

INTERNATIONAL UNION OF CRYSTALLOGRAPHY

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LETTER FROM THE PRESIDENT

Letter from the President



Henk Schenk

A Dutch proverb says: 'Who has the youth, has the future'. Therefore, young scientists are the key to the future of crystallography. As you may know, organisers of meetings can apply to the IUCr for a grant in order to sponsor young scientists (YS) to enable them to participate. The Sub-committee on the Union Calendar, with Professor Hartmut Fuess as Chair, reviews the applications and proposes the level of support to the Executive Committee. Organisers themselves often provide additional funds to support YS or find sponsors who sympathise with this scheme.

This summer I was able to see how well our YS grant scheme works. At both the ACA meeting in Los Angeles and the ECM in Krakow I spoke with many of the YS. Those who received a grant through our scheme expressed gratitude to the organisers and to the IUCr. Most YS are sponsored in part only. When they apply for additional funds at their home institutions or elsewhere, the potential sponsors are always impressed by the support provided by the IUCr and additional funds are more readily given.

We all know the history of our subject. For sure, the older among us remember the challenges and dreams of their young years and the excitement they felt when desired results were achieved or, unexpectedly, completely new ones were found. I, for instance, will never forget the exciting days when I found the 7-magnitude quartet relation in direct methods. I started with the thought that quartets H, K, L, -H-K-L are truly 3D relationships where triplets are 2D only. As such, for solving 3D structures, I had high expectations of them. However, when I checked the quality of these quartet relations based on four magnitudes, I was very disappointed by the results. Still, the 3D character of the quartet relation kept my mind busy. Then, on the next Sunday, my wife Coringe and I took a long walk in the dunes at the coast northwest of Amsterdam. In the last hour of the walk, I had the brainwave that three more reflections are involved in a quartet, H+K, H+L, and K+L. I still know exactly the place where that happened! A week of hectic programming and testing followed. The next weekend I could analyse the results and found that the three additional E-values, the crossterms as I called them, changed the picture completely. Strong crossterms appreciably enhanced the reliability of the quartet phase sum being zero, the positive quartets. Quartets with phase sums of 180 degrees were characterised by weak crossterms and predominantly found on the bottom of the list. These negative quartets proved to be very useful as well.

We all work on the present state of crystallography, but what the future will look like we do not know. Of course, there are plans for exciting new facilities and new possibilities will arise. And we all have dreams and challenges. However, youth has the future and for the future of crystallography it is important that the IUCr continues to focus its attention on the young women and men of our community.

Henk Schenk

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EDITORIAL

Editorial



This issue of the *Newsletter* contains yet another letter to the Editor concerning the relative ability of electron and X-ray diffraction to accurately reveal electron density in metals. A limit of 1/3 of a *Newsletter* page was arbitrarily imposed upon the author. The allocation of space to subsequent letters on the subject will follow a progression of 1/6, 1/12, 1/24, etc. of a page. While this progression may never end, the entries will soon become so small that they will be no imposition on the *Newsletter's* page limit and IUCr finances.

It has been brought to my attention that the individual identified as Aslanov in the picture on page 10 of Vol. 8 # 3 is actually Antipin. I am surprised that neither has written to complain. Perhaps neither detected the error or each felt it would be undiplomatic to complain. In any event, I apologize to both.

This issue contains important information concerning the XIX IUCr Congress and General Assembly now scheduled to be held August 6-15, 2001 in Geneva, Switzerland (page 8). The local Organizers have done an excellent job of arranging for very economical and convenient housing as well as a superb meeting venue.

I also draw your attention to the publication of Volume F of the *International Tables*, 'Crystallography of biological macromolecules'. Michael Rossmann and Eddy Arnold have done a remarkable job of editing this large, comprehensive and splendidly illustrated volume that upholds the tradition of quality characteristic of the *International Tables*, that collection of volumes essential to the conduct of crystallography (pages 24 and 25).

William L. Duax
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LETTER TO THE EDITOR

Letter to the editor

Dear Friends and Fellow Crystallographers,

We are deeply shocked by the terrorists' attack against America. We scientists are by nature international and cannot understand or accept such a horrible tragedy.

We shall even more than before, continue collaborating together to promote our science in all countries, especially the underdeveloped ones. We strongly believe and are convinced that this is a very important contribution to the world's peace.

With all our friendship,

Claude Lecomte

President, European Crystallographic Association

LETTER TO THE EDITOR

Letter

To the US National Committee for Crystallography

Dear friends,

Yesterday we all were very much shocked by the horrifying pictures of New York and Washington. Unbelievable what happened; this catastrophe goes beyond any imagination. At the time the first news came in, my complete group was gathered and we first did not believe that the message could be true. However, it just appeared to be the beginning of the terrorist's attack and the day changed into one of the real black days of history.

On behalf of the IUCr I want to express our sympathy in these difficult days with the American people and in particular with all our colleagues in crystallography and their relatives.

Henk Schenk

President, International Union of Crystallography

LETTER TO THE EDITOR

Letter to the editor

Dear Bill,

The Arizona electron-diffraction group has recently discussed 'three substantial points' in a 'Letter to the Editor' ([1] *IUCr Newsletter* **2001**, 9(1):2).

1. Accuracy of methods and published results: The reliability of the experimental and theoretical raw data may indeed be better than 1%. However, the validity of the published Figs. generated therefrom, e.g. the difference electron density plots, also depends on the applied approximation models. For instance, the good quality of the QCBED raw data does not automatically prove the existence of the hypothetically deduced novel type of $\text{Cu}^+ \cdots \text{Cu}^+$ bonding, no safe evidence of which could be found so far during a decade of serious experimental and theoretical searches (including the band structure calculation of [1]).

2. Attaching the word 'orbital' to difference densities: While the difference density under consideration exhibits the sign pattern of a *g*-function with 12 extrema (6 positive and 6 negative ones) in a plane around the Cu, it is stated in [1] that 'it would be perverse not to mention the resemblance of this shape to a *d*-orbital charge density', although the latter is characterized by 4 positive extrema (and 4 zeros), not to mention the shape of 'text-book orbitals'.

3. The significance of their difference density: The WIEN band structure calculations [1] resulted in an atomic orbital population on Cu of $3d_z^{21.6} 4s^{0.2} 4p^{0.1}$. Our Mo calculations resulted in a $3d_z^{21.5} 4s^{0.75} 4p^{0.25}$ MULLIKEN population. We note i) the different physical normalizations of different partial charge definitions (see *J. Phys. Chem.* **98** (1994) 8245), and ii) the *4s/4p* WIEN shorter range and MULLIKEN longer range population ratios of 2/1 and 3/1, respectively, which are not too different.

Summarizing, while most of the basic (exp. and theor.) data and their interpretations seem to agree with each other, the main discrepancy seems to concern the *interpretations* of the data advocated for by the Arizona group.

W.H.E. Schwarz

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LETTER TO THE EDITOR

Letter to the editor

Dear Bill

I wish to express my concern about the announcement that Kodak will stop the production of X-ray films. As far as I am aware, there are no other producers left. This is a serious problem for crystallographers, particularly of developing countries, who still use films for their research. Perhaps you or somebody else can provide information on how to solve this problem.

Mario Suwalsky (msuwalsk@udec.cl)

U. of Concepcion, Concepcion, Chile

LETTER TO THE EDITOR

Letter to the editor

Dear Professor Duax,

The structural chemistry group of the Institute at the Faculty of Science in Skopje, Macedonia, where I work, is looking for a used single-crystal diffractometer of any type. Our institute is ready to cover the complete transportation costs from any institution in Europe to Skopje.

*Pance Naumov, Tokyo Inst. of Technology,
Tokyo, Japan*

LETTER TO THE EDITOR

Letter to the editor

Dear Mr. Duax:

The recent issue (Vol. 8, No. 4, 2000) which I received has an incorrect picture caption in the Mineralogical Society of America “Notices” section (p. 24). The picture is of Quentin Williams (recipient of last year’s MSA Award), not Peter Burns.

David M. Jenkins, MSA - Secretary

MISCELLANY

Risky

In 1999, 17,000 people died by falling down, 41,000 died in motor vehicle accidents, and 3,000 died by choking on their food. Whether it's genetically modified food or not, we face the possibility of choking every time we eat, but it's a risk we must take every day. This risk cannot be eliminated, regardless of any amount of research conducted by bioethicists or scientists.

Mike M. Botz, Joliet, Mont., C & EN, June 25, 2001

MISCELLANY

So easy a child could do it

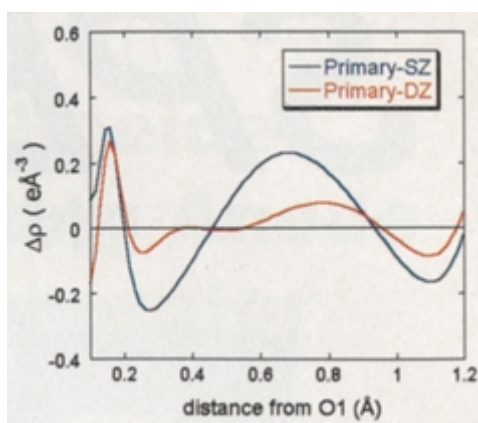
A certain portion of the research community has tended to regard crystal structure analysis as entirely too easy and the value of crystallographic results has been challenged as being irrelevant beyond the solid state, despite countless examples of correlations between structural features observed in the solid state and the chemical, physical and biological properties of the same molecules in vitro and in vivo, as measured by a wide range of techniques. The rapidity with which new structures are determined and the rate at which crystallographic databases are expanding fuels the argument that crystallography is easy and crystallographic instrument manufacturers reinforce this opinion by claiming that with today's instrument and software anyone can determine a crystal structure. Even Judith Howard, past BCA President was quoted out of context as saying 'instruments have been so advanced that you sometimes feel you can train a monkey to use it (ref)'. Unfortunately, a monkey so trained would know about as much about the underlying phenomena of diffraction, the proper use and analysis diffraction data and the structural information it provides as many other current users who lack formal crystallographic training.

Fine-tuning the rigid pseudoatom model

A. Volkov & P. Coppens, *Acta Cryst.* (2001). A57, 395–405

The recent adoption of high-speed data-collection methods, especially CCD detectors, and the wider availability of user-friendly software such as *XD* (Koritsanzky, Howard, Mallinson, Su, Richter & Hansen, 1995) have attracted new workers to charge-density studies from X-ray diffraction data, extending the variety of the systems studied, as well as leading to greater penetration of the results in mainstream chemistry and physics journals. However, it is increasingly clear that limitations of the rigid pseudoatom model (multipole refinement) upon which most studies are based may be compromising the more ambitious studies, especially topological analyses, where the objective is to determine the fine details of the curvature of the electron density.

There seem to be two ways forward: (i) fine-tune the rigid pseudoatom model, especially the radial functions, or (ii) abandon the model completely. Examples of the latter approach include maximum entropy methods and the derivation of 'experimental wavefunctions' from X-ray diffraction data. However, the vast majority of charge-density determinations still use the multipole refinement procedure, and numerous model studies have appeared recently that explore its strengths and limitations. Especially active in recent years has been the Coppens group in Buffalo, and the latest publication by Volkov & Coppens [*Acta Cryst.* (2001). A57, 395–405] explores the use of additional radial functions on non-H atoms.



Difference between primary electron density and multipole-derived electron densities along the C1–O1 bond in methyl carbamate. Two-term radial functions (DZ, red) show considerable improvement over conventional radial functions (SZ, blue).

Using model structure factors computed from periodic *ab initio* calculations on several molecular crystals, Volkov and Coppens applied the usual Hansen-Coppens multipole formalism, as well as augmenting it with an additional radial function for the higher multipoles on C, N and O atoms. These single exponential radial functions, $r^n \exp(-\alpha r)$, offer two degrees of freedom: the power of r , n , and the exponent α . For first-row atoms, conventional choices for n are between 2 and 4, and α is obtained from atomic orbital products. But it has long been known that alternative sets of n and α would produce fits to the data of comparable quality, although the nature of the radial functions differs substantially as n is increased.

A more flexible pseudoatom may be obtained by adding a second radial function per multipole, with a different set of n and α . But what are the optimum values to choose for each atom? To answer this question, Volkov and Coppens performed several thousand model refinements, optimizing α for choices of n between 4 and 22 for a second set of radial functions on first-row atoms. Inclusion of additional radial functions led to significant improvements in the agreement with the theoretical electron density and topological properties along the bonds, but discrepancies still remained, especially for polar bonds

such as N–O and C–O. The figure illustrates the improvement in the electron density for an O–C bond in methyl carbamate. Surprisingly, optimum values of n for the second deformation set were found to be as high as 20 and 22 in several instances, corresponding to quite narrow radial functions. The authors did not explore why this might be the case for some bond types, and do not provide a standard recipe for incorporating additional radial functions in multipole refinements. They conclude that application of this more flexible model will require experimental structure factors of exceptional accuracy, which is undoubtedly true if one aims to refine n and α simultaneously. However, it is worth remembering that Hirshfeld's multipole model (Hirshfeld, 1977), seldom used today, has always incorporated two-term radial functions for some higher multipoles, albeit in a constrained fashion, and its demands on the X-ray data are much more modest. It would seem desirable to compare its performance with the one- and two-term Hansen–Coppens models. This paper provides some valuable guidance and much-needed impetus for future studies aimed at fine-tuning the multipole model.

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Diffraction by the ideal paracrystal

J. L. Eads & R. P. Millane, *Acta Cryst.* (2001). A57, 507-517

Paracrystal was the name given originally by Hosemann and co-workers (Hosemann & Bagchi, 1962) to a class of models used to describe structures with highly distorted lattices that exhibit only very broadened diffraction peaks. The models describe structures that are still crystalline in the sense that each lattice site can be indexed by pairs (in 2D) or triplets (in 3D) of integers but the shape and size of the unit cell is highly variable. There are many examples of such materials: for example, polymers, glasses and alloys (Hosemann & Hindeleh, 1995); colloidal suspensions and block copolymer films (Matsuoka, Tanaka, Hashimoto & Ise, 1987); polymer fibres (Granier, Thomas & Karasz, 1989); muscle proteins, biopolymers such as nucleic acids and some synthetic polymers (Millane & Stroud, 1991). The lattice models themselves deal only with the shapes and sizes of unit cells and not their contents.

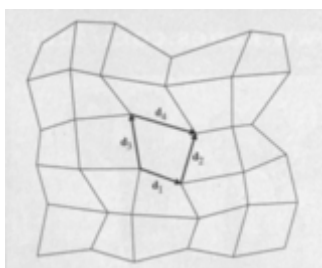


Figure 1. The cell closure constraint. The statistics of the intersite vectors must be specified such that $\mathbf{d}_1 + \mathbf{d}_2 = \mathbf{d}_3 + \mathbf{d}_4$.

In 1D the paracrystal model is well-defined and understood but extension to 2D and 3D is distinctly non-trivial, and has occupied numerous workers over the last ~40 years. The reason for this is easy to see by considering Fig. 1, which shows the general case in which the unit-cell edges can vary both in length and direction. Whereas for a 1D paracrystal the numbers of cell edges and lattice sites are equal, in 2D and 3D the number of edges far exceeds the number of sites, and this imposes severe constraints on the degree of variation that can occur.

This is the latest in a series of papers by Millane and co-workers that explore the properties of various types of such distorted lattice models. Their specific aim, not dealt with in any detail in the current paper, is to provide models suitable for describing more quantitatively the distribution of diffracted intensity from various real poorly crystalline materials. The aim is to be able to obtain better estimates of intensities of broadened Bragg peaks characteristic of these so-called fibre diffraction patterns, so that better structural information can be extracted from them. The work thus complements the authors' work in analysing such materials as cellulose and other biopolymers (see, e.g., Finkenstadt & Millane, 1998; Stroud & Millane, 1995).

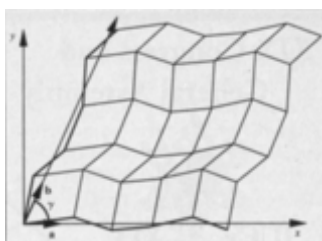


Figure 2. The ideal paracrystal defined in terms of two 1D paracrystals.

In the introduction section of the paper the authors review the development of the paracrystal and other paracrystal-like models. The *ideal paracrystal* model originated with Hosemann many years ago. The unit cell in the ideal paracrystal has cell edges that can vary both in length and direction but each unit cell is constrained to be a simple parallelogram (see Fig. 2). This latter feature was always considered to be an unsatisfactory aspect of the model as it resulted in a number of unwanted properties of the diffraction

pattern. In particular the model predicts low-angle scattering in excess of that observed in real systems and also shows a type of anisotropy in which the scattering behaviour in the direction of the lattice diagonal is different from that along the axial directions. There have been many and varied attempts to obtain models that do not have these shortcomings but despite this, the ideal paracrystal has continued to be of prime importance because of its amenability to analytical analysis, and consequent ease of computation.

The paper presents a description of ideal paracrystals in their most general form, develops the necessary equations by which their diffraction patterns can be calculated and explores the wide variety of peak-broadening characteristics they exhibit. The problem of incorrect low-angle diffraction is overcome by use of finite lattices, but the anisotropy between the axial and diagonal directions, however, remains. This is particularly problematical in attempts to construct an ideal paracrystal on a hexagonal lattice, an important case for crystals of molecules or assemblies that are approximately circular in cross-section. Despite this, the model described should provide a useful addition to the modelling possibilities in particular real example analyses. For example, it does seem likely that this anisotropy problem could be overcome for all practical purposes by taking an average of several different orientations of the ideal paracrystals described.

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Richard Welberry, Research School of Chemistry, Australian National U., Canberra, ACT, Australia

IUCR ACTIVITIES

Report of the Commission on High Pressure for the year 2000

High-pressure crystallography continues to develop very rapidly through the influence of modern synchrotron and neutron sources, with new techniques and areas of science opening up every year. The Commission sees as its principal activity the organization of symposia and workshops to keep the crystallographic community in touch with the latest developments, and to create opportunities to extend the boundaries of the Commission activities and draw in new people from the wider field of high-pressure science.

The principal activity of this year was the organization of an international workshop focused on the topic of Crystallography at High Pressure and High Temperature Using X-rays and Neutrons. Nearly 80 high-pressure scientists from 13 countries gathered at the picturesque site of the third-generation synchrotron facility Spring-8 at Hyogo, Japan for the four days from September 30 to October 3, 2000. The workshop was jointly organized by the Commission, the SRRC Japan Atomic Energy Research Institute (JAERI), and the Japan Synchrotron Radiation Research Institute (JASRI). The local organizer was Commission member Osamu Shimomura. The major topics of the oral sessions included structures and transitions in molecular and elemental liquids; novel (and often complex) structures in simple systems – like lithium, oxygen and xenon; theoretical studies of liquid carbon, molecular hydrogen and alkali metals under pressure; a wide variety of geoplanetary science – mineral phases and equations of state, the Earth's lower mantle and core, and planetary ices; high P-T synthesis of new materials like cubic boron carbonitride and 3D polymerization of C₆₀; and high P-T experimental techniques using x-ray synchrotron and neutron sources. Altogether, there were 25 oral and 43 poster presentations. The participants included 13 young scientists supported jointly by the IUCr and JAERI, from Germany, India, Russia, Switzerland, USA, UK and Sweden. Three young scientists were invited speakers. Considerable assistance with the excellent local arrangements was given by JAERI and JASRI staff.

In addition, Commission members have been involved during this year in the early stages of preparing an international workshop covering the full range of activities to be held at Orsay, France, in September 2001 with Commission member Igor Goncharenko as the local organizer. A preliminary bid has been prepared and submitted for sessions at the 2002 Congress. Planning has also continued for a School on High Pressure Crystallography to be held at Erice, Italy, in 2003 with Commission member Andrzej Katrusiak as Director.

The Commission maintains a regularly updated mailing list and an active web site, including a list of forthcoming meetings of interest to high-pressure crystallographers and detailed reports on past meetings. The Commission is preparing a list of information on central facilities for high-pressure crystallography, and on how to access them. These services to the community depend on the much appreciated efforts of John Parise, John Loveday, and Martin Kunz.

R.J. Nelmes, Chair

FEATURE ARTICLE

Crystallography of historical note: R.W. James on ice

In 1914, four days after the First World War began, Sir Ernest Shackleton and his crew of 27 seamen and scientists set sail from England for Antarctica on the 144 foot wooden ship *Endurance*. They would not be heard from again for nearly two years. Just one day before they reached Antarctica, temperatures plummeted and the ship was entrapped in pack ice. Frozen fast for 10 months, the *Endurance* was slowly crushed by the pressure of the ice. The crew was forced to abandon ship with three small lifeboats and limited supplies onto an ice floe. What followed were 22 grueling months of camping on different ice floes until they opened sufficiently to use the boats and reach Elephant Island. Then Shackleton and five others crossed some of the roughest seas in the world (Drake's Passage) in an open lifeboat to South Georgia Island and there traversed uncharted mountains before finding help. The most astonishing feat of all was that everyone survived. This harrowing story is now retold in the striking feature length documentary, 'The Endurance: Shackleton's Legendary Antarctic Expedition'. Produced by George Butler and author Caroline Alexander, the film resurrects astonishing Antarctic panoramas, the doomed ship, and the extreme hardships and miraculous climax of one of the greatest man-against-nature sagas to emerge in the 20th century.

We would like to point out that the renowned X-ray crystallographer Reginald William James (R.W. James of 'The Crystalline State, Vol. II, The Optical Principles of the Diffraction of X-rays') was a member of the Shackleton Antarctic Expedition. His duties as physicist were to study magnetism. In view of the documentary and the rumor that Hollywood is to make a movie of the epic, we thought today's crystallographers would appreciate knowing about James as they may view one or both of these films.

At Cambridge, James read physics, chemistry and geology for Part I and obtained a 1st Class in 1911 and physics for Part II. James was a classmate of W.L. Bragg in C.T.R. Wilson's Part II lab; both received 1st Class in their finals. They both attended lectures by Sir J.J. Thomson with whom James started research in 1912 and worked with until 1914. Although James received an appointment at Liverpool University after 5 years at Cambridge, a friend told him about Shackleton's Expedition. James said he might be interested and soon received a telegram from Shackleton. His interview with the latter lasted 5-10 minutes concluding with a 'very well, I'll take you.'

The Expedition was rescued in August, 1916 and James reached England that November. His diaries of the Expedition are now housed at the Scott Polar Research Institute, Cambridge University. After the war, James joined the Physics Department at Manchester University from 1919-1937 and then went on to Capetown, South Africa. He made a world-wide reputation for himself in his collaborations with W.L. Bragg, C.H. Bosanquet, C.G. Darwin and I. Waller. He measured the absolute reflecting power of rock-salt crystals for X-rays (between reflected rays and the incident X-ray beam). Another classical piece of work by James was the investigation of the intensity of reflections by rock-salt over a large temperature range with D.R. Hartree and Ivar Waller, which established the existence of zero-point energy in the lattice. One of R.W. James' most distinguished students is Sir Aaron Klug, winner of the Nobel Prize in Chemistry in 1982 for his development of crystallographic electron microscopy and the structures of nucleic acid-protein complexes.

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A. Tulinsky

MEETING REPORT

Crystals and films in India



Fundamental research on well characterized single crystal and epitaxial thin films is critical to the design of innovative and sophisticated devices. The area of materials characterization explores the relationship between properties of the materials and their structure. An International Workshop on Preparation and Characterization of Technologically Important Single Crystals (PCSC-2001) organized in February 2001 at National Physical Laboratory, New Delhi covered the following topics: •oxide optoelectronic and sensor applications; semi conducting materials; •thin films, multilayers, quantum wells, interfaces, and solar cells; •characterization of bulk single crystals, thin films, multilayers and their defects; simulation of crystal growth; and instrumentation for crystal growth and high resolution X-ray diffraction techniques.



Participants at the PCSC conference in February 2001 in New Delhi, India.

The Proceedings of the workshop (including 136 papers) were distributed to 180 registered participants.

A special session was organized to honor Krishan Lal on his 60th birthday.

Various dances of India were depicted in a cultural program.

An opening discussion lead to the following suggestions:

1. Future meetings should have an exhibition of industrial products.
2. Advanced facilities for characterization of materials at the national level should be established.
3. A Society on Materials Characterization should be formed in India and
4. Advanced courses on materials characterization should be introduced at post graduate level.

The workshop was sponsored by The Council of Scientific and Industrial Research, the National Physical Lab, Indian Nat'l Science Academy, the Dept of Science and Technology, the Ministry of Information Technology, the Ministry of Non-Conventional Energy Sources, the All India Council of Technical Education, the Indian Inst. of Technology, and the Int'l Union of Crystallography, Chester, England. An IUCr contribution helped support 37 young researchers who attended the workshop.

Invited speakers included: G. Heger, H. Klapper, R. Kohler of Germany; B.M. Arora, R.K. Bagai, D.N. Bose, P.N. Kotru, Krishnan Lal, J. Lakshmana Rao, V.D. Vankar of India; T. Fukada, Ken Suto of Japan; I. Lyubutin of Russia; J.N. Sherwood of UK; and M. Dudley, V. Greenhut, V. Prasad, I.L. Smolsky of the USA.

S.K. Halder

MEETING REPORT

Crystallography of molecular biology



Participants at the Erice Course, June 2000.

The June 2000 Erice Course on Crystallography of Molecular Biology consisted of two parallel meetings, sponsored by the IUCr and by the Int'l Union of Biochemistry and Molecular Biology, and financed by Nato under the ASI Program.

On Sunday, May 28 the main court of the E. Majorana Centre was dedicated to Dorothy C. Hodgkin, a former director of the Int'l School of Crystallography in Erice. The Erice Vaciago Prize for the most dynamical 'student' (under 35) in attendance was awarded to Bostjan Kobe. Canadian astronaut Julie Payette presented a special evening lecture on her ten days extraterrestrial flight.

Methods for macromolecular crystallography

Directors: L.N. Johnson and D. Turk

A. McPherson described new approaches to monitoring crystal growth by atomic force microscopy and G. DeTitta showed quantitative improvements to automate crystal growth – for high throughput structure analysis - 1536 simultaneous trials.

K. Branden gave an overview of macromolecular beam line facilities world wide (48 total, 20 in Europe and 20 in USA) and demonstrated their advantages for structural biology and the prospects for the future. Thompson described the experimental set up at synchrotron sources for multi-wavelength measurements including the parameters of the synchrotron required, the tuneable wavelength, and the basis of the method for phase determination. S. Ealick took up the theme of detector development, explaining the physical principles behind current detectors. E. Garman gave an account of the use of cryomethods (100 K), that have become so important in the field.



Lodovico Riva di Sanseverino and Maria Carrondo at the court of San Rocco building, a central point for those attending, was dedicated to Dorothy Hodgkin.

Data processing was admirably covered by A. Leslie with lectures and by Z. Otwinowski with hands-on computer tutorials in small groups: both practical aspects and considerations about errors that are still problematic were covered.

Phase determination was divided into *ab initio* and molecular replacement methods. G. Sheldrick and H. Hauptman described their application when high resolution data (1.2 Å) are available and the routine for location of anomalous scatterers at lower resolution (3 Å). J. Navaza and M. Rossmann described the powerful methods of molecular replacement. Only 9% of structures solved in 1999 contained a new fold. This also introduced non-crystallographic symmetry averaging and solvent flattening in phase determination. E. Weckert described the 3-beam method for experimental phasing.

Computer graphic displays and interpretation of electron density maps were covered by A. Jones, and R. Henderson illustrated the use of electron microscopy to determine structures from 2D arrays and the convergence of X-ray and EM methods was discussed.

Chemical Prospectives

Directors: M. Jaskolski and D.I. Stuart

The school reflected the 'state of the art' of the Crystallography of Molecular Biology bringing together experimentalists, theoreticians, biochemists, crystallographers and electron microscopists. Advances in macromolecular crystallography have led to an understanding of enzyme catalysed reactions, control of gene expression, regulation by phosphorylation and recognition in signal transduction pathways, and immune response, energy transduction, of membrane proteins and ion channels, and the assembly of viruses from component proteins. The most recent results presented by leading scientists in the field gave the audience the idea of the terrific improvements achieved in the understanding. Young participants presented their results as oral and poster presentations.

Recent results concerning membrane proteins, protein nucleic acid interactions, nucleosome structure, and the 30S subunit of the ribosome were presented.

Sessions were devoted to the combined utilization of Electron Microscopy and X-ray Crystallography, the potential of the new third generation synchrotron facilities, and the contributions of crystallography to structural genomics.

Advances in MAD and SAD phasing (W. Hendrickson & A. Brunger), high resolution structure determination (K. Wilson, York, UK), automatic structure interpretation (T. Terwilliger, Los Alamos, USA and D. Turk, Ljubljana, Slovenia), non-crystallographic averaging (R. Read, Cambridge, UK), maximum likelihood refinement (E. Dodson, York, UK) and *ab initio* phasing methods (G. Bricogne, Cambridge, UK) were described in detail. The school featured hands on tutorials in which small groups of participants learned first hand from the experts at the computer workstations.

MEETING REPORT

A protein structure course in Poland



Participants at the Determination of High-Resolution Structures for the Post-Genomic Age course in Poznan, Poland, June 2001.

A course entitled Determination of High-Resolution Structures for the Post-Genomic Age was held in Warsaw and Poznan, Poland in June 2001. The course was sponsored by the U.S. Nat'l Research Council, with funding provided by the Howard Hughes Medical Inst. Students from 11 countries of Central and Eastern Europe applied high-resolution NMR and X-ray crystallography to studies of protein structure. The curriculum was created by co-directors, X-ray Spectrometrists R.A. Byrd and X-ray Crystallographer A. Wlodawer (Nat'l Cancer Inst.). Crystallographic faculty members included M. Bochtler (Int'l Inst. of Molecular and Cell Biology, Warsaw), G. Bujacz (Technical U. of Lodz), Z. Dauter (NCI, USA), M. Jaskolski (Inst. of Bioorganic Chemistry, Poznan), A. McPherson (U. of California), and L. Sjolín (Chalmers Polytechnic, Sweden). For the first week in Warsaw, the students were instructed in the principles and application of NMR in structure determination. During the second week in Poznan, the students learned to use a Mar300 image-plate detector to collect diffraction data, and how to phase, trace, refine, and deposit protein structures. During the course the faculty members presented 10 public seminars on aspects of their own research, in addition to course-related lectures and classes. Many of the pre- and postdoctoral students that participated in the course will apply knowledge gained during these two weeks to various aspects of structural biology. The success of the course was possible thanks to K. Robins (Nat'l Academy of Sciences, USA), A. Stasiak (Warsaw) and J. Stepkowska (Poznan). Teaching materials created for this course are available to interested organizers of similar courses planned for the future.

Alexander Wlodawer

MEETING REPORT

Crystal Growth, Vail, Colorado



270 Registrants attended the Twelfth American Conference on Crystal Growth and Epitaxy (ACCGE-12) in **August, 2000**, which included 17 focused technical sessions, a poster session, an industrial exhibit and a photography contest. The conference covered a broad spectrum of topics from bulk crystal preparation to epitaxial film growth and included a Microgravity Workshop sponsored by NASA. The AACG Award was presented to C. David Brandle (Agere Systems) and the AACG Young Author Award went to Joan Redwing (The Pennsylvania State U.) ACCGE-13 will be held August 12-16, 2001 at the Radisson Hotel Burlington located in Burlington, Vermont.

American Association for Crystal Growth Spring 2001

MEETING REPORT

Croatian-Slovenian meeting

The 10th Croatian-Slovenian Crystallographic Meeting was held in Lovran, a famous holiday resort on the Adriatic coast. There were 80 participants from Croatia, Slovenia and other countries. Plenary lectures were Molecules in motion (K. Prout, Oxford); The transport of vitamin A in mammals: a crystallographer's view (G. Zanotti, Padova); Protein-peptide binding and its regulation (B. Kobe, Brisbane); and Crystallography of composite crystals (O. Milat, Zagreb). A half-day excursion was organized to the Krk (Vrbnik) island, where participants visited historic places and tasted smoked ham and wine. The meeting was supported by Pliva (Zagreb), Philips, Seifert, Molecular Structure Corp.-Rigaku, Nonius, Jeol and the Ministry of Science and Technology of Croatia. A full report is available at: www.chem.pmf.hr/~hkz/lovran01/.

Stanko Popovic and Ivan Leban

MEETING REPORT

British Crystallographic Association 2001 Spring meeting



Bragg Lecture. The first Bragg lecture was given by P.P. Ewald in 1962, the centenary of the birth of W. Lawrence Bragg's father, W.H. Bragg and the jubilee of the discovery of X-ray diffraction by crystals. The presentation of the 2001 Bragg lecture by David Stuart in the midst of the worst Foot and Mouth Disease outbreak since 1967 was remarkably timely. Determination of the structure of Foot and Mouth disease virus was published by Stuart in 1989. The structure of the virus was beautiful, but initially did not reveal the details of a surface loop, crucial for immune recognition of the virus. Further work including cryo-electron microscopy confirmed that the loop has multiple conformations, which could potentially be harnessed in vaccine design.

Stuart's lecture illustrated how far crystallography has travelled since Lawrence Bragg described a method to determine the structure of NaCl (28 Da) in 1912. Bragg can little have imagined that within a century it would be possible to use the same methods to visualize the atomic structure of a virus particle of 108 Daltons in the act of transcription.

Other Awards. The Alun Bowen Industrial Lecture, 'Crystallography in the Aerospace industry', was presented by C. Small (Rolls Royce, Derby). When a titanium fan blade failed a bird test despite no apparent structural changes, the texture was checked and a pole figure revealed dramatic differences between the texture of the failed blade and that of a normal blade. A particular forging process had caused the texture change. The lecture highlighted just how important it is for a crystallographer to be able to translate his/her analytical results into meaningful information for the engineer.

C. Wilson, U. of Nottingham, received the Cambridge Crystallographic Data Centre Prize for a series of variable temperature single crystal X-ray and neutron studies of di-copper complexes. The key structural change was a 3° variation in the angle between the magnetic planes over a 35 to 295 K temperature range. The David Blow poster prize (a piece of Blue John crystal) was presented to A. Carter from the LMB, Cambridge for his poster 'Crystal Structure of an Initiation Factor Bound to the 30S Ribosomal Subunit'. The 2001 Philips Award was given to J. Kreisel of ENS de Physique de Grenoble, for his work on phase transitions in perovskite and related phases. Poster Prizes were awarded to P. McGregor (Edinburgh) for 'The High Pressure Crystal Structure of Ethylene Glycol'; M. Gutmann (ISIS, RAL) for 'Charge Inhomogeneities in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ Evidenced from Pulsed Neutron Diffraction'; and H. Thompson (Heriot-Watt) for 'The Dehydration of α -Lactose Monohydrate'.



Attendees at the BCA meeting include (Seated left to right) Michael Hart, Judith Howard and Dave Stuart; (standing) Bill Duax, Geoff Mitchell, David Cardin, and Paul Fewster.

Visualization. A plenary session on visualization had relevance to all branches of the subject. R. Hubbard (U. of York) explored the structure and reactivity of the oestrogen receptor and the molecular biology of oestrogen action. S. Motherwell (CCDC) put graphics to new uses including visualization of hydrogen bonding networks, strong interactions, voids in crystals and the relationships among multiple copies of molecules within an asymmetric unit. P. Withers (Manchester U.) illustrated how visualization techniques in texture, stress and tomography can allow quick detection of grain boundaries. M. Dove (Cambridge U.) used animations of molecular dynamic simulations to visualize atomic motions in disordered materials including the diffusion of Na through quartz in an electric field and radiation damage in ZrSiO_4 . (Chris Gilmore)



Christine Cardin and Chris Gilmore spooning.

How MAD can you get? N. McDonald (ICRF) described the use of SeMet modified proteins as the most popular route to MAD structure determination. S. McSweeney used small anomalous signals at the ESRF to provide phase information, and reported that one Se per 20 kDa provided excellent phasing, one Se per 30 kDa was more difficult, and that anomalous scattering from sulphur, at $\alpha=1.77\text{\AA}$, required **very** careful data collection.

P. Rizkallah (Daresbury) described using longer wavelength radiation from second generation sources to collect anomalous signals from xenon and sulphur. The xenons were located with Shake'n'Bake, and the resulting phases used to locate the sulphur atoms. T. Schneider (Göttingen) described the latest software for solving the anomalous atom substructures, focusing on SHELXD and SnB (Shake'n'Bake) with which substructures of up to 60 Se atoms can be solved routinely. Z. Dauter discussed soaking crystals in high concentrations of 1M NaBr or 0.5M KI to incorporate large numbers of bromine or iodine atoms. Bromine substitution provided the best MAD data while iodine was best suited for SIRAS or SAD phasing. J. Löwe (LMB, Cambridge) illustrated that MAD can be successful even when the crystals diffract poorly ($3.1\text{\AA}$), have a high mosaicity and the resulting data have a high Rmerge (10%). In spite of these problems, a 3 wavelength Se MAD data set collected using inverse beam geometry on ID29 at ESRF gave a readily interpretable map in which sites were correctly located with SnB.

Atomic Resolution. E. Garman (Oxford) explained how data collection to resolutions around $1.0\text{\AA}$ allows refinement of atomic anisotropic displacement parameters, dual conformations of disordered residues, hydrogen atom positions and much improved water structure.

K. Wilson (York), described the computer program ACORN (Jia-Xing Yao) for *ab initio* protein structure determination using atomic resolution data starting with seed structures derived either from anomalous data or by molecular replacement. A dynamic density modification algorithm obviates the need for manual rebuilding of the molecule and has been successful in solving a number of structures where other direct methods packages failed.

Detection of electron density for catalytic hydrogen atoms on an active site histidine of human aldose reductase was reported from $0.66\text{\AA}$ data (A. Podjarny, Strasbourg).

The $0.8\text{\AA}$ resolution studies of pentaerythritol tetranitrate reductase uncovered significant errors in a previous $1.5\text{\AA}$ structure report (P. Moody, Leicester).

Hot and Cold Structures. J.A.K. Howard (Durham) described low temperature studies of electron densities, phase transitions and unstable samples. Below 100K, disorders can often be resolved, and different ordering at low temperatures can manifest itself in phase transitions. Howard described the variety of devices available at neutron sources including a high pressure device that uses nitrogen gas at 5 kBar.

R. Morris (St. Andrews) described 'Unusual Properties of Zeolites Studied by Single Crystal Synchrotron X-ray Diffraction'. Using 20 x 20 x 5 micron crystals, the structure determination of STT-SSZ-23 showed that it is essentially pure silica, with 9 atoms in one ring and 7 in the other, rather than the even-numbered rings expected.

P. Coppens (SUNY, Buffalo) combined crystallography, photochemistry, and laser irradiation and diffraction in the study of 'Light Induced Metastable States and Transient Species'. At liquid helium temperatures metastable species have essentially infinite lifetimes, and different species can be isolated by changing the wavelength of the laser or the temperature, and the population of excited states can be raised to a pseudo steady state.

S. Parsons (Edinburgh) described low temperature and high pressure crystallization of samples which are gases or liquids at ambient temperatures. Crystal growth is achieved by establishing a stable solid-liquid equilibrium in a capillary, and cooling slowly to induce crystal growth.

Diffraction at the Edge. G. Rosair (Heriot-Watt) outlined how absorption edges contain information on the local electronic and magnetic structures of crystalline, amorphous or liquid materials. The use of EXAFS and XANES to elucidate the number and type of atoms surrounding metals was expanded. Examples of studies of excited states, covalency in metal-ligand bonds, and the enhancement of the catalytic activity of Pt by Ge were presented. M. Helliwell (Manchester) described applications of anomalous dispersion in chemical crystallography and the essential features of phosphate-based molecular sieves. (*Sandy Blake*)

Why Industry Uses Crystallography. R. Copley (GlaxoSmithKline Pharmaceutical, Harlow, Essex) described how single crystal studies are used at all stages of the Drug Discovery Process (molecular conformation and absolute configuration studies of proteins, drugs and their complexes) in conjunction with powder diffraction, solid state NMR, IR and Raman spectroscopy.

X-ray diffraction analysis being used in the minerals industry from extraction, separation, blending, storage and transport was described by N. Elton (Exeter Advanced Technologies). Typical challenges to quantitative XRD analysis are: (a) complex mixtures, (b) solid solution polymorphs, (c) poor crystallinity, (d) low concentration, and (e) preferred orientation. In the cement industry these problems are compounded by lack of standards and peak overlaps in XRD patterns. Some European plants are using on-line XRD for clinker analysis. In the aluminum industry too, bauxite processing suffers from lack of good standards, variable crystallinity and preferred orientation, requiring the XRD/XRF mass balance approach. (*David Rendle*)

Future Powder Diffraction. Recent developments in the Powder Diffraction File (PDF) (J. Faber, ICDD), Line Broadening Analysis (R. Delhez, Delft U.), and Rietveld Refinement including dynamic studies and protein application were reported (J. Cockcroft, Birkbeck College). Technical presentations from Philips and Bruker AXS wound up the session. (*Stephen J. Maginn*)

Coherence Workshop. D. Laundy (CCLRC Daresbury) defined lateral and temporal coherence and described how both could be measured via synchrotron radiation. B. Tanner (Durham) discussed measuring coherence length using grazing incident surface scattering to determine near surface density. For the technique to be successful the coherence level needs to be larger than the grain size of the sample. Because the 'wobble' of the synchrotron electron beam decreases, the coherence of the x-ray beam experiments that are carried out over large time scales have a reduced coherence length. M. Hart

stated that coherence length is a function of sample, set-up, and apparatus, and recommended *Optical Physics* by Lipson & Lipson as the best reference.

Basic Powder Diffraction Workshop. The Basic Powder Diffraction Workshop consisted of three half-day sessions for people new to the field of powder diffraction. The sessions included a well-balanced introduction to the principles of crystallography, powder sample preparation, and sample identification. (Jo Jutson)

CRYSTALS Workshop. A CRYSTALS workshop was held at which R. Cooper explained the design aims behind the current release and gave a real-time demonstration of a structure analysis. Software aims to provide tools which will enable a synthetic chemist to make a reasonable attempt at performing a structure analysis on data that they have either collected themselves, or which has been provided for them. D. Watkin presented an overview of some of the crystallographic model building, manipulation, and analysis tools in CRYSTALS. Horst Puschman gave a demonstration of a structure archiving and tracking suite that assists in record keeping (Richard Cooper)

AWARDS AND PRIZES

Crystallography prize to J. R. Schneider



Jochen R. Schneider

The European Crystallographic Assn presented the second European Crystallography Prize to Jochen R. Schneider of the HASYLAB at DESY, Hamburg, Germany, for his pioneering work on the application of gamma-ray spectroscopy, his high energy synchrotron radiation studies, and his recent involvement in the development of the free-electron laser.

The European Crystallography Prize, which includes a monetary award as well as a certificate of recognition, was presented during the Opening Ceremony of the 20th European Crystallographic Meeting in Krakow, Poland, August 25-31.

Members of the European Crystallography Prize Committee: I. Olovsson (Coordinator), U. of Uppsala, Sweden; R. Boese, U. of Essen, Germany; M. Glazer, U. of Oxford, UK; B. Kamenar, U. of Zagreb, Croatia; Å. Kvik, European Synchrotron Radiation Facility, Grenoble, France; X. Solans, U. of Barcelona, Spain; A. Yonath, Weizmann Inst. of Science, Israel.

Prof. Schneider was born in Burgstädt, Saxony, Germany and studied Physics in Hamburg after an education as an electrical engineer. He did his PhD under the direction of H. Maier-Leibnitz at the Inst Laue-Langevin in Grenoble, France. His work on gamma-ray diffractometry and Compton scattering was performed at the Hahn-Meitner-Inst in Berlin, the synchrotron radiation work at DESY-HASYLAB in Hamburg. Prof. Schneider is presently Head of HASYLAB and Director of Research for Synchrotron Radiation and Free-Electron Lasers at DESY.

AWARDS AND PRIZES

Congratulations to...



J. Kuriyan

• **Pamela J. Bjorkman**, Howard Hughes Medical Inst. (HHMI) and California Inst. of Technology, Pasadena; **Russell J. Hemley**, Carnegie Inst. of Washington, Washington, D.C.; and **John Kuriyan**, HHMI and Rockefeller U. are among the 73 new members of the The Nat'l Academy of Sciences (NAS).

(*Science*, Vol. 292 11 May 2001)

• The 2001 Remsen Award of the American Chemical Society, Maryland Section was presented to **Ad Bax**, biophysical nuclear magnetic resonance spectroscopy section chief of the laboratory of chemical physics in the Inst of Diabetes & Digestive & Kidney Diseases at the Nat'l Inst. of Health (*C & EN*, June 18, 2001)

• **Stanko Popovic**, Physics Dept, Faculty of Science, U. of Zagreb, received the Annual State Award for 2000 for his scientific achievements in Powder Diffraction.

• **Ian A. Wilson** of the Scripps Research Inst. ranks fifth among the ten Top-Funded Basic Research PIs with respect to grants from the Nat'l Inst of Health. He holds grants worth over \$5.6 million for work in structural genomics. Most members of the top ten yearn for more time in the lab, but say they're driven to seek more research funding by a surfeit of ideas, as well as the trend toward big biology. (*Science*, 15 June 2001, Vol. 292)

• **Jerry L. Atwood**, Curators' Professor and chairman of the dept. of chemistry at the U. of Missouri, Columbia, has received the 2000 Izatt-Christensen Award in the area of Macrocyclic Chemistry. Atwood has made significant contributions in fields such as supramolecular chemistry, X-ray crystallography, organoaluminum chemistry, and green chemistry. The award is given annually by IBC Advanced Technologies, American Fork, Utah. (*C&EN*, May 7, 2001)

• Oxford Instruments Superconductivity has appointed **Frank Trundle** as marketing director. Mr Trundle joins the executive team to build on their current success, and develop a strong marketing strategy to help meet the challenges within existing and emerging markets.



G. Sheldrick

• The Royal Society elected 42 new members on May 14, including crystallographers **A.G.W. Leslie** (MRC Lab of Molecular Biology, U. of Cambridge) for revealing a number of biologically important structures in atomic detail, and **G.M. Sheldrick** (The Inst. for Inorganic Chemistry, U. of Göttingen, Germany) for major contributions to methods and his chemical X-ray crystallography computer program, SHELX. (*C & EN*, June 18, 2001)

MISCELLANY

Peace talk

The continuing overwhelming focus on weapons and military technology ignores history and prevents interdependence. The cell phone and Internet will likely do far more to ensure future peace than any gadgets developed at seemingly unlimited expense by scientists working on secret defense projects. The biggest contributions that the scientific community can make for world peace are to encourage young scientists and engineers to shun military work; to focus on the challenges in energy, civilian communication, and the environment; and to promote leaders who recognize these priorities.

Eric W. McFarland

U. of California, Santa Barbara

from Physics Today (July 2001)

NOTICE

Second hand generator needed in Cuba

Dear colleagues, our old high voltage tube-based generator from the GDR has definitely died albeit our care to have it working. This generator used to feed an x-ray tube for a texture and a double crystal goniometer, the only ones available in Cuba. Our Bragg-Brentano goniometer is presently working very well with an ENRAF NONIUS Diffractist 581 generator donated by Utrecht U., which encourages us to ask for help from our researcher colleagues. Making the aforementioned goniometers operational will benefit not only Havana U., where we work, but also the Cuban materials science community, taking into account the limited availability of x-ray diffraction equipment in the country.

A. Gómez, ariel@lae.ff.oc.uh.cu / ariel_g_g@yahoo.com, U. de la Habana, San Lazaro y L, Vedado, Havana, Cuba

NOTICE

Oxford Diffraction Limited

Oxford Diffraction Limited, a new company resulting from an alliance between Oxford Instruments plc and Kuma Diffraction, an X-ray diffraction equipment manufacturer from Wrocław, Poland will focus on X-ray crystallography and structural proteomics. Proteomics sets out to define the tens of thousands of proteins in the human body. Oxford Diffraction will use the new investment from TTP Ventures for further developments in detectors, X-ray sources, and cryogenics and to strengthen its distribution network. TTP (The Technology Partnership) Ventures is a Cambridge-based company formed in 1998 as the venture capital arm of TTP Group plc. TTP Ventures manages a £35m fund, which focuses on UK and European innovation technology businesses at an early phase.

For information contact: P. Loeffen, FAX: 44 01235 528 005.

MISCELLANY

Anything they can do...

A mass spectrometry technique for identifying folding patterns of proteins that is potentially faster and requires less sample than x-ray crystallographic or NMR structural methods has been developed by Irwin D. Kuntz who believes the time needed to determine the fold family of a protein can be reduced to one week and the amount of protein required reduced to less than 10 µg. The technique may provide sufficient resolution to elucidate function, conformational states, macromolecular interactions, and leads for the design of protein mimetics.

C & E News, June 5, 2000

MISCELLANY

Structure and drug design

Several marketed drugs, including protease inhibitors used in the treatment of AIDS, have been designed using the 3-D x-ray structure of a target protein as a template for structure based antagonist design. Current and future developments in the high-throughput expression, purification, crystallization, and x-ray structure determination of large numbers of proteins promise to yield many more successes in the future.

M.E. Wolff, President, Intellepharm Inc., C & E News, Sept. 18, 2000.

MISCELLANY

Bernal on collaboration

J.D. Bernal said 'we have in the practice of science the prototype for all human common action. The task which scientists have undertaken – the understanding and control of nature and of man himself – is merely the conscious expression of the task of human society. The methods by which this task is attempted, however imperfectly they are realized, are the methods by which humanity is most likely to secure its future. Scientists have learned consciously to subordinate themselves to a common purpose without losing the individuality of their achievements. Each knows that one's work depends on that of one's predecessors and colleagues, and that it can only reach its fruition through the work of one's successors. Scientists collaborate not because they are forced to by superior authority or because they blindly follow some chosen leader, but because they realize that only in this willing collaboration can one's goals be achieved. Facts cannot be forced to our desires, and freedom comes by admitting this necessity and not by pretending to ignore it'.

MISCELLANY

Are crystallographers not physicists?

In the March 2000 issue of *Physics Today*, N. David Merman pleads for elegance in Physics and instructs crystallographers in the correct way to describe and explore aperiodic and quasicrystals. Distressed at crystallographer's failure to appreciate his 'beautiful and illuminating shift from the structure of the crystal to the structure of its diffraction pattern', Merman concludes that crystallographers are 'not physicists' and 'not interested in electronic properties'.

Physics Today, March 2000, 11-12.

Ed.: He certainly isn't reading my mail.

MISCELLANY

What good are synchrotrons?

Nobel Laureate physicist Pierre Gilles de Gennes, College de France disparaged the value of synchrotron radiation (*Science*, Vol 287 P. 1733) saying 'if we are speaking of major unexpected discoveries made during the last 5 years, the result is practically nothing'. In response, Roger Fourme, head of Biology at LURE, provided a list of proteins whose crystal structures were determined using the facility. de Gennes opinion does not appear to be widely shared as new and better synchrotron sources and additional beam lines continue to be added around the globe.

MISCELLANY

Scientists for sale?

The Int'l Congress of Scientific Unions (ICSU) sponsored a World Conference on Science (WCS) that was attended by a number of members of the Third World Academy of Science (TWAS). A report on the WCS was published in the ICSU newsletter. In his report, Muhammed Akhtar, U. Southampton, UK, a founding fellow of TWAS, stated 'I am afraid that more and more scientists are selling their souls to corporate concerns in return for adequate resources to pursue their research, particularly scientists from developing countries where this trend promises to render its most adverse consequences'.

MISCELLANY

Reflections on a mature discipline

Now we live in a technological age, computers of unprecedented capacity and speed, and almost instantaneous communication with colleagues anywhere in the world. But I have a question: When do we have time to think? One can only applaud the improved efficiency of modern equipment, but the frenetic pace of so much research today results in undue stress that can be detrimental in human terms. In a recent book on the genetic basis of cancer, I came across an extreme example of research under pressure. The author cites the case of a crash effort involving 24 hour days by one group to beat a competing group to a deadline. Such an extreme course of action seems to me unworthy of science and has led to some questionable ethics. A saying I encountered years ago suggests a useful response to a competitive situation: 'Compete with your possibilities and not with your neighbor'.

Lyle H. Jensen's Buerger Award address, July 24, 2000

BOOK REVIEW

Just published

***International Tables Volume F: Crystallography of Biological Macromolecules*, edited by Michael G. Rossmann and Eddy Arnold, Kluwer Academic Publishers, ISBN 0-7923-6857-6, 832 pp, 2001, \$275 for institutions, \$137.50 for individuals. (www.iucr.org/iucr-top/it/itf/itf.html)**

Crystallography of biological macromolecules was commissioned by the IUCr in recognition of the extraordinary contributions that knowledge of macromolecular structure has made, and will make, to the analysis of biological systems, from enzyme catalysis to the workings of a whole cell, and to the growing field of structural genomics. The volume covers all stages of a crystallographic analysis from the preparation of samples using the techniques of molecular biology, through crystallization, diffraction data collection, phase determination, structure validation and structure analysis.

Although the book is written for experienced scientists, it is recognized that the modern structural biologist is more likely to be a biologist interested in structure than a classical crystallographer interested in biology. Thus there are chapters on the fundamentals, history and current perspectives of macromolecular crystallography, as well as the availability of useful programs and databases including the Protein Data Bank. Each chapter is written by an internationally recognized expert.

Table of Contents: 1. Introduction 2. Basic Crystallography 3. Techniques of Molecular Biology 4. Crystallization 5. Crystal Properties and Handling 6. Radiation Sources and Optics 7. X-ray Detectors 8. Synchrotron Crystallography 9. Monochromatic Data Collection 10. Cryocrystallography 11. Data Processing 12. Isomorphous Replacement 13. Molecular Replacement 14. Anomalous Dispersion 15. Density Modification and Phase Combination 16. Direct Methods 17. Model Building and Computer Graphics 18. Refinement 19. Further Experimental Information 20. Energy Calculations and Molecular Dynamics 21. Structure Validation 22. Molecular Geometry and Features 23. Structural Analysis and Classification 24. Crystallographic Databases 25. Macromolecular Crystallography Programs 26. A Historical Perspective.

***Handbook of Hydrothermal Technology: Technology for Crystal Growth and Materials Processing*, K. Byrappa and M. Yoshimura, William Andrew Publishing, ISBN 0-8155-1445-X, 875 Pages, 2001, \$175.**

A single source for understanding how aqueous solvents or mineralizers work under temperature and pressure to dissolve and recrystallize normally insoluble materials, and decompose or recycle waste material.

Quartz, zeolites, gemstones, perovskite type oxides, ferrites, carbon allotropes, complex coordinated compounds and many other products are now produced using hydrothermal technology. This handbook gives a detailed description of all the major hydrothermal methods.

The full table of contents and ordering information is available at www.williamandrew.com/jw0501.html.

OBITUARY

José Tormo (1960-2001)



José Tormo, who played a major role in the development of structural biology in Spain, died of cancer in Barcelona on June 21, 2001. He graduated in Biology from the U. of Barcelona and was the first to achieve a doctorate in Protein Crystallography in Spain. He spent eight years in postdoctoral positions: in the laboratories of T. Steiz (Yale, New Haven, USA), D. Stuart and Y. Jones (Oxford, UK) and R. A. Mariuzza (CARB, Rockville, USA). These postdoctoral years resulted in more than twenty five publications including two *Nature* papers of which he was first author. His main achievements were in the field of structural immunology with results such as the recognition of CD8 by MHCs that can be found in textbooks of the field.

José Tormo had a passion for research that allowed him to overcome the inertia of the Spanish academic system contributing decisively to prove, both to scientists and administrators alike, the need that the country had for crystallographic research in Structural Biology. He obtained a permanent position in the Spanish Research Council (CSIC) and, as a member of the National Center of Biotechnology (CNB), was initiating Protein Crystallography in the Madrid Autonomous U. (UAM). He was a remarkable young scientist communicating greatness and strength to all those who met him and had the privilege of working with him. His untimely passing will undoubtedly affect the future of structural biology in Spain.

Colleagues, collaborators and friends of José Tormo will gather at a scientific meeting honoring him on November 19-20th, 2001 at the CNB in Madrid. Information concerning his life achievements and the meeting can be found at <http://ibmb.csic.es/J.Tormo>.

Ignacio Fita and Celerino Abad-Zapatero

OBITUARY

G.N. Ramachandran (1923-2001)

G.N. Ramachandran, an outstanding figure in the field of protein structure, passed away at the age of 78, on April 7, 2001, in Chennai (the erstwhile city of Madras), India. Ramachandran (G.N.R. or Ram to his friends and associates) was the founder of the 'Madras school' of conformational analysis of biopolymers. His discovery of the triple helical structure of collagen in 1955 and his analysis of the allowed conformations of proteins through the use of the 'Ramachandran plot' rank among the most outstanding contributions in structural biology, along with Pauling's description of the α -helix and Watson and Crick's discovery of the double helical structure of DNA. Ramachandran became a professor of physics at the U. of Madras at the age of 29 and set up a fully equipped modern X-ray crystallographic lab at Madras. The IUCr awarded the 5th Ewald Prize to Ramachandran for his outstanding contributions to the field of crystallography. Specifically, the award was 'in the area of anomalous scattering, ...in the analysis of the structure of fibers, collagen in particular, and, foremost, for his fundamental works on the macromolecular conformation and the validation of macromolecular structures by means of the Ramachandran plot'.

Ramachandran was a man of many talents. He was interested in classical Indian and Western Music, as well as in the philosophical systems of India and the West. During his brilliant and illustrious academic career, the number of awards, medals and citations conferred on him are too numerous to be listed. As a man who breathed science, and in terms of his lasting contributions to structural biology, Ramachandran belonged to the same intellectual class as Srinivasa Ramanujan in mathematics and Subrahmanya Chandrasekhar in astrophysics. To know more about the life and times of Ramachandran, the reader is referred to *Ramachandran – a biography*, by R. Sarma. Ramachandran's death is a grievous loss not only to his family members but also to the Indian and International scientific community and marks the passing away of a brilliant mind with great passion for structural biology. His scientific contributions will remain as monuments to his superb intellect.

E. Subramanian, Nature Structural Biology, Vol. 8 No. 6 June 2001

OBITUARY

Clifford G. Shull (1915-2001)

MIT Professor Emeritus Clifford G. Shull died on March 31, 2001 aged 85. He was co-recipient of the Nobel Prize in physics in 1994, awarded for his pioneering work in neutron scattering. Prof. Shull started work in 1946 at what is now Oak Ridge Natl Lab. He teamed up with the late Earnest Wollan, and for the next nine years they explored ways of using the neutrons produced by nuclear reactors to probe the atomic structure of materials. In his opinion the most important problem he worked on at the time dealt with determining the positions of hydrogen atoms in materials.

As he refined the scattering technique, Prof. Shull studied the fundamental properties of the neutron itself. He also initiated the first neutron diffraction investigations of magnetic materials. This yielded information about the magnetic properties of materials at the atomic level, opening up an entirely new field of study. Shull's awards include the Buckley Prize, which he received from the American Physical Soc. in 1956, and election to the American Academy of Arts and Science (1956) and to the Natl Academy of Sciences (1975). In 1993 he received the Royal Swedish Academy of Sciences' Gregori Aminoff prize for his 'development and application of neutron diffraction methods for studies of atomic and magnetic structure of solids'.

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OBITUARY

Jan Kroon (1937-2001)



Jan Kroon, Professor in Crystallography at Utrecht U., The Netherlands, died unexpectedly on May 3, 2001 due to heart failure. Jan was born July 18, 1937 in Oudschoonebeck and received his PhD in 1964 on a thesis entitled 'The Crystal Structures of Potassium Mesotartrate Dihydrate and Tartronic Acid' with J.M. Bijvoet. Interest in tartrates and the investigation of derivatives arose from the work of Bijvoet, Peerdeman and van Bommel on the determination of the absolute configuration of Sodium Rubidium-*d*-Tartrate published in 1951. Much of Jan's subsequent work, with over 225 published papers, had its roots in his PhD work. Hydrogen bond interactions were his lifelong interest. Together with his former supervisor, Jan Kanters, and Loes Batenburg, who later became his wife, many studies were published on carboxylic acids and sugars. Jan attended and often organized regular meetings of the hydrogen-bond research community. Interest in Direct Methods, used in solving the tartronic acid structure, was shared with his colleague and friend, Henk Krabbendam (deceased 1995). Together, as members of the small theoretical Direct Methods community, they published many innovative papers. When Jan succeeded Peerdeman as head of the department in 1985, it was a typical small molecule research group with a staff having expertise in various fields. It was clear to him that in the future, (funded) challenges in crystallography would be mainly in bio-crystallography. It is here that his organizational qualities made a seamless transition possible to bio-crystallography. Through Jan's efforts, traditional crystallography was sustained within the National Facility for Single Crystal Studies. Although Jan spent all of his scientific life in Utrecht, he developed an impressive international network that brought many postdocs to Utrecht. He always encouraged young students. We have lost a leader and a father figure who created an excellent work environment for his staff and students.

Ton Spek