

INTERNATIONAL UNION OF CRYSTALLOGRAPHY

IUCr Newsletter

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Collected archival edition

Original article text and available illustrations

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LETTER FROM THE PRESIDENT

Letter from the President



First of all I wish you a happy and prosperous 2001. According to some this is the real first year of the century, as important as 2000 itself. On the other hand, through our involvement with computers we start counting at 0 so for us 2001 may not be special at all. However, for the IUCr it will be special as we will have the first back issues electronically available for subscribers to our journals. The number of these will then quickly increase until all are available, unleashing the real power of **Crystallography Journals Online**. Also it is the year that we prepare for the General Assembly in 2002 and we hope all of you will participate in this process by coming up with initiatives, suggestions and nominations. Just a comment as so many of you have approached us: the Executive Committee is aware of the concerns about the site of the Congress and General Assembly and is working on it.

Whereas at the start of the last century science was a minor subject in society, now it has a much different stature. For instance, in 1900 diffraction was still to be discovered and now the number of X-ray diffractometers is numerous. Nevertheless, as far as I can see, the position of science is no longer changing positively. Money, as we all know, is necessary for mankind to use imagination and skills to make new discoveries, develop new products etc. But lately it looks like money is being used less for this purpose and is more and more just focused on itself. Changes in society are dynamic processes and all of us have an influence, so let us try to do what we can to facilitate imagination and skills to continue playing a leading role.

As you may know, the IUCr is member of the International Council for Science (ICSU), comprising 26 international, single-discipline Scientific Unions and 126 other bodies. ICSU closely works together with UNESCO. I call your attention to the web site of UNESCO and, in particular, to the Newsletter about the follow-up of the **1999 World Conference on Science** at http://www.unesco.org/science/wcs/newsletter/wcs_newsletter.shtml, where you will find very interesting information. There is also a section about the International Forum of Young Scientists, a continuous platform to discuss general issues and challenges to science. I cite their main conclusions:

- Scientists should increase their responsibility to inform the public openly about research and its wider implications and therefore learn communication skills;
- Science education at all levels should be strengthened and scientists should collaborate with educators;
- Education should present science in a cross-disciplinary manner;
- Ethical aspects should be a part of all scientific undertakings and a special focus on ethics should be included in all education programmes;
- Scientists should take full responsibility to provide help to the scientific communities in less developed countries and should urge their governments to support long-term grants for fundamental research to maintain sustainable growth;
- Scientists should assume increased responsibility for environment and development programmes;
- Young scientists should participate in decisions made about science.

Henk Schenk
schenk@chem.uva.nl

EDITORIAL

Editorial



I wish to express the appreciation of the Executive Committee of the IUCr to the people in dozens of countries throughout the world who devote time, energy and financial support to assist in the distribution of the *IUCr Newsletter* in their part of the world. These individuals and, in some cases, the organizations they represent are listed in the table. These people maintain mailing lists in their country and see to it that the *IUCr Newsletter* is distributed within their country in a timely fashion. They have expressed a willingness to expand the distribution of the *IUCr Newsletter* to include new crystallographers and other scientists and friends of physical sciences who are interested or should be interested in the world of crystallography and the activities of the IUCr. If you know of individuals in those countries who are not receiving the *IUCr Newsletter* and could benefit from doing so (including yourself) please send names and addresses directly to the appropriate distributors listed to the right. If you are in a country that does not benefit from the assistance of a local or regional distributor, and you are willing to assist in distribution in your country, either personally or by arranging with a national society to implement such a distribution, please contact me.

The Crystallographic Society of Japan distributes 1000 copies of each issue to its members. B. W. Skelton includes some issues of the *IUCr Newsletter* with the mailing of the Newsletter of the Australian crystallographers. The most recent additions to the list are Cuba and Portugal. The service provided by the crystallographers usually results in more timely delivery as well as permitting inexpensive wider distribution.

This is also a good time for me to express my appreciation to the editors of the Newsletters of the British Crystallographic Association (Kate Crennell), the American Crystallographic Association (Judy Flippen-Anderson and Ron Stenkamp), and the Society of Crystallographers in Australia and New Zealand (Brian Skelton) and the Commission on Powder Diffraction (rotating editors recently include Bill David and Lachlan Cranswick) for generously allowing me free use of material in their publications for inclusion in the *IUCr Newsletter*.

Bill Duax

duax@hwl.buffalo.edu

LETTER TO THE EDITOR

Women in crystallography

Dear Bill

On behalf of all women crystallographers, I want to thank you for the recent IUCr Newsletter featuring Dorothy Hodgkin. As the only surviving member of the group you referred to as being 'in the early days of crystallography' I feel honored to be included among them. Those in that group all knew each other well. I visited Carolyn MacGillavry and Dorothy Hodgkin in their homes and Kathleen Lonsdale stayed in my home when she came to this country.

Kathleen Lonsdale wrote to me about a visit from Dorothy Hodgkin when she was in the hospital, terminally ill with cancer of the bone marrow. She said that when she asked Dorothy what bone marrow did, Dorothy replied, "I'm afraid it does rather a lot". I can just imagine the quiet way in which Dorothy would say that.

It is to the credit of all crystallographers that women are welcomed in their field more than in other science fields, with the possible exception of astronomy. What matters in any field is that the person comes to it with interest and competence. Gender is irrelevant.

Elizabeth Wood
New Jersey, USA

LETTER TO THE EDITOR

Dorothy Hodgkin

Dear Bill

I enjoyed reading the recent newsletter. John Robertson's article captured the flavour of Dorothy very well. I recall an incident in Oxford in which Dorothy had just got into her car and was sitting with the door open carrying on a conversation with John who, in order to get down to Dorothy's level, was on his knees on the sidewalk in a position that was more reminiscent of worship! Unfortunately, I had no camera handy.

I. David Brown
McMaster U., Canada

LETTER TO THE EDITOR

Reuse of books and journals

Dear Sir

In Vol. 8#2 of the *IUCr Newsletter*, I read [the note from Bill and Kirsten Streib](#) on the Letters to the Editor page about the volumes of *Acta Cryst.* and the basic X-ray crystallography texts which they wished to offer to the public rather than recycle.

Since retirement I should also like to dispose of many of my basic crystallography books for which I have no further use. I am enclosing a list of them in the hopes that potential recipients may be found via Newsletters and websites.

Ethel J. Watts

California, USA

Dear Mrs Watts

I feel certain that your collection of basic crystallographic books would be very welcome in many laboratories and universities in countries that are just beginning to develop crystallographic capabilities, particularly in Africa, Asia and Latin America. Please ship your books to the ACA/IUCr office in Buffalo for storage pending distribution.

Bill

The Streib *Acta* collection is being shipped to Jordan, and three boxes of Mrs. Watts' books are now in Buffalo

MISCELLANY

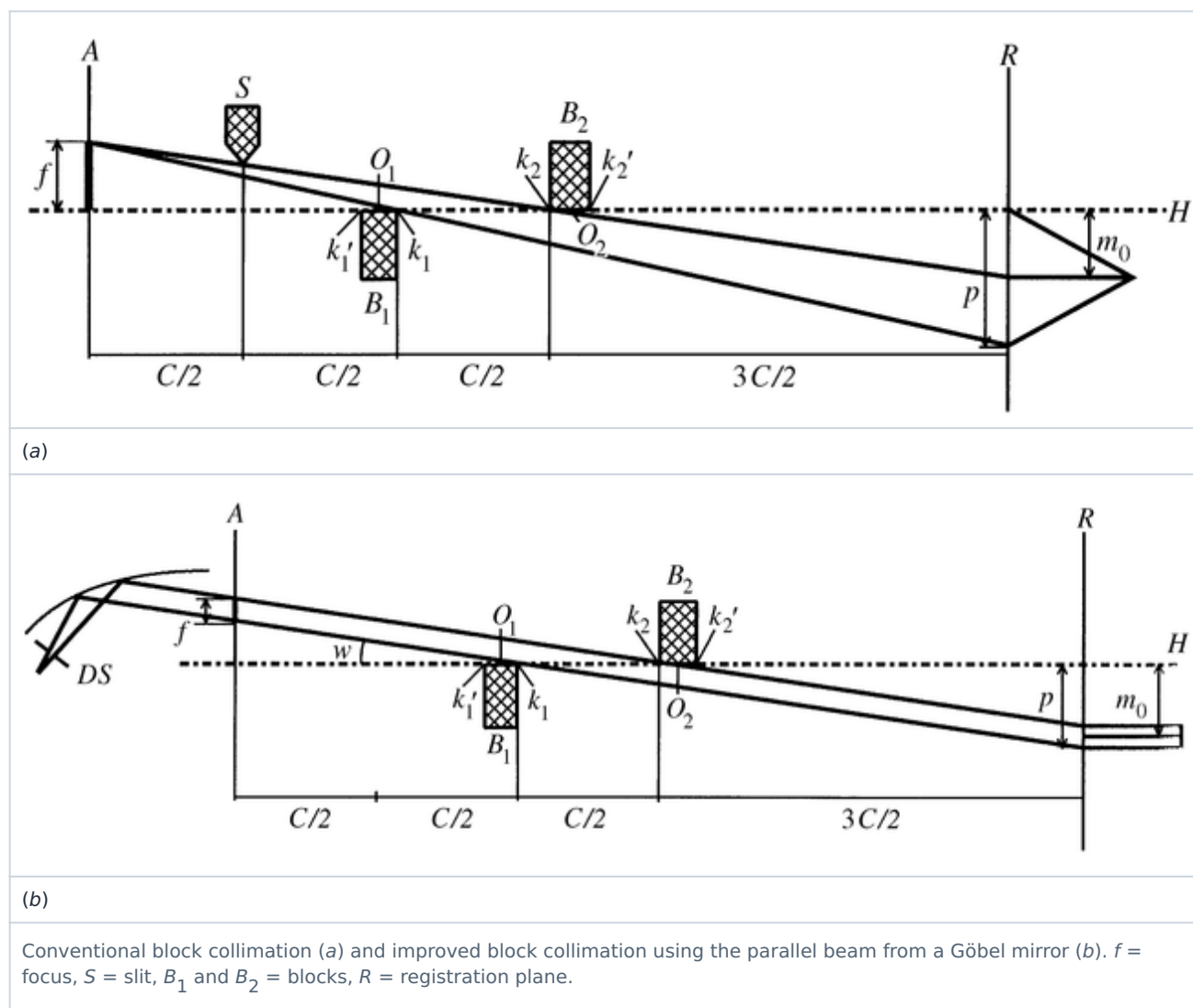
Farewell to Arnold



It is with sorrow that we report the death of Arnold Beevers on January 16, 2001. Anyone who ever sang “My Bonny Lies Over the Ocean” under his delightful direction is forever reminded of the very Bonnie Arnold when they hear that song. Arnold is seen here in fine fettle at the J. Monteath Robertson Symposium in Glasgow with (left to right) J. Trotter, R. Bryan, Arnold, S. Abrahams, M. Rossman, J. Dunitz, and N. Isaacs.

New apparatus combination creates outstanding performance of Kratky SAXS systems

J. Appl. Cryst. (2000). **33**, 869-875 [doi:10.1107/S0021889800000881]



Small-angle X-ray scattering (SAXS) is a powerful technique to study electron density fluctuations on a nanometer scale. The essential prerequisite for SAXS measurements is an X-ray beam of low divergence and high intensity. For a long time, with conventional X-ray sources, these requirements have been met to some degree only by using long-slit collimation geometry, realized for example with the widely used Kratky camera (Kratky, 1982). Nowadays, technical developments such as rotating-anode X-ray generators, two-dimensional position-sensitive detectors, and in particular, new X-ray optics like parabolically bent, graded multilayers ('Göbel mirrors', Schuster & Göbel, 1995), allow pinhole cameras to be built that meet or even exceed the performance of classical long-slit systems in terms of resolution and primary beam intensity. Pinhole cameras overcome the most serious drawbacks of long-slit systems, namely the slit-smearing of the signal and the loss of information for anisotropically scattering samples. One might thus even ask why long-slit systems are still of interest today.

In this context, Bergmann, Orthaber, Scherf & Glatter [*J. Appl. Cryst.* (2000). **33**, 869-875] have recently reported on a significant improvement of long-slit systems by taking advantage of the above-mentioned technical developments (Göbel mirrors) for the Kratky camera. Using a parallel, monochromatic X-ray beam from a Göbel mirror, a slight modification of the Kratky block collimation system leads to an intensity gain of a factor of four without loss of resolution. This is simply due to the fact that in contrast to the classical system the whole focus illuminates the registration plane R and that the parallel beam results in a rectangular instead of a triangular beam profile (see figure). Together with the advanced characteristics of the Göbel mirror (15-20 mrad angular acceptance from the source) and the use of a rotating-anode X-ray generator, a total intensity gain of a factor of about 40 in comparison with a conventional Kratky system was reached by the authors. In terms of primarybeam intensity, this would nearly be comparable with some SAXS instruments on second-generation synchrotron radiation sources (bending magnets). This remarkable gain puts Kratky cameras again on a competitive basis for laboratory SAXS instruments, as long as fully isotropic scattering systems are concerned. As quite a significant number of SAXS applications deal with solution scattering (e.g., particles or polymers in solution), the improved Kratky camera can be expected to cover a wide field of applications with up to now unmatched primary-beam intensity.

References

Kratky, O. (1982). *Small Angle X-ray Scattering*, edited by O. Glatter and O. Kratky. London: Academic Press.

Schuster, M. & Göbel, H. (1995). *J. Phys. D Appl. Phys.* **28**, 270-275.

Oskar Paris, Metal Physics Inst., U. of Leoben

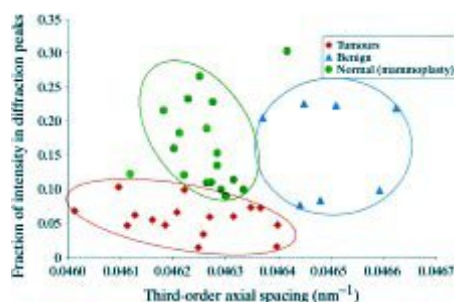
Erich Schmid Inst., Austrian Academy of Sciences, Leoben, Austria

Breast cancer diagnosis using scattered X-rays

***J. Synchrotron Rad.* (2000) **7**, 348-352 [doi:10.1107/S0909049500009973]**

Breast cancer is a leading cause of cancer deaths in women and the lifetime risk of a woman developing breast cancer is as high as 10-13% in some western countries. Screening mammography is widely used in developed countries for the detection of tumors as early detection offers the best hope of treatment to improve life expectancy. Currently diagnosis is based on the so-called triple assessment - a combination of physical examination, mammography using X-rays and/or ultrasound, and fine needle aspiration cytology or core-biopsy. The histopathological assessment relies on alterations to cellular morphology and tissue architecture. Although triple assessment is effective in detecting most malignant lesions, its suboptimal specificity means that in some cases open biopsy surgery is required to exclude malignancy. There is therefore a considerable interest in developing diagnostic methods that are specific for the presence of malignant breast tissue.

Using the Daresbury SRS at beamline 2.1, Lewis, Rogers, Hall, Towns-Andrews, Slawson, Evans, Pinder, Ellis, Boggis, Hufton & Dance [*J. Synchrotron Rad.* (2000). **7**, 348-352] carried out synchrotron X-ray diffraction studies of core-cut biopsy specimens taken from normal breast tissue, from benign tumors and from malignant tumors. They found that the diffraction patterns obtained from the three types of specimen showed significant differences in the spacing and scattered intensity of a prominent axial peak (see below). This peak arises from the collagen fibrils in the connective tissue of the breast and is associated with the regular packing of the tropocollagen molecules in the fibril. The intensity of the axial peaks is very sensitive to the degree of order in the orientation and packing of the collagen fibrils, and as might be expected, the disruption of the connective tissue associated with malignancy reduces the intensity of these peaks.



Scatter plot of the fraction of scattered intensity in the diffraction peaks versus the spacing of the third-order axial reflection. Ellipses are shown to illustrate the clustering.

An unexpected finding was that the measured values of the third-order spacings in benign and malignant tumors were grouped in separate clusters, as shown in the figure. The *D* period in tendon collagen is known to be sensitive to mechanical deformations, hydration and ionic environment, and further work would be required before these differences in spacings could be attributed with confidence to *in vivo* differences between the collagens.

This is an exciting development; the authors have succeeded in identifying a specific test for malignancy in breast tissue - the big challenge will be to develop a procedure suitable for routine use. In their closing remarks they state that they are currently considering the possibility of collecting diffraction data *in vivo*. This would have the great advantage of being non-invasive, but it is difficult to see how this could be achieved as the wavelengths of the X-rays used for diffraction studies are such that they will only penetrate a few millimeters into breast tissue before they are extinguished.

R.D.B. Fraser DSc, FAA, Noosa, Queensland, Australia

S.E. Fraser MB BS FASBP, Cairns Breast Cancer Screening Facility, Queensland, Australia

Authors' reply

The reviewers are certainly correct that the change in the collagen repeat spacing (the D spacing) could be explained by mechanical deformation or varying hydration levels. We were aware of this at the time of the experiment and took great care to maintain full hydration at all times and mounted all the samples in a similar manner. However, it is quite possible that this effect could arise from different stretching occurring for different tissues within the capillary tubes even though we did allow considerable time for relaxation between sample mounting and measurement. Nevertheless, we agree with the reviewers that there are multiple possibilities for our observation and intend to study this effect further. The absorption problem referred to by the reviewers would be reduced if the measurement were performed in a manner similar to a localized compression view in mammography. Furthermore, we would use a technique similar to our colleagues at Philips Research (Harding & Schreiber) who have shown it is possible to identify materials in baggage scanning systems with very few scattered photons. Our current ideas for bringing the technique closer to the clinic are based around modified mammography equipment operating at doses and wavelengths commensurate with a normal mammogram. Obviously there is a very long way to go before we could see this used in the clinic, and these are only ideas at present, but sometimes we need to dream.

Reference

Harding, G. & Schreiber, B. (1999). 'Coherent X-ray scatter imaging and its applications in biomedical science and industry,' *Rad. Phys. Chem.* **56**, 229-245.

IUCR JOURNALS NEWS

E is for electronic

- and exciting, and enterprising, and edifying, and perhaps even entertaining! But certainly ESSENTIAL



January 2001 will see the first issue of the IUCr's new electronic-only journal, *Acta Crystallographica Section E: Structure Reports Online*. It is being launched by the IUCr in collaboration with the Cambridge Crystallographic Data Centre (CCDC) to provide rapid and efficient publication of organic, metal-organic and inorganic crystal structures. As such it replaces the 'electronic papers' published in *Section C* recently, and seeks to build further on our experience with that medium.

The section editors are Bill Clegg (U. of Newcastle) and David Watson (CCDC).

A number of important enhancements are being made in the introduction of *Section E*:

- All communication between authors and the journal, from web-based submission through checking and review, to proofs and publication, is entirely electronic.
- Author services provided will include a new free easy-to-use CIF editor, and we are developing tools for incorporating output of popular word-processing and chemical drawing software in the submission, to make life easier: no more crude text-editing of CIFs!
- Published articles, available to readers in PDF and HTML formats, can include graphical illustrations of many kinds; even multi-media supplements are possible. Extensive supplementary material is also provided, including the complete CIF, diffraction data, and output of the automatic checking procedures.
- The length of textual comment by the author is flexible and it can be quite brief in many cases.
- Although the journal will not publish fundamentally flawed work, and is not going to act as a repository for poor quality results, acceptance criteria are more flexible than hitherto in *Section C*. The publication of more difficult and challenging structures is encouraged, with appropriate comment by authors on the problems encountered.
- Each published report (of a single structure) includes a set of 'key indicators' for precision, completeness, and validation of the results, enabling readers easily to make their own assessment of how these might be used appropriately in their own work.

So here is your chance to use a new and fast publication method and perhaps make an impression on those piles of unpublished structures that the world should hear about. Can we catch up on the flow of data from modern diffractometers?

For further information on the journal and how to submit and subscribe, see the IUCr web page for **Crystallography Journals Online**, at <http://journals.iucr.org>

Bill Clegg

Dept of Chemistry, U. of Newcastle, Newcastle upon Tyne, UK

IUCR JOURNALS NEWS

Journal Grants Fund

The International Union of Crystallography is pleased to announce the establishment of a Journal Grants Fund providing journals at reduced subscription rates. Grants are only open to Institutions taking out new subscriptions. In the first year of operation, only institutions that have not held a subscription in the past three years will be considered.

The granting procedure is determined by a Sub-committee of the Executive Committee, chaired by a member of the Executive Committee. The Sub-committee reports to the Executive Committee by providing a list of applicants in order of priority. The procedure is organised as a competition with some constraints such as:

- the grants should be distributed on a fair regional basis
- member countries have priority over non-member countries
- institutions publishing papers in IUCr journals receive preference

Grants will last 3 years and cover from 25% to 85% of the costs of subscriptions. Successful applicants will be invoiced for 15% to 75% of the list price. Each year 20 grants will be available for each of the six print journals and free online access is included. The first year starts with 60 grants for each journal: 20 with a duration of 1 year, 20 with a duration of 2 years, and 20 with a duration of 3 years. When the one-year and two-year grants expire, Institutions are eligible to re-enter the competition up to a maximum grant period of three years.

IUCr ACTIVITIES

IUCr Executive Report



IUCr Executive Committee (seated) M. Tanaka, H. Schenk, and S. Larsen, (standing) M. A. Carrondo, Z. Zhang, E. N. Baker, H. Fuess, J. C. A. Boeyens, M. J. Cooper, L. A. Aslanov, and W. L. Duax.

The IUCr Executive Committee met in Nancy, France August 22-24, 2000. Principal topics discussed were plans for the 19th Congress and General Assembly of the IUCr in Jerusalem, the launching of a new electronic journal, a program of partial grants to needy countries for IUCr publications (see Page 11), a major initiative to support the development of crystallography in African nations, and the appointment of the Ewald Prize Committee.

Excerpts from the minutes of the Executive Committee meeting

Review of Journals

It was noted that crystallization papers in *Acta D* were an important category and were well suited to electronic-only publication, analogous to electronic papers in *Acta C*. This would be discussed within the Commission on Journals with 2002 as a possible start date. The Managing Editor reported that IUCr journal publication times had been reduced significantly.

The Executive Committee agreed with a proposal from the Working Group on Journals of the Promotion Committee that plenary speakers at IUCr Congresses should be invited to write Lead Articles for inclusion in IUCr journals. The papers would be spread across the journals and could also be collected together on a CD-ROM. Recipients of the Ewald Prize should be encouraged to provide a Lead Article.

The Editor-in-Chief reported on progress with the electronic-only journal *Acta Cryst. Section E* that would be launched in January 2001.

World Directory of Crystallographers

The next edition of the Directory (WDC-11) would be published in early 2002. March 2001 is the deadline to update entries via the web.

Internet services

The Committee on Electronic Publishing, Dissemination and Storage of Information acts as the IUCr Web Editorial Board. Currently there are nine mirror sites for IUCr Web services (in Australia, France, Israel, Japan, Russia, South Africa, Sweden, Switzerland and the USA). The Crystallography Journals Online service was hosted by the Internet service provider UUnet. This site received about 19,000 requests per day.

Database linking

The Managing Editor planned to consult the Committee on Crystallographic Databases concerning the best way to link **Crystallography Journals Online** to appropriate databases.

The Executive Committee approved the publication of *Crystallography Across the Sciences* (CATS II) with Prof. Schenk as Guest Editor as the first issue of Acta A in 2002. Subscribers to other IUCr journals would receive on line access to this Special Issue.

Donations

W. E. Klee donated EUR 9,500 to the IUCr to be used to purchase volumes of *International Tables* for institutions in developing countries and countries of the former Eastern bloc.

The Executive Committee approved the Finance Committee recommendation that the allocation should be in the form of partial grants, similar to the model for the subscriptions initiative.

Ewald Prize

P. W. Coddling has agreed to chair the Selection Committee for the Sixth Ewald Prize, to be presented in Jerusalem in 2002.

Jerusalem programme

Chairs of Commissions and Secretaries of National Committees had been asked to supply recommendations for members of the Jerusalem Programme Committee. Draft Guidelines for IUCr Congress Programme Committees had been sent to members of the Executive Committee and the Chair of the Jerusalem Congress Programme Committee on June 30, 2000.

Crystallography in Africa

At the Glasgow meeting Prof. Boeyens reported that the Cambridge Crystallographic Data Centre (CCDC) agreed to provide free copies of the Cambridge Structural Database as part of the Crystallography in Africa project. The Executive Committee had agreed to underwrite the distribution costs for three years. Boeyens reported that matching funds had been found from the South African National Science Foundation (NSF). T. Koritsanszky runs the CCDC Affiliated Centre in South Africa.

The President reported that he and Prof. Boeyens would prepare a proposal for support for African Ph.D. students to work in a South African university. The Executive Committee approved the Finance Committee recommendation that support of up to USD 6,000 p.a. for five years be allocated for two students throughout their Ph.D. studies. Additional financial support might be obtained through the ICSU/ UNESCO grants program, the South African NSF, South African industry and charities such as the CCDC.

Audited accounts for 1999

The Executive Committee approved the audited accounts for 1999. The IUCr was operating at a loss of 7% of turnover owing to the strong pound and to significant expenditure on developing online services and preparation of new volumes of *International Tables*. The temporary operating loss is supported by the assets.

Status of membership

Ukraine was suspended for being in arrears for four years. Venezuela is three years and Argentina two years in arrears. The Executive Committee agreed that efforts should be made to attract new member

countries. The President and Prof. Fuess reported that Greece and Turkey had expressed interest in applying for membership.

The summer 2001 meetings of the Finance and Executive Committees will be held in Los Angeles, CA, USA, prior to the American Crystallographic Association (ACA) meeting, July 21-26, 2001. The Congress Programme Committee will meet July 17-19, 2001.

Mike Dacombe

IUCR ACTIVITIES

Electronic publishing pace accelerates

Members of the IUCr Commission on Journals convened meetings at ECM 2000 in Nancy and at the ACA meeting in St. Paul, Minnesota. Matters discussed and actions recommended included the following:

- *Acta Crystallographica Section E: Structure Reports Online* will provide for rapid publication of small-molecule and inorganic crystal structures beginning in January 2001. Bill Clegg and David Watson are Editors. The Acta E home page is at <http://journals.iucr.org/e/journalhomepage.html>.
- Manuscripts submitted to *Acta D* for the CCP4 Proceedings were used as a pilot study of electronic review. The lessons learnt will be applied initially to *Acta E*, which will require web submission of papers. Pilot electronic submission and review procedures will also be introduced for other journals during 2001.
- Crystallization papers in *Acta D* were discussed and considered well suited to electronic-only publication, with 2002 as a possible start date.
- Improved linking of **Crystallography Journals Online** was discussed. The IUCr will become a member of the CrossRef linking service.
- The digitization of all back issues of the journals is underway. Over 50,000 articles (170,000 pages) are to be scanned and converted to PDF pages. A sample issue (*Acta Crystallographica* Volume **15**, Part 3) is now available from **Crystallography Journals Online** at <http://journals.iucr.org>.
- Free printed reprints were replaced by electronic reprints at the start of 2000.
- A document on archiving policy is being developed in conjunction with the IUCr Electronic Publishing Committee.
- A lighter grade of paper has been selected for printing.

William L. Duax

IUCR ACTIVITIES

CIF news 5



Most crystallographers are familiar with the CIF (Crystallographic Information File) dictionaries. Those working with small structures have used the core dictionary to write CIFs submitted to Acta Cryst. B, C or E. Those in the macromolecular field will be acquainted with the macromolecular dictionary used to submit protein structures to the Protein Data Bank, and those working with powders will know of the dictionary being adopted for the Powder Data File.

Several groups have been developing dictionaries for other fields of crystallography. These are now in the process of being approved by Comcifs, the IUCr committee charged with approving all changes and additions to the CIF standard. One of the more interesting dictionaries that has recently been approved is designed for storing multidimensional images produced by 2-dimensional detectors. Synchrotron laboratories produce large numbers of these images for transfer to other laboratories for processing.

Two-dimensional detector images are produced as large binary files. Unfortunately, the CIF standard is restricted to ASCII characters since ASCII is the most robust standard. An image can only be stored in a CIF if it is converted to ASCII. There are several standards for conversion, the most familiar being MIME, the conversion used to prepare binary files as attachments for transmission by email. Because of the large number of images that a synchrotron source can generate, it was necessary to devise a standard as part of the CIF suite that allows binary image files to be transmitted without conversion. Such a file cannot be a CIF since a CIF must be written in ASCII. The solution is to define a binary file that looks as much like a CIF as possible.

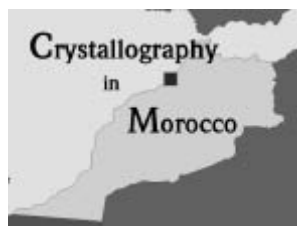
The new dictionary defines two standards, an imgCIF format in which the image is first converted to ASCII characters, and a Crystallographic Binary File (CBF) identical to the imgCIF except that the image field itself is written in binary. The two files map directly onto each other, the only conversion being of the image itself from binary to ASCII and vice versa. Even though everything in a CBF except the image is written in ASCII, the fact that the image is in binary makes the whole file a binary file and therefore not a CIF. This allows an image to be read and manipulated in the form of a binary CBF. The CBF can be converted to an imgCIF if, for example, it is to be archived, but in any case the additional information needed to characterise the image (details of the sample, the experimental arrangements and the mode in which the detector was read) can easily be extracted and incorporated into a CIF reporting the results of the study. The imgCIF is a fully conforming CIF and everything except the image conforms fully to the CIF standard.

This project was initiated by Andy Hammersley and has been brought to completion by Paul Ellis, Bob Sweet, Herbert Bernstein and others. Software is being written to store and process images in imgCIF/ CBF and synchrotron users can expect to find themselves using these files soon. The full text of the dictionary can be found at: www.bernstein-plus-sons.com/software/CBF/doc/cbftxt98.html.

I. David Brown

REGIONAL NEWS

Crystallography in Morocco



About 500 permanent Moroccan researchers use the techniques of X-ray crystallography, Scanning Electron microscopy (SEM), and Transmission Electron Microscopy (TEM) to characterize materials. They represent 20% of all researchers in the physical and chemical sciences. The majority of these researchers received training in crystallography in foreign laboratories, especially in France. These researchers work in about 50 laboratories in 23 universities, schools of engineering, and institutes of technology.

In university laboratories, the techniques are used as a tool for routine investigation to check the purity of synthesized compounds and to characterize their reactivity and surfaces. These techniques also allow crystal chemical characterization, single-crystal structural determination, and analysis of thin films. In chemistry, crystallography remains a speciality of inorganic chemists. Only recently have organic chemists and biochemists adopted diffraction as a technique complementary to their conventional techniques (NMR, Mass spectrometry). They use X-ray analysis for structural studies and the purification of natural products. Other researchers have developed computer models of crystallographic or defect structures and tested the models using the X-ray, SEM or TEM techniques. Industrial laboratories use these techniques to analyze and characterize the products of mining, cement manufacture, and the processing and production of building materials.

Teaching of crystallography

1,500 students who have basic knowledge in crystallography obtain a Bachelor's degree in physics and chemistry in Moroccan universities. Crystallographic teaching begins in the second year of undergraduate study. The students receive instruction in the theory of crystallography, description of metal and ionic structure, practical exercises, and in the rare cases where instruments are available, diffraction data acquisition.

Crystallographic research



The Bab Mansour (Mansour Gate) is a wall typical of Moroccan imperial cities. The gate is located in Meknes, the capital of Morocco under the reign of the King Moulay Ismael in the 17th century, an ancestor of the current King, his majesty Mohamed VI.

In Morocco 90% of scientific research is conducted in universities and schools of engineering via the individual initiatives of researchers. Research involving crystallography covers a broad range of topics.

Materials growth

- crystallized or vitreous compounds, oxides, ceramics
- growth of single crystals by flow method and sol-gel

Surfaces and interfaces

- treatment of the metal surfaces against corrosion
- the coating of metal surfaces
- semiconductor thin films
- characterizations of crystal defects

Structural studies and modeling

- structural analysis of minerals
- properties of surfaces
- determination of the structure of powders
- mineralogical characterization and studies of the physicochemical properties of clays
- electrostatic modeling based on high-resolution X-ray diffraction

Distribution of resources

This diversity of research topics is related to the distribution of human and material resources. 45% of the research groups have 4 members. Only 11% of the laboratories employ more than 10 researchers. More than 50% of the researchers are not affiliated with any laboratory. The absence of coordination at the national and regional level and the limited support allocated to research (0.3% of the G.D.P. which represents 100 million US dollars) are the principal causes of this distribution. Many scientists turn to the foreign laboratories in which they were trained to continue an active research program.

The majority of the research in materials sciences is due to International Programs of Co-operation such as the Integrated Actions (I.A.), Concerted Actions (C.A.), and International Programs of Scientific Co-operation (I.P.S.C.), which account for 58 programs in Marrakesh and 470 in all of Morocco since 1985.

While these programs educate and sustain a potential research capability, they have little relevance to national needs, are seldom sustained, and fail to build the science infrastructure or lead to acquisition of modern equipment needed in the country. They do generate joint publications and doctoral theses (369 at the U. of Marrakesh since 1985).

Research in materials sciences



B. Tanouti, N. Bouhaida and A. Thalal (left to right) in the Scanning Electronic Microscope room (the arabic calligraphy at the top of the photo means Electron Microscope).

Research in materials sciences is hampered by outdated equipment, inadequate infrastructure, and the isolation of researchers.

The national laboratories have only ten powder diffractometers, three scanning electronic microscopes and three transmission electron microscopes that are fifteen years old and subject to breakdowns. The age of the equipment makes it difficult to conduct experiments of good quality. In the absence of a single-crystal diffractometer, local crystallographers must depend on foreign partners. Almost all structures determined by Moroccan crystallographers have been solved using powder data.

In addition to the purchase price, the cost of maintenance is also prohibitive. In general, scientific equipment costs 1.8 times more in Morocco than in France. The average budget allocated to a laboratory in Morocco is about 1000 US dollars per annum.

Moroccan research suffers from the lack of a scientific infrastructure. The National Center of the Planning and Coordination of Scientific and Technologic Research (C.N.P.C.R.S.T.) created in 1978 has only recently organized some actions in support of research.

The cost of subscriptions to scientific journals limits the scientific literature. The high cost of the registration fees, transport and living expenses prohibits attendance at scientific conferences. The Internet, now present in almost all the laboratories, helps combat isolation, but restrictions on access to scientific articles and papers is still a problem.

Achievements and outlines

Conscious of the importance of scientific research for the development of the country, Moroccan researchers are working together to improve conditions and increase scientific output.

In the last three years solid state physicists and theoreticians founded the 'Moroccan Society of Statistical Physics' and published an annual review entitled *Moroccan Journal of Condensed Matter*. Solid state chemists formed a group 'REMCES' (Moroccan Meetings of Solid State Chemistry) and organized 8 international meeting in 17 years. The proceedings of these meetings are published in international reviews such as *Journal of Alloys and Compounds*, *Advanced Materials Research*, and *Phase Transitions*.

A School of Crystallography and the creation of a Moroccan Crystallography Association are being planned.

Research scientists in universities are cooperating in the design and support of shared facilities to achieve shared goals, including:

- the coordination of research activities and the revitalization of structures already in place,
- the creation of a national fund for the promotion of scientific research and engineering,
- the gathering of major equipment in research centers,
- the creation of an internal communication network to ensure better diffusion of scientific information,
- the financing of research projects through **P.A.R.S.** (Programme d'Appui à la Recherche Scientifique) and **P.R.O.T.A.R.S.** (Programme Thématique d'Appui à la Recherche Scientifique).

International cooperation needed

In spite of the goodwill of all involved, financial support remains inadequate and international collaboration is essential for the development of scientific research in general and crystallography in particular.

We need the assistance of foreign partners and international organizations. Specific needs include:

- donation of equipment,
- discounts on major equipment which take into consideration the income per capita of the purchasing countries,
- assistance with equipment maintenance,

- creation of regional centers to train crystallographers and technicians,
- development of regional research programs in connection with African needs to encourage cooperation among African countries,
- sources of support for traveling and training of crystallographers,
- reduction of the prices of subscription to the scientific journals and registration for international congresses,
- support for Moroccan publications to ensure their continued survival.

Conclusion



A. Thalal.

As is true of most developing countries, Morocco did not make scientific research a priority. Research in Morocco survived because of individual researchers and international cooperation (particularly with France). The state has recently become sensitive to the importance of scientific research to economic and social development. Although concrete measures have been taken to promote scientific research, they remain inadequate. This effort would benefit from the support of international organizations. Theoretical research in crystallography offers few outlets and does not allow the laboratories to obtain subsidies to maintain their activities. To develop research related to crystallography it is necessary to have very expensive equipment. Research in this field decreases annually. Because of the high cost of equipment many Moroccan crystallographers have changed fields. The teaching of crystallography is likely to decline. The assistance of the international community of crystallographers is needed if crystallography is to survive in Morocco.

A. Thalal, B. Tanouti, N. Bouhmaida and F. Bensamka
Cadi Ayyad U., Marrakesh, Semlalia Morocco

MEETING REPORT

9th Slovenian-Croatian Meeting

The 9th Slovenian-Croatian Crystallographic Meeting was held at The Julian Alps, Slovenia, **June 2000**. There were four plenary lectures: G. Giacovazzo (Italy) 'Phasing – From Powders to Proteins'; A. Tonejc (Croatia) 'Nano-Sized Crystalline and Amorphous Materials'; C. Baerlocher (Switzerland) 'Structure Solution from Powder Data'; and I. Turel (Slovenia) 'Quinolones and Their Metal Compounds'. A full report is available at <http://rcul.uni.lj.si/~fn01leban/report9.html>.

I. Leban (Ljubljana, Slovenia) and S. Popovic (Zagreb, Croatia)

MEETING REPORT

Indaba III, Symmetry and Structure

About 60 delegates flocked to Skukuza, South Africa in the Kruger National Park, to attend the third Indaba of the South African Crystallographic Society, sponsored by the IUCr. The theme of the **August 2000** workshop, 'Symmetry and Structure', was well suited to the 'Indaba' spirit, the study of a subject in depth from many different angles.



IUCr President Henk Schenk visited crystallographers at the U. of Cape Town in July 2000. The group is carrying out research in the field of supramolecular chemistry (structure, thermal analysis, kinetics of description of inclusion compounds) as well as studying drug-cyclodextrin interactions. Front row (left to right): Eliane DeVries, Main Kilkeny, Henk Schenk, Ayesha Jacobs, Dejana Vujonz. Back row: Vincent Smith, T. van Schalkwyk, Mino Cauva, Welcome Mhlono, Peter Linder, Clive Oliver, John Bacsá, Luigi Nassimbeni.

Henk Schenk, president of the IUCr, opened the proceedings with a review of the structure and activities of the Union, after which J. Boeyens (Pretoria) gave an overview of the interplay between symmetry, the time-space universe, and the fundamental laws of nature. D. Avnir (Jerusalem) discussed qualitative and quantitative measurement of symmetry, and speculated about the relation between symmetry, information content, and entropy. C. Graham (Pietermaritzburg) discussed chirality and time reversal symmetry in molecular and crystal optics, and a flamboyant H. Flack (Geneva) discussed the problems and pitfalls of the determination of absolute structure and absolute configuration.

The social highlight of the day was a game drive through the chilly winter night in the bushveld surrounding the camp. The spirits of the shivering participants flared up when they were treated to the rarely witnessed spectacle of a large herd of buffalo being attacked by a pride of lions.

The next morning A. Janner (Nijmegen) compared the symmetry of snowflakes with that of DNA molecules. O. Vassilyeva (Kiev) reported on the structure and properties of copper complexes. P. Comba (Heidelberg) entertained everyone with a pair of chiral apples, the similarity between the 'Ascending and Descending' painting by Escher and German politics, and the amount of 'leftness' and 'rightness' in the faces of his twin daughters. M. Lofener presented a paper by A. Amann (Innsbruck) who was unable to attend, on the substance problem in chemistry and the use of large deviations theory.

E. Osawa (Toyohashi) kicked off the afternoon session with a new model to describe hydrogen bonds based on data extracted from the Cambridge Structural Database. After showing some interesting McGillavry memorabilia, H. Schenk (Amsterdam) discussed the influence of symmetry on direct methods.

Wednesday brought the first reports of participants having spotted the 'big five': elephant, lion, buffalo, rhino and leopard before breakfast. Undisturbed by the exuberance of the visual hunters, G. Desiraju (Hyderabad) discussed relationships between molecular and supramolecular symmetry. After tea, L. Nassimbeni (Cape Town) eloquently spoke about physico-chemical aspects of inclusion compounds. N. Harada (Sendai) demonstrated (on paper!) the mechanism of a light-powered molecular motor, and D. Levendis (Johannesburg) discussed the relation between pseudo-symmetry, superlattices, and disorder.

J. Flippen-Anderson (Washington) opened the last day with comments on rapid data collection and increased computing power, and a discussion of 'twins, disorder and other demons'. A cheerful A. Roodt

(Bloemfontein) then discussed examples of chirality in coordination chemistry, and the new Cambridge Structural Database software was described by M. Fernandes (Johannesburg).

In the final session, K. Tornroos (Bergen) spoke about order-disorder phase transitions, W. Depmeier (Kiel) covered structural disorders in microporous materials, and J. Cai (Guangzhou) discussed racemic and enantiomeric complexes.

After a final game-spotting excursion, all attendants enjoyed tribal Zulu dancing, traditional 'potjiekos' for dinner, and a nonsense speech by the nestor of South African crystallography, Jan Boeyens, and a very witty Peter Comba. During the evening, Manuel Fernandes (Johannesburg) and Armin Wagner (Johannesburg/Berlin) shared a prize for presenting the best poster. Indaba III achieved its goal of being a highly stimulating and successful 'meeting of minds'.

Jan Dillen, U. of Stellenbosch



Participants of Indaba III in August 2000.

MEETING REPORT

The borders of hydrogen bonds

The problem of what interactions should be considered 'hydrogen bonds' is as old as the field of hydrogen bond research. In the 1920s when the field was in its infancy, liberal views held sway and borders were open. In the late 1930s, rigid and exclusive hydrogen bond definitions became the order of the day and remained practically unchanged (though not unchallenged) for about 50 years. Typical definitions held that in a hydrogen bond $X-H\cdots A$, X and A must be 'very electro-negative atoms' and that $H\cdots A$ or even $X\cdots A$ must be significantly shorter than the sum of the van der Waals radii. In the 1980s and 90s, conflicts with experimental data reached such a level that stringent criteria were increasingly ignored by researchers. A modern and useful definition of a hydrogen bond has not yet been found. In an informal meeting arranged by Roland Boese in Essen on **September 19, 2000**, the current state of this matter was explored to determine where borderlines should be drawn between interactions that are of the 'hydrogen bond type' and interactions that are clearly not hydrogen bonds. (Participants included R. Boese, G.R. Desiraju, A. Gehrke, R. Goddard, S. Harder, M. Kirchner, C. Lehmann, M. Mazik, T. Steiner, R. Sustmann.)

It was agreed that as a primary requirement, a hydrogen bond must involve a hydrogen atom, however trivial this might sound. The question of whether the term 'hydrogen bond' should be applied only to interactions formed by protic X-H groups (where H carries a positive partial charge relative to X), or be extended to include interactions involving hydridic X-H groups of opposite polarity, is more controversial. In fact, structural and functional features of $X^{\delta+}-H^{\delta-}\cdots A^{\delta+}$ interactions (e.g. agostic interactions, diboranes, 'inverse hydrogen bonds', etc.) in many significant ways parallel 'normal' $X^{\delta-}-H^{\delta+}\cdots A^{\delta-}$ hydrogen bonds. Nevertheless, the electronic nature of the interactions are different, being formally three center.four electron in one case, and three center.two electron in the other. This difference makes it possible to define a borderline on a chemical basis and term as a proper 'hydrogen bond' only the four-electron interaction.

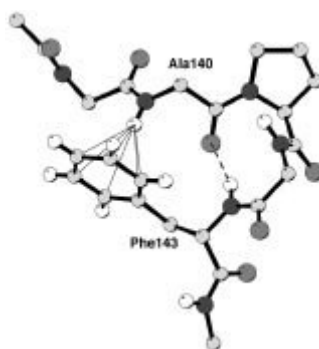


Figure 1: Example of a hydrogen bond type that does not fit early hydrogen bond definitions: typical $N-H\cdots Ph$ interaction in a protein (from T. Steiner, G. Koellner, *J. Mol. Biol.*, **305**, 2001, 535).

However, the use of the three center.four-electron condition as a stringent criterion is inappropriate because it would exclude such acceptors as the π -faces of benzene rings (see Figure 1). In fact, it is only required that the acceptor is a sterically accessible concentration of negative charge.

A hydrogen bond is a complex interaction composed of electrostatic, covalent and van der Waals forces that can be further divided (e.g. electrostatics into monopole, dipole and multipole contributions with different distance and angular characteristics, and van der Waals forces into attractive dispersion and exchange repulsion terms). In different kinds of hydrogen bonds, these constituents have different weights. In 'normal' hydrogen bonds, for example, electrostatics are dominant, while very strong hydrogen bonds can be dominated by covalent interactions and weak hydrogen bonds have electrostatic and van der Waals contributions of similar weight. In some cases, continuous transition to 'pure' interaction types is observed as in the transition to covalency that occurs with strong hydrogen bonds. Symmetric hydrogen bonds ($X-H-X$ with two equal $X-H$ distances) can be characterized as two half

covalent bonds. It is more difficult to evaluate a transition to purely ionic (*i.e.* non-directional) electrostatics that occurs if the partners carry large charges but only small dipole or quadrupole moments. Here, a liberal view was favored that concedes a certain hydrogen bond nature to an X-H...A interaction if some positive directionality can be detected, *i.e.* discernible favoring of linear over bent X-H... angles.

Most difficult to define is the transition to pure van der Waals forces. If donor or/and acceptor are only weak dipoles, such as in typical C-H...A or X-H...Hal-C interactions, positive directionality was again accepted as the primary criterion for the definition of a hydrogen bond. If the distance fall-off of the electrostatic component is fast, a dividing line can only be drawn subjectively. A possible borderline that can be drawn between dipole-quadrupole and quadrupole-quadrupole interactions was discussed.

It is currently fashionable to assign hydrogen bond character to a given contact by locating 'bond-critical points' in electron density distributions. After intense discussion, the group concluded that the existence of a bond critical point is a necessary though not a sufficient criterion for hydrogen bonding. It appears that a simple definition of the hydrogen bond is not possible. The complexity of the phenomenon, the large number of different contributing factors and the gradual transition to other types of interactions, does not permit the definition of clear borderlines. Once the openness of borders is acknowledged, a more general view of hydrogen bonding becomes possible. It is noteworthy that throughout the discussion, the 'van der Waals cutoff '-criterion was not mentioned. This criterion, which ruled the field for decades, is now completely abandoned - clearly a sign that the field has evolved.

Thomas Steiner, Freie U. Berlin

MEETING REPORT

Heart of Europe Bio-Crystallography

The Third Heart of Europe Bio-Crystallography Meeting (HEC) took place at the Polish Academy of Sciences in Poznan in **September 2000**. The HEC meetings are annual three-day workshops of structural biology and crystallography groups located in central Europe (Czech Republic, East Germany, and Poland). This year Mariusz Jaskolski, U. of Poznan, organized an exciting meeting with a well-balanced schedule of presentations and ample room for extensive discussions. All correspondence with the 55 participants and announcements were handled over the internet (www.man.poznan.pl/~jabies/HEC/).

The emphasis of the meeting was to give young scientists, PhD students and postdocs the chance to present their research to a larger scientific community and to meet with peers to discuss practical crystallographic issues. The 25 oral presentations spanned areas from protein production, crystallization, phasing and crystallographic refinement to the analysis of atomic resolution crystal structures. The keynote speaker, George Sheldrick (U. of Göttingen), talked about structure refinement and applications of *ab initio* structure determination methods in biological crystallography using the SHELX program suite.

Although participation is limited geographically, the number of groups involved continues to increase substantially each year, reflecting the growth of structural biology in the center of Europe. The fourth HEC meeting is scheduled to take place in the Czech Republic during the autumn of 2001, hosted by Jindrich Hasek and Juraj Sedlacek.

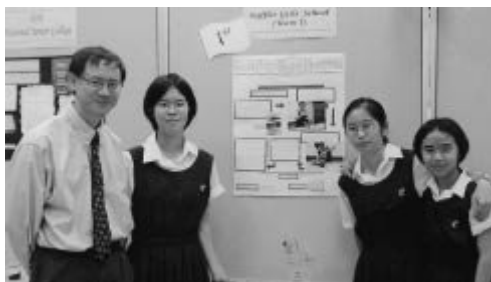
Yves A. Muller, Max-Delbrück-Center, Berlin



Participants of the Third Heart of Europe Bio-Crystallography Meeting in Poznan, Poland.

MEETING REPORT

4th Singapore National Crystal Challenge



With the prize winners of the Open level, Prof. T.S. Andy Hor, Head of the Chemistry Department, National U. of Singapore.

Large beautiful single crystals are fascinating and aesthetically pleasing. Growing crystals of a desired size and shape is still considered more of an art than a science. To stimulate student interest in the art of growing crystals, the Dept of Chemistry at the National U. of Singapore organized the 4th Singapore National Crystal Growing Challenge in **September 2000** for secondary school, junior college and polytechnic students. The school provided instruction in technique and gave students an opportunity to be creative in growing crystals. This year's competition included Junior, Senior, and Open levels, with cash awards of \$400, 300, 200 and 50, and trophies in each category.

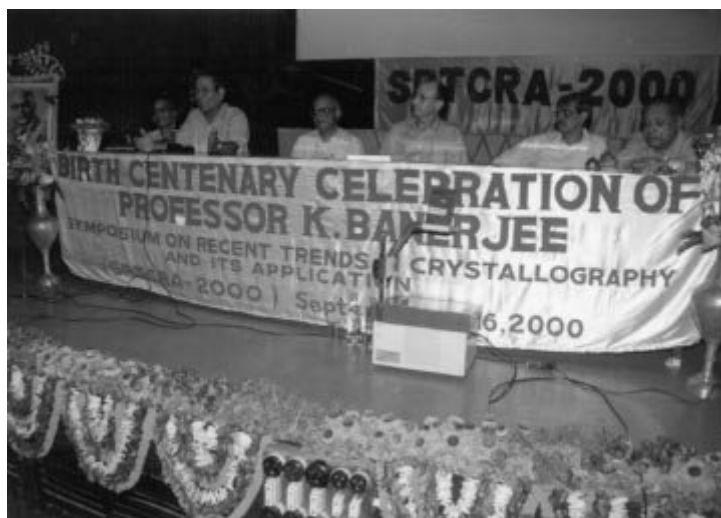
At the Junior level students were challenged to grow the cubic or tetrahedral form of sodium chlorate (NaClO_3) crystals. The Senior level students were challenged to grow blue-green nickel sulfate hexahydrate ($\text{NiSO}_4 \cdot 6\text{H}_2\text{O}$) crystals (tetragonal) and not the heptahydrate that would usually come out of solution first. The Open level students were allowed to grow organic/metallo-organic compounds of their choice to exercise their creativity, individuality and scientific knowledge. There were 109 entries from 41 secondary schools and 11 junior colleges and polytechnics. Mr. Werner Schittenhelm, Managing Director Bruker AXS, Germany, was the guest of honor for the prize presentation ceremony. This year's competition was sponsored by Bruker Singapore Pte Ltd and Lee Foundation of Singapore. Details of the challenge and the names of the winners are available at the website: www.chemistry.nus.edu.sg/ncgc1.htm.

Jagadeese J. Vittal and Yulin Lam

MEETING REPORT

Recent trends in crystallography, Calcutta, India

To commemorate the 100th anniversary of the birth of Professor K. Banerjee, the pioneer crystallographer of India, a Symposium on Recent Trends in Crystallography and its Applications (SRTCRA 2000) was organized at the Indian Association for the Cultivation of Science (IACS) in Calcutta, on September 15-16, 2000. The inaugural ceremony was attended by more than 200 participants including J.R. Helliwell, U. of Manchester, students, and family members of Prof. Banerjee. S.K. Sikka, Chairman of the Indian National Committee on Crystallography and Director of the Solid State & Spectroscopy Group of Bhabha Atomic Research Centre (BARC) of Trombay, opened the Symposium. D. Mukherjee, Director, IACS, discussed the role of crystallography in interdisciplinary research and the heritage of IACS including the contributions of C.V. Raman (Nobel Laureate), M.N. Saha, K.S. Krishnan, K. Banerjee, S. Bhagavantam and many others. The Chairman of the Organizing Committee, S.P. Sengupta, a member of the IUCr Commission on Powder Diffraction (CPD), described how Banerjee initiated modern crystallographic research in India and played a key role in establishing active research centers across the country. Messages from eminent crystallographers including H. Hauptman, J. Karle, M.M. Woolfson, and H. Schenk revealed deep appreciation of Banerjee's contributions to the development of direct methods. A.K. Sharma, President, IACS, emphasized the importance of crystallographic research in the current context of the genome project. To mark the occasion Professor Sharma announced the publication of 'A Collection of Professor Banerjee's Work', including research publications and lectures on scientific policy, and unveiled a bronze relief of Banerjee at the IACS campus.



Concluding session of SRTCRA 2000.

In the opening scientific session M. Vijayan, Indian Inst. of Science, Bangalore, delivered the keynote address on the 'Structural diversity and functional specificity of proteins - A case study involving lectins'. There were 21 talks by speakers from India and abroad. In his lecture on the 'Complementarity of Neutron and Ultra-high resolution Synchrotron X-ray protein crystallography' J. Helliwell gave an overview of recent advances in the field of high-resolution and neutron protein crystallography. T.P. Singh (AIIMS) presented the threedimensional structure of phospholipase A2 and a structure-based design of its inhibitors. A. Banerjee (Bose Inst.), A. Banerjee (IACS) and D. Mukherjee, (SINP,) discussed molecular design in living systems, reverse turns in proteins, synthetic peptides and pseudo-peptides and the crystal structure and functions of a chymotrypsin inhibitor protein isolated from the seeds of the winged bean.

K. Lal (NPL) and S.K. Sikka (BARC) highlighted recent advances in Dynamical diffraction from crystals and High pressure studies using synchrotron radiation sources while D. Pandey (BHU) spoke on structural

phase transitions in mixed perovskites. Other speakers in the Materials Science session, D. Chakraborty (IACS), K. Chattopadhyay (IISc), J.K. Bhattacharjee (IACS), A. Mukherjee and S.N. Bose (National Centre for Basic Sciences, Calcutta) delivered lectures on Nanoscale magnetic heterostructures, Quasicrystals, Second order structural phase transitions and Properties of materials from first principles.

The lectures by M. Mukherjee (IACS) and D. Velmurugan (U. of Madras) were on ab-initio Phasing of proteins by multiresolution Direct methods and Combination of Direct Methods with Anomalous scattering/ Isomorphous replacement. The topics of the last session with speakers G.D. Nigam (IIT Kharagpur) and A.K. Mukherjee (Jadavpur U.), S. Paul (North Bengal U.) and S. Gupta (IACS) covered Probability distribution functions, Crystallographic disorder and Structures of Liquid Crystals.

A special 'Reminiscences' session on Prof. K. Banerjee was arranged in the evening with some of his senior students A.R. Chowdhury, R.K. Sen, S.C. Chakraborty, K.C. Banerjee, A.K. Datta and A.K. Pant as speakers, chaired by B.S. Basak.

An Endowment fund was established by the family, students and admirers of Prof. Banerjee with a proposal for an annual lecture in his name. Professor J.R. Helliwell, the recipient of the Professor Banerjee Silver medal, delivered the first Professor Banerjee Endowment Lecture. An article based on the lecture will appear in the January 2001 issue of the Indian Journal of Physics.

S. P. Sen Gupta, Monika Mukherjee (IACS, Calcutta) and John Helliwell (Manchester, UK)

FEATURE ARTICLE

Kedareswar Banerjee - India's first crystallographer



Unveiling of a bronze relief of Prof. K. Banerjee at SRTCRA 2000.

Professor Kedareswar Banerjee, a pioneer X-ray crystallographer, was born in Bikrampur, Dacca (now in Bangladesh) on September 15, 1900. In 1923, after a brilliant academic career in Dacca U. and the U. of Calcutta, young K. Banerjee joined the research group of Sir C.V. Raman at the Indian Association for the Cultivation of Science (IACS), Calcutta, a premier Indian research institute of India. He worked in various institutions including IACS, the Indian Meteorological Department, Dacca U. and Allahabad U. and finally retired as the Director of IACS, Calcutta in 1965.

Banerjee laid the foundation of X-ray Crystallographic research in India. In 1924, when only a few crystal structures had been determined throughout the world, Banerjee's work on the determination of atomic arrangements in crystalline naphthalene and anthracene received international attention. Banerjee was awarded the DSc degree of the U. of Calcutta in 1930. He had close associations with almost all the leading crystallographers of his time including W. H. Bragg, W. L. Bragg, J. M. Robertson, P. P. Ewald, J. D. Bernal, K. Lonsdale, N. V. Belov and M. Avrami. In 1933, Banerjee proposed a new approach to the crystallographic phase problem, which not only broke new ground beyond the 'trial and error' structure solution method of that time, but also heralded the extremely powerful direct methods of crystallography of the modern era. His seminal paper (*Proc. Roy. Soc.*, 1933, **141**, 188) on direct methods was cited in the Nobel Lecture of Dr. Jerome Karle in 1985.

Apart from structural X-ray crystallography, Banerjee's research pursuits covered a wide field of crystal physics. His research contributions in various fields including low angle scattering, thermal diffuse scattering of X-rays from crystals, diffraction of X-rays by liquids, jute fiber and organic polymers, structures of coal and glass, determination of the elastic constants of crystals by X-rays, theoretical modelling of the vibrational spectra of crystal lattices and some topics in crystal optics have received international recognition. Perhaps his most significant contribution to the advancement of science in India was the creation of active schools of research wherever he went leaving behind a band of young, energetic research workers who became the torch bearers of his scientific tradition.

Banerjee was elected a Fellow of the Indian Academy of Science and the National Academy of Science (N.A.Sc.). He was the sectional President for the Physical Science Group at the Indian Science Congress in 1947, Vice-President of the N.A.Sc. from 1958 to 1960 and General President of the N.A.Sc. in 1967. He was a member of the first National Commission for cooperation with UNESCO from 1947 to 1951, a member of the Scientific Advisory Committee of the Planning Commission from 1953 to 1956 and a member of the review committee and advisory boards of several National Laboratories. In 1948, he was invited as a 'Guest of Honour' to the inaugural Congress and General Assembly of the International Union of Crystallography.

Apart from being a stellar scientist, Prof. Banerjee possessed a rare and pleasing personality. He was extremely kind and affectionate yet strong in his convictions. He lived a life of noble deeds and thoughts that brought him self-composure, freedom from fear and made him a truly international scientist. On April 30, 1975 Prof. Banerjee died at Barasat, a suburb of Calcutta.

NOTICE

Mineralogical Society of America



The MSA invites applications for the 2002 grant for Research in Crystallography from the Edward H. Kraus Crystallographic Research Fund. This is a \$5000 grant for support of research beginning January 2002. Some restrictions apply. Application instructions and form for the grant may be obtained from the MSA website at www.minsocam.org. Completed applications must be returned by June 1, 2001.



Outgoing President Bill Carlson passing the gavel of the MSA presidency to new President Kase Klein. Photo courtesy of MSA.

Elected to office for 2001: **Cornelis Klein** (U. of New Mexico) as President; **Rodney C. Ewing** (U. of Michigan) as Vice President; **James G. Blencoe** (Oak Ridge National Lab) as 2001-2002 Treasurer; and **Craig E. Manning** (U. of California, Los Angeles) and **Kathryn L. Nagy** (U. of Colorado) as 2001-2002 Councilors. Remaining in office are **William Carlson** as Past President; **David Jenkins** as 2000-2001 Secretary; and **Michael Carpenter**, **Sorena Sorensen**, **David L. Bish**, and **Jeffrey E. Post** as Councilors.



Peter C. Burns. [\[correction\]](#)

The Mineralogical Society of America is pleased to announce that **Peter J. Wyllie**, California Inst. of Technology, is the 2001 Roebling Medallist; **Peter C. Burns**, U. of Notre Dame, is the 2001 MSA Award recipient; and **Jeffrey E. Post**, Smithsonian Inst., is the 2001 Mid-Career Award recipient. The 2001 recipient for the research grant in crystallography from the Edward H. Kraus Crystallographic Research Fund is **Steven D. Jacobsen**, U. of Colorado, for his study of 'Elasticity of singlecrystal (Mg,Fe)O and a new method for generating GHz-frequency shear waves'. The 2001 recipients for the research grants in mineralogy and petrology from MSA's Mineralogy/Petrology Research Fund are **Carlotta B. Chernoff**, U. of Arizona, for her study 'Distribution of trace metal contents in black shales and their metamorphic equivalents' and **Kaye Sawyer Savage**, Stanford U., for her study of 'Efflorescent uptake of trace oxyanions: effect on crystal structure and distribution'. New Fellows of the Society are: **Michael B. Baker**, **Jay D. Bass**, **Patrick R. L. Browne**, **Anastasia Chopelas**, **Patricia M. Dove**, **Thomas W. Sisson**, **Takamitsu Yamanaka**, and **Michael E. Zolensky**.

J. Alexander Speer, Administrator Mineralogical Society of America
(www.minsocam.org/)

NOTICE

2000 Future Investigator Award winners announced

Molecular Structure Corporation proudly announces the recipients of the first annual MSC Future Investigator Awards. These awards are designed to reward outstanding and promising researchers early in their careers. The inaugural MSC Future Investigators were selected on the basis of their scientific accomplishments in the field of structural biology, their publications, and the expectation that they will contribute to the field of macromolecular crystallography. Each received an unrestricted \$2,500 cash award. The four winners are: M.J. Bennett (California Inst. of Technology), J.C. Boyington (LIG/NIAID, National Inst. of Health), P. Cramer (Stanford U. School of Medicine), and C. E. Stebbins (Yale School of Medicine).



Melanie Bennett.

The work of **Melanie Bennett** on the hereditary haemochromatosis protein HFE and its complex with transferrin receptor (TfR) may help in our understanding of this iron-overload disorder. Dr. Bennett is a former Fellow of the Damon Runyon-Walter Winchell Foundation.



Jeffrey Boyington

Jeffrey Boyington has recently determined the structure of the complex of the immunoglobulin-like natural killer (NK) cell receptor KIR2DL2 with its ligand, the class I MHC protein HLA-Cw3. The cytolytic activity of NK cells is tightly regulated by both activating and inhibitory NK cell receptors. This particular receptor inhibits NK cell-mediated lysis upon recognition of certain class I MHC molecules on the surface of healthy host cells. The KIR/MHC interaction is strikingly different from the interaction observed between T-cell receptors and MHC molecules and reveals a mechanism of allotypic specificity.

Patrick Cramer along with colleagues solved the structure of yeast RNA Polymerase II, the central enzyme of gene expression that synthesizes all messenger RNA in eukaryotes.

C. Eric Stebbins has worked on the ternary complex of the tumor suppressor VHL bound to Elongin B and Elongin C; the complex of Hsp90 with its inhibitor, geldanamycin, an antitumor antibiotic; and the bacterial GreA transcript cleavage factor involved in regulating the processivity of RNA polymerase. Dr. Stebbins is a Fellow of the Damon Runyon-Walter Winchell Foundation. He now studies the structural basis for the modulation of signal transduction pathways by bacterial virulence factors that are translocated into host cells for the benefit of the pathogen.

Textbooks of the future will be updated with the knowledge gleaned from the fundamental research of our winners. It is gratifying to award these creative thinkers with the MSC Future Investigators award to show our appreciation.

For information regarding the 2001 MSC Future Investigator Awards please visit our website at www.msc.com/msc/awards.html.

NOTICE

Struchkov Prize



Professor Yuri T. Struchkov (1926-1995) was an outstanding Russian crystallographer who made substantial contributions to the structural chemistry of organic and organometallic compounds. He was the founder and long time director of the X-Ray Structural Centre of the Russian Academy of Sciences, one of the most productive laboratories in the field of 'small molecule' organic crystallography. He served as a member of the Executive Committee of the IUCr in 1990-1993 and was elected the Vice-President of the IUCr at the XVIth General Assembly in Beijing in 1993. He did not finish his term as a VP, as he passed away in August, 1995.

In order to commemorate the life achievements of Prof. Struchkov, his friends and former colleagues have established the Struchkov Prize, which since 1997 has been awarded annually to a young (<35 years) scientist from the Former Soviet Union (FSU) for the best research work in the field of X-ray crystallography. The jury, chaired by the present director of the X-ray Structural Centre, M. Yu. Antipin, and composed of members of the FSU crystallographic community, selects the winner from submitted applications. The winner receives a diploma and a prize of approximately \$500. In the past three years the prizes were awarded to A. V. Virovets, Inst. of Inorganic Chemistry, Novosibirsk (1997), A. M. Abakumov, Chemistry Dept, Moscow State U. (1998), and T. I. Ivanova, Geology Dept, St Petersburg State U. (1999). Over the years the competition has grown tougher, with the number of applications increasing from 8 in 1997 to 17 in 1999.

Early in 2000 the Struchkov Prize underwent an organizational change. Initially the funds for the Prize were provided by the X-ray Structural Centre. This year a group of more than 15 former students and co-workers of Prof. Struchkov, working in crystallographic labs all over the world, formed the Struchkov Prize Society (registered in San Diego, USA), whose goal is to promote individual contributions towards the funding of the Struchkov Prize. Growth of the Struchkov Prize fund will permit an increase in the monetary value of the award as well as allow the award of additional prizes honoring top ranking candidates. Anyone wishing to contribute to the Struchkov Prize fund should contact M.Yu. Antipin at mishan@xray.ineos.ac.ru or A. I. Yanovsky at yan@xrpent.ineos.ac.ru for details.

A. I. Yanovsky

NOTICE

SESAME

Synchrotron-light in the Middle East

Developed under the umbrella of UNESCO, Synchrotron-light for Experimental Science and Applications in the Middle East (SESAME) is to be the Middle East's first international research center. It will have as its centerpiece a synchrotron radiation source based on an anticipated gift from Germany of the 0.8 GeV BESSY 1 storage ring and injector system. Programs planned for SESAME include structural molecular biology, molecular environmental science, surface and interface science, microelectromechanical devices, X-ray imaging, archaeological microanalysis, materials characterization, and medical applications. SESAME will be a propeller for regional science and the economy of the Middle East as well as promoting peaceful cooperation among scientists.

On April 6-7, 2000 the first meeting of the Structural Molecular Biology (SMB) Scientific Subgroup of the SESAME Scientific Committee was held at the U. of Athens. Participants from each of the countries in the Middle East summarized the present status of work in SMB in their countries and the prospects for such work with SESAME. Several hundred scientists from the region are expected to use SESAME.

The top priority for the SMB Scientific Subgroup is to see a research institute established alongside SESAME for the development of SMB projects and infrastructure in the region. There was also discussion of a meeting of the powder diffraction scientific subgroup in Turkey.

More information is available at www.sesame.org.jo/

Herman Winick

from Crystallography News, No. 74, September 2000

NOTICE

2002 Patterson Award



The next presentation of the A.L. Patterson Award will be made at the San Antonio, TX, meeting of the American Crystallographic Association in May, 2002. The A.L. Patterson Award, established in 1980, is to recognize and encourage outstanding research in the structure of matter by diffraction methods. This may include one or more of the following: (i) significant contributions to the methodology of structure determination, (ii) innovative application of diffraction methods, (iii) elucidation of biological, chemical, geological or physical phenomena using new structural information. There are no restrictions as to nationality, race, sex, religion, or ACA membership. The award is given in memory of Arthur Lindo Patterson, Senior Member, Inst. for Cancer Research, Philadelphia, whose most important contribution to crystallography was the function named after him. Previous recipients were: Wayne A. Hendrickson, 1981; Jerome Karle and Herbert Hauptman, 1984; David and Lieselotte Templeton, 1987; Michael Woolfson, 1990; George Sheldrick, 1993; Christer E. Nordman, 1997; and Gérard Bricogne, 1999. Nominations are invited from throughout the crystallographic community. The major contributions of the nominee should be identified, with supporting documentation. The closing date for nominations is March 31, 2001; earlier nominations would be welcomed. The members of the 2002 Patterson Award Committee are: Philip Coppens, Dave Duchamp, Jane Griffin, and Andy Howard. Nominations and supporting documents should be sent, in writing, to the ACA office, 73 High Street, Buffalo, NY 14203-0906, USA.

NOTICE

Honorary BCA Members



The list of Honorary Members of the British Crystallographic Association consists of: A. Beevers, B. Cochran, B. Evans, B. Forsyth, R. Jenkins, A. Klug, H. Megaw, M. Perutz, J.E. Walker, and T. Willis. You can find links to pages describing their achievements on the BCA website at: <http://bca.cryst.bbk.ac.uk/BCA/admin/Hons.html>

NOTICE

European Crystallography Prize



The European Crystallographic Association (ECA) invites nominations for the second European Crystallography Prize to recognize a significant achievement or discovery in crystallography in the past 5-10 years. Nominees should be affiliated or identified with the European crystallographic community, as broadly defined in the charter of the ECA (see the ECA-news site www.ba.cnr.it/eca/).

The prize, including a monetary award and certificate of recognition, will be awarded at the opening ceremony of the 20th European Crystallography Meeting (ECM-20) in Krakow, Poland, August 25-31, 2001.

The first prize was awarded to Professor Ada Yonath of the Weizmann Institute of Science in Israel at the ECM-19 in Nancy, France in August, 2000 for 'her pioneering achievements in structural studies on the ribosome'.

Nominations should include a statement of the contribution for which the prize is to be awarded, a 2-3 page curriculum vitae of the nominee and the signature of at least three additional nominators, preferably with supporting nominating letters. They should be postmarked no later than February 28, 2001 and should be sent to: Davide Viterbo, Dip. di Chimica IFM, U. di Torino, Via P. Giuria 7, I-10125 Torino, Italy; FAX: 39-011-6707855, E-mail: viterbo@ch.unito.it.

AWARDS AND PRIZES

The Aminoff Prize in Crystallography to Dan Shechtman



Sitting (left to right): Kristina Olovsson, Sven Lidin, Dan Shechtman, Janne Carlsson (President of the Academy); standing: Ivar Olovsson and Zipora Shechtman.

The Royal Swedish Academy of Sciences has awarded the Aminoff prize in crystallography for the year 2000 to *Professor Dan Shechtman, Israel Institute of Technology, Haifa, Israel, for his discovery of quasicrystals*. He received the prize at the Academy meeting on September 13, 2000.

The Wenner-Gren Foundation hosted an international symposium, 'Symmetry 2000', September 13-16, organized by Istvan Hargittai and Torvard Laurent. The program spanned vast areas, from symmetry in arts and architecture, crystals and tilings to mathematics and theoretical physics. Over 100 participants took part in the symposium, including B. Grünbaum, H.S.M. Coxeter, J. Dunitz, A.L. Mackay, B. Mandelbrot, D. Schattschneider and M. Senechal. The interdisciplinary character of the symposium stimulated interesting discussions among participants with widely different backgrounds.

Shechtman's discovery at the beginning of 1980 of an ordered material with classically forbidden fivefold symmetry, 'quasicrystals', was something of a crystallographic bomb. The discovery constitutes a fundamentally new step in our understanding of basic concepts about order and symmetry in the crystalline state. Intensive research into those fascinating solids revealed extraordinary physical properties and has led to novel practical applications. Shechtman's discovery also stimulated theoretical studies of quasicrystalline arrangements by mathematicians and theoretical physicists.

Ivar Olovsson, Chairman, Swedish National Committee of Crystallography

AWARDS AND PRIZES

Congratulations to ...

Gautam R. Desiraju (U. of Hyderabad, India) has been awarded the Third World Academy of Sciences (TWAS) Award in Chemistry for 2000 which consists of a check for \$10,000 and a citation that reads: 'For his pioneering contributions to the area of crystal engineering, the designed synthesis of solid state supramolecular entities, and for increasing the awareness in the properties and consequences of the weak hydrogen bond'. Dr. Desiraju is also the recent recipient of the prestigious Alexander von Humboldt Research Award which allows him to visit and conduct research in laboratories in Germany.

Uli Arndt (Cambridge, UK) received the Dorothy Hodgkin 2000 Prize. His major research interest lay in the development of new apparatus and techniques. The majority of his more than 100 publications are in the field of instrument design. He was elected a Fellow of The Royal Society in 1982.

Sean Langridge (ISIS, UK) was presented with the 2000 Philips Physical Crystallography Award for his work in magnetic structure using both X-rays and neutrons. His prize lecture was entitled 'Quantifying magnetic domain correlations in antiferromagnetically coupled multilayers'.

Jacqui Cole (Cambridge, UK) was awarded the inaugural CCDC/CCG Prize for her work in the field of developing materials with useful optical properties. Dr Cole's award lecture, entitled 'Crystals and glasses in non-linear optics and lasers: structural requirements', covered aspects from designing molecular and crystal structures, to the determination of the structure of rare-earth phosphate glasses, to attempting to harness the vibrational characteristics of molecules.

The Rutgers' Board of Governors has named **Helen M. Berman** a Board of Governors Professor of Chemistry. 'The Board of Governors Professorship is the highest academic honor that Rutgers U. (USA) can give a member of its faculty,' said Joseph J. Seneca, university vice president for academic affairs. 'This is an affirmation of Professor Berman's international reputation for scholarship and recognizes her dedication to the missions of teaching and research at Rutgers.'

Dave Stuart FRS (Oxford U., UK) will give the Bragg Lecture at the Reading BCA Meeting (April 7-10, 2001) on his work on viruses, virus receptors and related cell surface proteins.

Melvin R. Churchill received the 2000 Jacob F. Schoellkopf Medal from the Western New York Chapter of the American Chemical Society. Dr Churchill, a prolific crystallographer, is ranked 183rd on a list of the '1000 Most-Cited Chemists in the World. The title of his talk was 'Order, Disorder and Surprises in the Crystallography of Organometallic Materials'.

OBITUARY

Lydia Leonyuk (1950-2000)



Lydia Leonyuk died on September 23, 2000, after a struggle of three years with cancer. She was born in St.-Petersburg and graduated from Moscow State U. in 1972. Lydia had a very successful career in solid state physics, crystallography and crystal growth. She received a PhD in Crystallography and Crystal Physics under Nikolas V. Belov (1978) and published more than 200 papers and two books. In 1995, she was awarded a DSc degree by the Faculty of Physics, Moscow State U. for her contributions to the field of superconducting cuprates. In 1996, she prepared and described a new family of superconducting cuprates with a ladder-type structure. Recently, she applied the knowledge of cuprate motifs in oxysalts to minerals.

She was the Head of the Laboratory of Crystal Growth and a leader of research projects supported by the Russian National Program on Superconductivity, the European Community and the USA. She received grants for work in laboratories in London, Paris, Nantes, Geneva, and Warsaw and had joint projects with universities in Sweden, Germany, Japan, and China. She was a dedicated teacher and a member of the Russian Academy of Natural Sciences.

Lydia loved her research, and it was exciting to work with her. With the support of her husband, Nikolai, she accepted her terminal illness courageously. I am sure that, like myself, many other crystallographers around the world will miss the superb experimental expertise of Lydia and remember her as a charming person and a precious friend.

Elena V. Sokolova