting of the American Crystallographic Association in Buffalo, NY, in recognition of his pioneering work in the field of crystallography, his landmark studies of sugar structures by X-ray and neutron diffraction, his studies of the properties of the hydrogen bond, and his founding of the only university crystallographic department in the U.S.

Jeff was an enthusiast, always full of life and a great supporter and advisor for many of us in the generation that followed his pioneering actions. "His" Crystallography Department in Pittsburgh was known and visited by many colleagues, post-docs and students to whom he always offered advice with his strong teaching and friendship. Many of us learned from him the basic principles of Crystallography, how to write a winning grant proposal or even how to organize a conference or a course. He was very proud of the Department's list of visiting scientists and students, with more than 200 names, some more than once, for whom he always had an open door, a word of encouragement and good moments of relaxed, well humored and friendly atmosphere!

I shall never forget the way I first met him as a crystallographer. Back from my Ph.D. in London I was in Portugal, with nothing more than an old Weissenberg camera, trying to start research work at my University. I met Jeff and Maureen in 1980 at the European Crystallographic Meeting in Barcelona and after five minutes of conversation he offered me the possibility of going to Pittsburgh for the period that my teaching duties would allow, to do my own research work, using all the facilities available in his Department, including a salary as Visiting Professor. Since then, a great friendship started that, with time, was extended to many other Portuguese Crystallographers. We were all very happy and proud, later on, to see Jeff receive in 1991 a "Honoris causa" Doctorate from the Technical University of Lisbon. In his fluent, direct and humorous style, he then made a speech, zooming from science to human behaviour, that immediately conquered the Portuguese academics, even those who did not have the privilege of knowing him before.

I am sure that, like myself, many other crystallographers around the world, will remember Jeff as a great scientist, a man of vision and wisdom, a charming, deep human being and a precious friend. Maureen, a perfect and gentle partner, further reinforced his qualities during their long marriage and companionship.

Beyond the frontiers of life, Jeff is surely now part of another world of Peace and Love, a state to which he much contributed during his earthly existence.

Maria Arménia Carrondo

To honor Jeffrey, a fund to support graduate student attendance at IUCr Congresses is being established by the Pittsburgh Diffraction Society. The Jeffrey Awards will be open to students of crystallography throughout the world. Please send donations in US currency to Dr. Bryan Craven, Chemistry Dept, Indiana U. of Pennsylvania, Indiana, PA 15705. Checks should be made out to "The Jeffrey Fund/Pittsburgh Diffraction Society". Donations are tax-deductible in the USA.

Paul B. Sigler (1934-2000)

Paul Sigler suffered a sudden and fatal heart attack on January 11th while walking from his home in New Haven to his laboratory at Yale University. His unexpected death came as a shock to all who knew him, and is particularly distressing to those of us who were privileged to call him student, mentor or colleague. Paul's engaging personality, his intense enthusiasm and his passion for science will be missed by many.

Paul's remarkable scientific versatility as chemist, structural biologist and crystallographer stems from his early training. He graduated *summa cum laude* in chemistry from Princeton University, and then trained in medicine at Columbia University. After completing both internship and residency at Columbia-Presbyterian Medical Center, he switched careers to pursue basic research. Paul was introduced to crystallography in David Davies' laboratory at the NIH, and he received his Ph.D. from the University of Cambridge in 1967 for his role in the structure determination of γ -chymotrypsin in collaboration with David Blow, Richard Henderson and Brian Matthews. As a faculty member of the University of Chicago, Paul conducted pioneering structural investigations of initiator tRNA^{met}, phospholipase A₂, and *trp* repressor. His career reached new heights of excellence after his move to Yale University in 1989 to become an HHMI investigator and Henry Ford II Professor of Molecular Biophysics and Biochemistry. In his last and most productive decade, Paul led a large and extremely capable group of young scientists in groundbreaking investigations of eukaryotic transcriptional control, transmembrane signaling, and protein folding.

Paul's ambition to understand biological phenomena in structural terms often challenged the limits of the crystallographic method, and was a driving force for many significant advances. His highly inventive mind and keen ability to motivate others created a fertile environment for scientific exploration. Paul liked to compare protein crystallography to a decathlon, where the competitor may excel in certain events, but must be proficient in each one. Paul was more often coach than competitor, but he had a deep understanding of the game, and an instinct for bringing out the best in his people. Among his many contributions are innovations in crystallization, preparation and analysis of heavy atom derivatives, cryogenic techniques, optics, data process-



Photo courtesy of Yale U., Office of Public Affairs

ing and density modification. In many ways Paul's laboratory defined the cutting edge of modern protein crystallography.

My first interactions with Paul were in the graduate course he taught at the University of Chicago in the spring of 1983. An enduring memory is the huge beaker of chalk he brought up to the classroom, with which he would illustrate every concept with incredible clarity and detail. Despite temperamental comments when the chalk would slip away from him, his love of the crystallographic method and his enthusiasm for its use shone through loud and clear. When I subsequently joined Paul's laboratory I discovered that the effort he took in the classroom was redoubled in the supervision of his graduate students and postdoctoral fellows. He would frequently leave handwritten notes, sometimes several pages long, with suggestions of how to get the experiment of the day to work. But he also insisted that we think for ourselves, rather than operate as "trained baboons." The message was often passionately delivered, and we all listened and matured as scientists. Beyond the experiment, Paul was a great conversationalist, a terrific party host, and a good friend.

Paul trained and nurtured over seventy students and postdocs, many of whom have gone on to independent scientific careers. He also had many warm and lasting relationships with scientists from around the globe. I am grateful to colleagues who have generously shared their memories of Paul to aid the writing of this tribute, which has been a labor of love. Paul's love for his family was obvious to us all, and we extend our deepest sympathies to his wife Jo, their five children and eight grandchildren.

Cathy Lawson

Yale U. will honor Paul's memory by creating a permanently endowed lectureship in structural biology at Yale, which will be held by leading scientists who will be chosen as exemplars of the approaches and style that Paul represented. Please send contributions to Office of the Chair, Dept of Molecular Biophysics and Biochemistry, Yale U., PO Box 208114, 260 Whitney Ave., New Haven, Connecticut 06520-8114. Checks should be made out to Yale University and marked "Paul Sigler Lecture Fund".



Jerome Cohen (1933-2000)

Jerome B. Cohen, past president of the ACA, spearheaded a transformation of the engineering school at Northwestern University, revamping the curriculum, recruiting top-flight faculty members and presiding over an ambitious building plan. A graduate of the Massachusetts Inst. of Technology, Jerry Cohen came to Northwestern in 1959 as an assistant professor of materials science and engineering. He became dean in 1986. Cohen oversaw a \$125 million renovation of the university's Technological Inst. and the \$45 million construction of a Materials and Life Sciences Building. It was his innovations in undergraduate course work for which he was most noted, transforming the methodology of

teaching engineering at the college level. Rather than limiting theoretical and applied science courses to higher-level learning, he saw the benefit of introducing students to real-life problem-solving situations early in their academic careers. He encouraged engineering students to participate in joint studies in medicine, music, law, journalism, education and management, believing they could use their talents in applying math and logic to become leaders in any field. Mr. Cohen continued to carry out important research in the use of X-ray diffraction in understanding the nature of materials. He performed work at Argonne Nat'l Laboratory under funding from Dow Chemical and the DuPont Corp. and has several patents attributed to him, including one for a method of making beryllium alloy.

Megan O Matz, Chicago Tribune

Imre Tarján (1912-2000)



Professor Imre Tarján, a member of the Hungarian Academy of Sciences, died on January 19, 2000, at age 88. He arranged for Hungary to join the IUCr in 1963. He was first the secretary of the Hungarian National Committee of IUCr, and later its president (1966-1973).

Imre Tarján excelled in teaching, research and scientific administration.

He received his Ph.D. from the University at Debrecen in 1939.

After teaching physics in a leading secondary school, he headed the Biophysical Institute of the Medical University at Budapest from 1950 until his retirement in 1982.

In the early fifties, together with Professor Zoltán Gyulai, he grew synthetic quartz crystals and he and his co-workers produced NaI(Tl) and other single crystals for the detection of nuclear radiation. In the mid-sixties he extended his activity and applied solid state physical methods to the investigation of bio-

logical macromolecular systems. He and his team developed a method for the fast quantitative characterization of the mutagenic activity of chemicals and automatic equipment for its measurement. He was a co-author of a "Laboratory Manual on Crystal Growth" (Akadémia Kiadó, by arrangement with UNESCO, Budapest, 1972.). C.W. Bunn commented about the book "It should be in the hands of all teachers and students of crystal growth". His textbook "An Introduction to Biophysics with Medical Orientation" had 9 editions in Hungarian and was translated into Russian, Polish, English, and German.

He was a founding member of the Editorial Board of the Journal of Crystal Growth (1967-1971) and the Crystal Research and Technology (1966-1989). He was active in the Physical section of the Hungarian Academy of Sciences. He was dean (1959-63) and vice-rector (1970-73) at the Medical University in Budapest, head of the Research Laboratory for Crystal Physics of HAS (1961-1976), and honorary president of the Crystal Physical Section of the Hungarian Roland Eötvös Physical Society.

His numerous awards included the Kossuth Prize, the Hungarian State Award, and the Gold Medal of the Hungarian Academy of Sciences.

Ervin Hartmann

Metals in the PDF



The International Centre for Diffraction Data is expanding cooperation with the National Institute of Standards and Technology with respect to crystallographic data on metallic substances. While there are about 25,000 experimental metal and alloy patterns in the Powder Diffraction File (PDF), there are several thousand alloys not represented in either the PDF or the NIST Crystal Data File for which only single crystal data are available. Powder patterns will be calculated on the basis of their data to fill the gaps in the PDF. Similar agreements are already in place with the CCDC that maintains the Cambridge Structure Database and FIZ that maintains the Inorganic Crystal Structure Database. The size of the PDF has more than doubled in the past 3 years, as a result of these agreements, and with expansion of the ICDD Grant-in-Aid program.

High Wire Act

Eighty-three life sciences journals will make their back issues - representing more than 137,000 articles - free on the web through High Wire Press (<http://highwire.stanford.edu/lists/freeart.dtl>).

High Wire Press is a not-for-profit outfit set up in 1995 by Stanford University Libraries and Academic Information Resources to help universities and societies to publish on the web at low cost.

Most journals taking part in the High Wire scheme will make their content free one or two years after print publication. *PNAS* is making its content freely available one month after print publication, and *Molecular Biology of the Cell* after two.

Declan Butler in *Nature*, 404, Mar. 9, 2000

Mineralogical Research Grants

The Mineralogical Society of America announces the 2001 Grant for Research in Crystallography from the Edward H. Kraus Crystallographic Research Fund with contributions from MSA membership and friends.

Eligibility for the \$3,500 grant: applicant must have reached his or her 25th birthday but not yet have reached his or her 36th birthday on the date the grant is given. Selection will be based on the qualifications of the applicant, the quality, innovativeness, and scientific significance of the research, and the likelihood of success of the project. Application forms may be obtained from the MSA website (www.minoscam.org) or by contacting J.A. Speer, MSA Business Office, 1015 Eighteenth St., NW Ste 601, Washington, DC, 20036-5274; Tel: 202 775-4344; FAX: 202 775-0018; E-mail: j_a_speer@minsocam.org. Completed applications must be returned to the MSA Business Office by June 1, 2000.

FUTURE MEETINGS

High Pressure and High Temperature, Japan

A Workshop on "Crystallography at High Pressure and High Temperature using X-rays and Neutrons" organised by the IUCr Commission on High Pressure, the Dept. of SR Research, the Japan Atomic Energy Research Inst., and the Japan Synchrotron Radiation Research Inst., and supported by the Japanese Society of Crystallography **September 30 - October 3, 2000** at L Spring-8, Hyogo Japan.

Richard Nelmes' son, Malcolm, whom he resembles.

physics, Frontier topics and novel techniques.

International Advisory and Program Committee: R.J. Nelmes (UK), Chair; Organizing Committee: O. Shimomura, Chair.

Further information is available at www.iucr.org or www.spring8.or.jp/index.html or contact the HPC-3 Workshop Office, A. Shimamura, Spring-8, Kouto 1-1-1, Mikazuki, Sayo, Hyogo 679-5143, Japan, Tel: 81-7915-8-2701, Fax: 81-7915-8-2740, e-mail: IUCr2K@spring8.or.jp

Richard Nelmes

Malaysia 2000

The 2nd Asian Conference on X-Rays and Related Techniques in Research and Industry (ACXRI 2000) will be held from **November 20-22, 2000** in Kuala Lumpur, Malaysia. The conference is venue for introducing new ideas and innovations related to X-ray and other radiations. Special sessions will be held on XRD, XRF, SANS, microscopy and microanalysis in materials research and industrial applications. There will also be a scientific exhibition.

For further information visit www.mint.gov.my/mns/Seminars/ACXRI2000/Fisrt%20Announcemnet.htm

Meor Yusoff, Executive Secretary, ACXRI 2000

Motor Proteins

Jack Tuszynski and Bob Hodges U. of Alberta, Edmonton, Canada, on behalf of the Organizing Committee help to spread the word about "Banff 2000". A symposium on The Biophysics and Biochemistry of Motor Proteins which will take place in Banff, in the heart of the Canadian Rockies, **August 27-September 1, 2000**. For further information, visit <http://www.phys.ualberta.ca/~biophys/banff2000/>.

MEETING CALENDAR

A selection of future meetings. Extensive lists appear regularly in *J. Applied Crystallography*, the *BCA Newsletter* and the *ACA Newsletter*. Corrections and new listings are invited by the Editor.

JULY 2000

- 22-27 ♦ American Crystallographic Assn Annual Meeting (ACA '00). St. Paul, MN, USA. Contact: www.hwi.buffalo.edu/ACA.
31-4 ♦ 2000 Denver X-ray Conference. Denver, Colorado, USA. Contact: D. Flaherty, Conf. Coordinator, ICDD, FAX: 610-325-9823, flaherty@icdd.com, www.dxcicdd.com.

AUGUST 2000

- 6-11 ♦ Indaba III: Symmetry Breaking, Chirality and Disorder of Molecules and Crystals. Skukuza, Kruger Nat'l Park, So. Africa. Contact: <http://hobbes.gh.wits.ac.za/indaba>.
13-18 ♦ Twelfth American Conf. on Crystal Growth and Epitaxy. Vail Colorado Contact: www.aml.arizona.edu/aacg/conferences/acge12/index.html.
27-1 ♦ The Biophysics and Biochemistry of Motor Proteins. Banff, Alberta, Canada. Contact: www.phys.ualberta.ca/~biophys/banff2000/.
28-8 ♦ New Materials and their Dynamics: Advances through Synchrotron Radiation, Euro Summer School. Rostock, Germany. Contact: <http://euroschoool.physik.uni-rostock.de>.

SEPTEMBER 2000

- 3-9 ♦ Seventh BCA Protein Crystallography Summer School. Bristol, England. Contact: www.bch.bris.ac.uk/staff/lb/pxss/sumsc2.htm.
3-9 ♦ Sagamore XIII. Conf. on Charge, Spin and Momentum Densities. Jablonki, Poland. Contact: <http://alpha.uwb.edu.pl/sagamore>.
4-7 ♦ XVIII Conf. on Applied Crystallography. Wisla, Poland. Contact: www.us.edu.pl/universytet/konferencje/2000/cac/tekst/index.shtml.
5-8 ♦ Naples Workshop on Bioactive Peptides (Peptides as Templates, Artificial Receptors and Spacers; Membrane Active Peptides/ New Peptide Foldamers; Peptides in Material Science). Anacapri, Italy. Contact: <http://challenge.dichi.unina.it:8000/capri2000/index.html>.
7-10 ♦ Int'l Workshop on the Rietveld Method. Wisla, Poland. Contact: www.us.edu.pl/universytet/konferencje/2000/cac/tekst/index.shtml.
9-11 ♦ Dalton Discussion 3 – Inorganic Crystal Engineering. Bologna, Italy. Contact: www.rsc.org/lap/confs/daltondisc3.htm.
15-16 ♦ The Int'l Conference on Recent Trends in Crystallography/Centenary Celebration of K. Banerjee. Calcutta, India.
24-29 ♦ First Int'l Workshop on Physical Characterization of Pharmaceutical Solids (IWPCPS-1). Lancaster, PA, USA. Contact: A. Zakrzewski, FAX: 610594-2082, Angeline@ASSCI.com; www.assci.com/~marekz/IWPCPS-1.htm.
30-3 ♦ Crystallography at High Pressure and High Temperature using X-ray and Neutron. Hyogo, Japan. Contact: www.iucr.org (High Pressure Commission).

NOVEMBER 2000

- 20-22 ♦ 2nd Asian Conference on X-Rays and Related Techniques in Research and Industry (ACXRI 2000). Kuala Lumpur, Malaysia. Contact: www.mint.gov.my/mns/Seminars/ACXRI2000/Fisrt%20Announcemnet.htm

MAY 2001

- 23-3 ♦ Strength from Weakness: Structural Consequences of Weak Interactions in Molecules, Supermolecules, and Crystals. Erice, Italy. Contact: www.geomin.unibo.it/orgv/erice/accurate.htm or P. Spadon, paola@pdchor.unipd.it, FAX: 39 049 8275239.

JULY 2001

- 29-3 ♦ Int'l Conf. on Crystal Growth 13 in conjunction with Vapour Growth and Epitaxy-11 (ICCG-13/ICVGE-11). Kyoto, Japan. Contact: info@iccg.doshisha.ac.jp.

AUGUST 2002

- 6-15 ♦ XIX Congress and General Assembly of the IUCr. Jerusalem, Israel. Contact: <http://www.iucr.org/>.

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