

INTERNATIONAL UNION OF CRYSTALLOGRAPHY

---

# IUCr Newsletter

Volume 10 · Issue 1

Collected archival edition

Original article text and available illustrations

# Contents

## Letter from the President

|                           |   |
|---------------------------|---|
| Letter from the President | 4 |
|---------------------------|---|

## Editorial

|           |   |
|-----------|---|
| Editorial | 6 |
|-----------|---|

## Letter to the Editor

|                                 |   |
|---------------------------------|---|
| Request for equipment           | 7 |
| Gratitude for equipment donated | 8 |
| Relations with Armenia          | 9 |

## IUCr journals news

|                                                                                                                                                           |    |
|-----------------------------------------------------------------------------------------------------------------------------------------------------------|----|
| Controllable variation of the intensity of diffracted X-ray beams and double modulation of such beams for transmission and reception of audio information | 10 |
| Symmetry survives pressure                                                                                                                                | 12 |

## IUCr activities

|                                          |    |
|------------------------------------------|----|
| CIF news 7: CIF and symmetry             | 14 |
| IUCr sponsorship and support of meetings | 16 |
| Powder Diffraction update                | 17 |
| IUCr Congress in Geneva ...              | 18 |

## Feature article

|                                                               |    |
|---------------------------------------------------------------|----|
| Optical rotation of tartaric acid crystals finally determined | 21 |
|---------------------------------------------------------------|----|

## Regional news

|                    |    |
|--------------------|----|
| US science adviser | 23 |
|--------------------|----|

## Notice

|                                                         |    |
|---------------------------------------------------------|----|
| Canadian Light Source (CLS)                             | 24 |
| Crystallographic Society of Japan                       | 25 |
| In the news                                             | 43 |
| The Chatt lecture 2002                                  | 44 |
| A Critical Assessment of Predicted Interactions (CAPRI) | 45 |

## Meeting report

|                                                |    |
|------------------------------------------------|----|
| BCA Winter 2001 meeting reports                | 26 |
| Student views down under                       | 28 |
| Protein crystallography in the heart of Europe | 29 |
| Young people's guide to ACA - LA               | 30 |
| High throughput structures                     | 31 |
| Materials microstructure                       | 33 |

|                                              |    |
|----------------------------------------------|----|
| ECM20 - Krakow                               | 34 |
| <b>Awards and prizes</b>                     |    |
| Honors                                       | 42 |
| Mineralogical Society awards                 | 47 |
| <b>Book review</b>                           |    |
| BOOKS                                        | 46 |
| <b>Miscellany</b>                            |    |
| Rietveld on Rietveld                         | 48 |
| The very model of a protein crystallographer | 54 |
| <b>Obituary</b>                              |    |
| Don C. Wiley (1944-2001)                     | 49 |
| Norio Kato (1923-2002)                       | 51 |
| Jim Graham (1929-2001)                       | 52 |
| Ryoichi Sadanaga (1920-2002)                 | 53 |

## LETTER FROM THE PRESIDENT

# Letter from the President



Henk Schenk

I congratulate Michael Woolfson on winning the sixth Ewald Prize. As most of you know, Michael made many great contributions to direct methods. I recall the famous program MULTAN that solved so many crystal structures all over the world. He will receive the prize this summer on 6 August at the Opening Ceremony of the Geneva General Assembly and Congress of the IUCr. As Ewald laureate he will also present the opening lecture of the Congress. I have known Michael personally since 1970 as we shared (with many others) the excitement for direct methods. Not only is his work fantastic, but also the way he socialized direct methods through the famous summer schools was remarkable. Many of us became friends because we attended one of these schools. I am looking forward to listening to his talk.

Through direct methods I also had the pleasure to meet P. P. Ewald. He was the invited speaker at the Workshop on Direct Methods in Buffalo in 1973. With twenty other young scientists I listened to very interesting talks. At the time, Paul Ewald was already 85 years old, a very nice and bright person and a brilliant lecturer. He was not only one of the founders of X-ray crystallography but also the main driving force behind the International Union of Crystallography. In 1944 he started discussions about setting up an IUCr-like organisation and an independent crystallographic journal. He was the President of the Provisional International Crystallographic Committee, which in 1947 prepared the official start of the IUCr and the launch of *Acta Crystallographica*. He was the first Editor of *Acta* and also President of the IUCr from 1960-1963. I invite you to read his Editorial Preface in the first issue of *Acta Cryst.* in 1948, maybe through Crystallography Journals Online.

Here I give two citations:

'Much is yet to be learned about the general mechanism of crystallization, including the reasons for the transitions of a substance from one crystalline form to another; about the mechanical, electrical, optical and plastic properties of crystals in relation to atomic forces and structure; about the internal perfection and imperfection of crystals and the consequences thereof; about chemical bonds, surface forces, diffusion and chemical reactions within the solid; about the diffraction of atoms, electrons, neutrons and, possibly, of other particles by crystals. Many problems arise from the study of substances which show a periodicity less perfect than the three-dimensional one of true crystals. Fibres, high polymers, and high molecular substances in general require the study of the weak intermolecular forces which are determined by the surface of the molecule rather than directly by its internal constitution, and the same is true for the mesomorphic states of matter.'

'Acta is intended to offer a central place for publication and discussion of all research in this vast and ever-expanding field. It borders, naturally, on pure physics, chemistry, biology, mineralogy, technology and also on mathematics, but is distinguished by being concerned with the methods and results of investigating the arrangement of atoms in matter, particularly when that arrangement has regular features. Ever since crystals became the object of scientific investigation it has been felt that they are the most precisely defined form of matter, and that the understanding of their atomic structure introduces clarity and detail into concepts which must in other cases be expressed in more general terms. This is particularly apparent in all types of diffraction experiments, but it is also true for elastic, optical, electric, magnetic and thermodynamic properties, and the whole field of crystal structure may be

regarded as the ultimate development of stereochemistry, amplified by a wealth of quantitative geometrical information.' I hope to meet you this summer in Geneva.

*Henk Schenk*  
*[schenk@science.uva.nl](mailto:schenk@science.uva.nl)*

## EDITORIAL

# Editorial



Urszula Rychlewska is truly the rose between two thorns Derek Hodgeon and the editor) at the XIth Symposia on Organic Crystal Chemistry in August, 2001. More pictures on page 12.

The XIX IUCr Congress in Geneva is the premier Crystallographic event of the triennium. No other meeting brings together leaders from all over the world working in all aspects of diffraction physics and its applications. The gathering will include innovators and experts, pioneers and novices. Because crystallography is vital to physics, mineralogy, chemistry, biology, and a plethora of cross disciplines, the meeting will cover the latest advances in all of these areas. An update on the Geneva program appears on page **10** and the program for an open commission meeting on the Future of Macromolecular Crystallography appears on page **11**. This issue contains microsymposia reports from ECM 20, reports of BCA meetings in 2001, and Young Scientists' comments on meetings in Australia and the USA (page **16**). There is a commonly expressed concern that the future of science depends upon our ability to explain to the general public what we do and why it is important. How have studies of materials translated into stronger, safer, more reliable every day products? How does detailed knowledge concerning the structures of drugs, hormones and proteins contribute to improved health?

Unfortunately, most of us are engaged in such specific applications of crystallography that our work is not only difficult for the public to understand, it is often difficult for us to explain to other crystallographers. My father said, "If you don't toot your own horn, nobody is going to toot it for you". In that spirit and in an effort to encourage crystallographers to find the right words to effectively explain the significance of their work, I invite all readers to toot their own horns. If you have recently published results that you would like to shout about, send a 200 word description, one illustration with a caption, and your photograph to the editor.

All submissions will be given careful consideration, but not all will be accepted for publication. Papers published in IUCr journals will receive preferential consideration. No more than one item per author will be published per triennium. The idea for such a feature arose from an unsolicited contribution from Artem Organov that appears on page 7. Items will be evaluated on the basis of scientific significance and its successful communication.

## LETTER TO THE EDITOR

# Request for equipment

Dear Colleagues

Despite years of intensive care, our old high voltage tube-based generator from the GDR has definitely died. This generator previously used for texture analysis and a double crystal goniometer are the only ones available in Cuba. Our Bragg-Brentano goniometer is presently working well with an ENRAF NONIUS 581 generator donated by Utrecht U., which encourages us to ask for donated equipment from our colleagues. Acquisition of a functioning generator would benefit not only Havana U., but the Cuban materials science community in general.

*A. Gómez, U. de la Habana, Havana, Cuba;  
ariel@lae.ff.oc.uh.cu/ariel\_g\_g@yahoo.com*

## LETTER TO THE EDITOR

## Gratitude for equipment donated

Dear Bill

As you may know, Argentina is going through very difficult times, and the pursuit of Science in general, and Crystallography in particular, is not an exception to this state of affairs. Fortunately, the international community has a remarkable sense of solidarity, which helps us to go on working. We at the Atomic Energy Commission in Argentina, wish to express our indebtedness to Judith Howard and her research team, from Durham U., UK, for the donation of a four circle diffractometer vital to our scientific survival. We sincerely hope that her generosity, will stimulate similar generous acts to promote science in the lesser developed regions of the world.

*Daniel Vega, CNEA, Buenos Aires, Argentina*

## LETTER TO THE EDITOR

# Relations with Armenia

Dear Andrea Sharpe

I am grateful that my article has been selected for review in the next issue of the *IUCr Newsletter* (Vol. 10 No. 1). It is a great honor to me. I will do my best to justify your positive opinion to my article. I would like to be acquainted with you. Unfortunately our Republic of Armenia has been isolated from the external world for the last decades. So the development of civilized relations between our colleagues abroad is temporarily stopped. Superficial knowledge of English language impedes our progress. Your suggestion that my article to be included in the *IUCr Newsletter* (Vol. 10, No. 1) makes us hope that we live in our civilized and kind world again.

*Marut Navasardyan*

*Dept of Physics, Yerevan State U., Armenia*

# Controllable variation of the intensity of diffracted X-ray beams and double modulation of such beams for transmission and reception of audio information

M.A. Navasardyan, *J. Appl. Crystallogr.* (2001). 34, 763-766

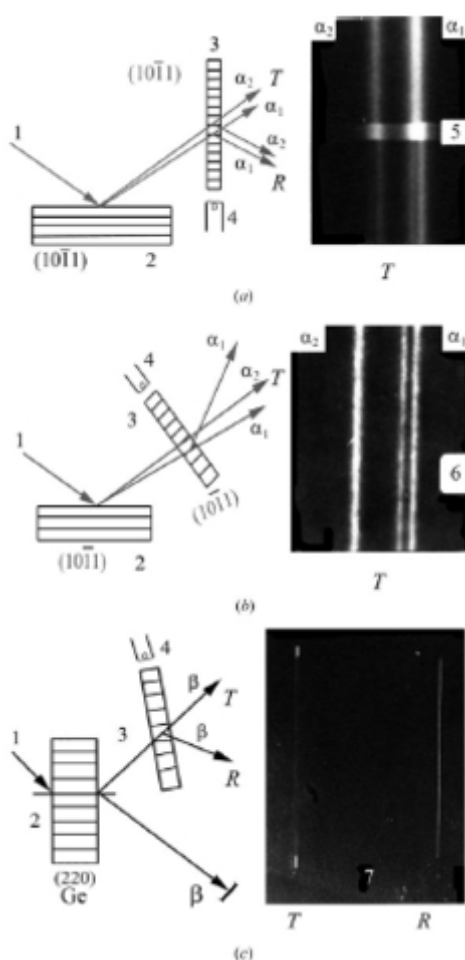


Figure 1. Geometry of the experiment for observation of the phenomenon of controllable complete reflection in the case of a quasi-plane wave in the following settings of a double-crystal spectrometer: (a) (+, -)quartz-quartz, (b) (+, +) quartz-quartz, (c) (+, -)germanium-quartz. 1: the X-ray tube with Mo anode; 2: crystal monochromator; 3: studied crystal (crystal analyser); 4: heater; 5: profiles of transmitted Mo  $K\alpha_1$  and Mo  $K\alpha_2$  beams in the absence (from the top) and in the presence (from below) of a temperature gradient; 6: transmitted  $K\alpha_1$  and  $K\alpha_2$  beams, when only the  $K\alpha_1$  beam is reflected (from the right-hand side); 7: transmitted (T) and reflected (R) Mo  $K\beta$  beams. The thickness of Ge is  $t = 0.3$  mm and of quartz is  $t \approx 1$  mm. On beam R in position 7, the size of the reflected beam corresponds to the vertical size of the quartz plate.

Communicating acoustic information with the help of Bragg reflections may seem surprising at first sight. Prof. Navasardyan of Yerevan State U., Armenia addresses the topic in a recent issue of the *J. Applied Crystallography*.

The story starts in the 1930s, when the diffracted X-ray intensity from a quartz crystal was noticed to increase when applying a temperature gradient or ultrasonic oscillations. Such investigations gathered momentum after the discovery (in 1941) of the Borrmann effect, or anomalous transmission, through relatively perfect single crystals. Two régimes were of interest: those with  $\mu t \leq 1$  or  $> 10$ , where  $\mu$  is the linear absorption coefficient and  $t$  the thickness of the crystal. Explanations for unusual behaviour of the transmitted beams were sought in X-ray standing waves and in a decrease in primary extinction. With a temperature gradient of a certain magnitude and direction (perpendicular to the reflecting atomic planes), the energy of the incident beam was wholly diverted into the reflected beam.

Controllable complete reflection in the Laue case, 'forced' by a temperature gradient or ultrasonic oscillations, is distinguished from the total reflection in Bragg geometry within the angular range of Darwin reflection. Controllable complete reflection has been demonstrated for quasi-plane waves in double-crystal (+,+) and (+,-) geometries (see Fig. 1).

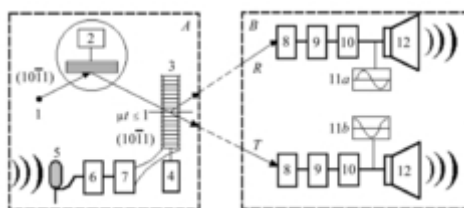


Figure 2. Scheme of a practical device for the transmission and reception of acoustic oscillations (speech) by means of diffracted X-ray beams. 1: source of X-radiation; 2: monochromator; 3: crystal modulator; 4: goniometer; 5, 6, 7: microphone, low-frequency and high-frequency generators; 8: scintillation detectors; 9: integrating circuits; 10: amplifiers; 11a, 11b: oscilloscope with appropriate oscillograms; 12: loudspeakers. A and B are the transmitting and receiving parts of the device, respectively.

Of interest is the time-dependence of the X-ray intensity from the crystal, simultaneously excited by ultrasound resonance (of high frequency  $\nu$ ) and audio oscillations (of low frequency  $\omega$ ): that is, double modulation. In crystals of medium thickness ( $\mu t \leq 1$ ) under conditions of controllable complete reflection, the diffracted (R) beam intensity can equal the initial intensity of the transmitted (T) beam. During one oscillation period, there can be several hundreds to hundreds of thousands of photons in a beam from an X-ray tube (35 kV and 15 mA) and a detector registers a continuous photon count varying by a low frequency ( $\omega \leq 20$  kHz). It is thus possible to transmit and to receive audio information (e.g., speech) by the X-ray beam and a possible scheme is shown in Fig. 2.

The quartz crystal modulator is set for Bragg reflection in Laue geometry and resonance oscillations ( $\nu = 2880/t$ ) so that the condition  $t = \lambda/2$  is fulfilled, where  $\lambda$  is the wavelength of the acoustic wave in quartz. The diffracted beam intensity increases (by a tenfold factor) and the low-frequency ( $\omega$ ) generator (a microphone or tape recorder) modulates the crystal. The diffracted beam intensity also oscillates with frequency  $\omega$ , which is registered on the scintillation counter after it has travelled some distance, possibly penetrating barriers inaccessible to other forms of radiation. In this paper, Navasardyan also lists other uses, including the study of fast chemical reactions, the tracking of time-dependent processes in crystals and the characterization of synchrotron and other sources of X-radiation.

*Reviewed by Moreton Moore*

*Dept of Physics, Royal Holloway U. of London, UK*

# Symmetry survives pressure

'Theoretical investigation of metastable  $\text{Al}_2\text{SiO}_5$  polymorphs'  
A.R. Oganov, G.D. Price, J.P. Brodholt (2001)

*Acta Cryst.* A57, 548-557



Isosymmetric transition in sillimanite ( $\text{Al}_2\text{SiO}_5$ ). Top: sillimanite, bottom: its high-pressure isosymmetric successor. The new phase has 5-coordinate Al (light grey) and Si (dark grey). The 5-coordinate Si, so rare in inorganic compounds at low pressures, may be important in the Earth's mantle.

Most phase transitions involve changes in crystal symmetry. However, there are examples of isosymmetric transitions, where the full space group is preserved and atoms occupy the same Wyckoff positions in both phases. Such transitions have interesting properties: being necessarily first-order, they disappear above the critical temperature and become fully continuous (just like liquid-gas transitions!).

Isosymmetric transitions involve changes in either the electronic (Ce, SmS), or atomic ( $\text{KTiOPO}_4$ ,  $\text{PbF}_2$ ) structure, and often are metastable.

The number of known isosymmetric transitions is rapidly increasing.

Using quantum-mechanical simulations, we predicted a metastable isosymmetric transition in *sillimanite* ( $\text{Al}_2\text{SiO}_5$  – see Figure) at pressures of ~30-40 GPa. Detailed structural study revealed that the transition occurs when non-bonding Al...O and Si...O contacts become too short (<2.25 Å for Si...O), and transform into bonds. The existence of suggested critical bond distances would be useful in defining coordination numbers of atoms and explaining properties and phase transitions of condensed matter.

Forces in crystals obey space group symmetry, and tend to preserve it. Most phase transitions, however, change crystal symmetry, usually by a group-subgroup scheme. Isosymmetric transitions remain a rare, but fundamentally important phenomenon. Their study can lead to new important discoveries.

*Highlights of article submitted by Artem R. Oganov  
U. College London*

## IUCR ACTIVITIES

## CIF news 7: CIF and symmetry



David Brown

A good definition of a crystallographer is someone who can find their way around International Tables for Crystallography Vol. A since it is symmetry that lies at the heart of crystallography and is what distinguishes it from other condensed matter sciences. It is surprising therefore to find how few symmetry items are defined in the CIF dictionaries. This is all the more strange given that the precise definitions of space group theory ideally lend themselves to handling by computer. That omission has now been corrected with the recent release of the CIF Symmetry Dictionary which can be found on the IUCr web site [ftp://ftp.iucr.org/pub/cif\\_sym.dic](ftp://ftp.iucr.org/pub/cif_sym.dic).

Because the concepts of space group theory are precisely defined, one would expect it to be easy to provide them with good CIF definitions, but the working group that prepared the dictionary ran into some unexpected problems. A space group cannot be fully described without choosing a setting, and since each space group can be found in many possible settings none of which is unique, there are many ways in which it can be described. The choice of which description to use is arbitrary and depends on how the information is to be used.

There are 230 space groups and each of these is defined by the set of symmetry operations that comprise the group. However, these symmetry operations can only be properly described by expressing them in an explicit algebraic form, and this can only be done by choosing a specific coordinate system or setting. What is then the best way to represent a space group in a CIF? One method is to list the symmetry operations of the group in the setting of choice. This is the option most often found in the current CIF archives of crystal structures where the setting is chosen to give the simplest description of the structure. In theoretical studies, on the other hand, it is better to choose one invariant reference setting for each space group, even though the choice is arbitrary, since this permits a consistent description of the relationships between space groups.



N-dimensional Rubics cube

In a printed work, such as International Tables, it not feasible to display the space group in all possible settings, so the setting chosen becomes, *de facto*, the reference setting needed for theoretical studies, but a computer is more flexible. The symmetry operations and special positions can be calculated on the fly in any desired setting from the Hall space group symbol (International Tables Vol B (1993) 1.4 Appendix B) using a computer application such as the Windows program WGETSPEC ([www.ccp14.ac.uk/ccp/web-mirrors/Impg-laugier-bochu](http://www.ccp14.ac.uk/ccp/web-mirrors/Impg-laugier-bochu)). This opens up possibilities that are not available to printed tables.

Space groups are identified by their name or symbol. There are two types of symbol, those that define the space group in terms of its setting and those that are independent of the setting. Each has its advantages and disadvantages. The Schoenflies symbol and the International Tables (IT) number are unique identifiers of the space group that are independent of the setting. Their disadvantage is that the name itself, e.g., IT-62, contains no explicit information on the operations the space group. To get this information one must consult a separate listing of the symmetry operations, but any such listing immediately implies a particular setting. On the other hand, names such as the Hall symbol, which contain complete information about the symmetry operations, necessarily imply a particular setting, with the result that different symbols are needed for different settings of the same space group. Because so many different Hall symbols describe the same space group, it is not easy to identify the space group from a cursory examination of the symbol.

The Hermann-Mauguin (H-M) symbols can be decoded to give the symmetry operations, but they cannot reach all possible settings since they contain no information about the choice of origin, or the axis system for rhombohedral space groups. They are of limited use as generators of the space group operations, but, because they are setting dependent, many different H-M symbols can be used to describe the same space group.

Since the symbol cannot be precisely defined as either a space group generator or as a setting independent space group name, the CIF Symmetry Dictionary defines several different versions of the H-M symbol. One of these, `_space_group.name_H-M_ref`, is tightly defined. Only one form of the symbol, defined by an enumeration list, may be used for each space group. It can therefore act as a setting-independent space group name, but it can also be decoded to give the symmetry operations of the reference setting (normally the first setting given in International Tables Vol A). An alternative H-M symbol, `_space_group.name_H-M_alt`, is provided for people who like to use the Hermann-Mauguin symbol in other ways, such as to indicate the setting used as well as the space group. There are no rules about how this symbol is to be written or used and, for this reason it cannot be reliably used as a space group generator. The CIF stores this symbol solely for the information of the user and it is not intended to be used as an instruction to a computer program.

Version 1.0 of the CIF Symmetry Dictionary defines the basic terms encountered in space group symmetry such as the different space group symbols, the symmetry operations, the reference setting and transformations between the reference setting and the setting adopted in the CIF. There are also items describing the special positions, their symmetry and Wyckoff letters. Future versions of the dictionary will include symmetry in higher dimensions (used for incommensurate structures and quasi-crystals) and group - subgroup relationships (useful in analysing displacive phase transitions). In the meantime the new set of `_space_group` items will be added to the core and macromolecular dictionaries as the old `_symmetry` items are phased out.

*David Brown*  
*Chair, COMCIFS*

## IUCR ACTIVITIES

## IUCr sponsorship and support of meetings

The Sub-committee on the Union Calendar receives and considers requests for IUCr sponsorship and financial support and makes recommendations to the Executive Committee. Organizers of meetings (which must be international in character) wishing to seek IUCr sponsorship should submit applications at least nine months in advance of the meeting. Applications for sponsorship of satellite meetings require the approval of the Chair of the Organizing Committee of the main meeting. The IUCr continues to support and uphold ICSU's policy of non-discrimination and adheres to its decisions and procedures concerning the free circulation of scientists. Organizers of any meeting seeking IUCr sponsorship or support must assure the Calendar Sub-committee that the authorities of the country in which the meeting is to take place guarantee free entrance of bona fide scientists from all countries.

Application forms are available from the Chair of the Sub-committee: H. Fuess, Technische Hochschule Darmstadt, FB 21 Materialwissenschaft Strukturforschung, Petersenstrasse 23, D-64287 Darmstadt, Germany; (email: fuess@friedel.st.mw.tudarmstadt.de)

*'Science is the search for truth – it is not a game in which one tries to beat his opponent, or do harm to others. We need the spirit of science in international affairs to make the conduct of international affairs an effort to find solutions.'*

Linus Pauling in *No More War*

## IUCR ACTIVITIES

# Powder Diffraction update



The Commission on Powder Diffraction (CPD) Newsletter now reaches 2000 recipients around the world. All the Newsletters since the first issue of 1989 will be published on CD-ROM soon. The congress on Accuracy in Powder Diffraction III (APD3, Gaithersburg, MD, USA, 22-25.47.2001) was a major event for the year 2001. Future meetings will include EPDIC 8 (Spring 2002) in Sweden and the IUCr World Congress (Geneva, August 2002) where eight microsymbiosia will be dedicated to powder diffraction and related topics and Structure solution and refinement will be central themes.

Issue No. 26 of the CPD Newsletter focused on structure determination from powder diffraction data. The field has developed rapidly and a diverse set of Crystallographic tools allow *ab initio* structure solution from powder diffraction data alone. Whilst not yet as routine as single crystal determinations, the application of structure determination from powder diffraction methods can be routine in many circumstances. Although computing power has catalysed many advances, especially in the area of global optimization, algorithmic developments, experimental ingenuity, chemical intuition and a refusal to accept the conclusion that certain things 'just can't be done using powder diffraction' have all contributed to recent successes.

## Quantitative phase analysis round robin

The IUCr Commission on Powder Diffraction (CPD) sponsored a Round Robin on the determination of quantitative phase abundance from diffraction data. The aims of the Round Robin were: (i) to document the methods and strategies commonly employed in quantitative phase analysis, (ii) to assess levels of accuracy, precision and lower limits of detection, (iii) to identify specific problem areas and develop practical solutions, (iv) to formulate recommended procedures for QPA using diffraction data, and (v) to create a standard set of samples for future reference.

The preliminary report and analysis of results are available at [www.boulder.nist.gov/div853/balzar](http://www.boulder.nist.gov/div853/balzar), CPD and CCP14 websites.

*Bill David, Paolo Scardi*

## Rietveld refinement

Issue No. 26 of the CPD newsletter is devoted to various aspects of modern Rietveld refinement. The basic idea behind the Rietveld method is to calculate the entire powder pattern using a variety of refinable parameters and to improve a selection of these parameters by minimizing the weighted sum of the squared differences between the observed and the calculated powder pattern using least squares methods. That way, the intrinsic problem of the powder diffraction methods with systematic and accidental peak overlap is overcome. Hugo Rietveld invented the method a few decades ago, to extract as much information as possible from powder patterns. Applications of the Rietveld method range from the refinement of small protein structures to quantitative phase analysis of industrial importance.

*Robert Dinnebier*

## IUCr ACTIVITIES

# IUCr Congress in Geneva ...



The XIX IUCr Congress and General Assembly in Geneva (August 6-15, 2002) offers an opportunity to enjoy a full and varied scientific program, meet with industry representatives at the exhibition, and sample a variety of social events - all in the beautiful setting of Geneva.

The daily program is available on the web, with the abstracts online. As of this writing, we have already received close to 1,500 registrations from 48 countries - a truly international event!

Registration is still open for the Pre-Congress workshops on Tuesday, August 6, though space is limited. The Opening Ceremony will take place at the Noga Hilton that evening, with the presentation of the 6<sup>th</sup> Ewald Award to Professor Michael M. Woolfson who will deliver the Ewald Lecture. A reception will follow, against the beautiful background of Lake Geneva.

The always-popular Student Mixer is scheduled to take place on Thursday, August 8 where the student registrants are invited to dance to dawn at the Liquid Club, courtesy of Oxford Cryosystems. More dancing on Saturday, August 10, when participants will have an opportunity to learn Israeli folk-dancing.

Sunday, August 11 offers everyone a chance to rest from scientific sessions and social events alike with a day free for touring. The scientific program recommences on Monday, August 12 and the social event that evening is a concert by the much-respected Sine Nomine quartet, sponsored by Emerald Biostructures.

Tickets are still available for the Gala Dinner on Wednesday, August 14 and should be reserved in the advance (price US\$65). The number of seats is limited! The menu, and all other information can be found at the Congress website.

## New news

The IUCr is pleased to announce that the CCDC is again sponsoring three Poster Prizes in chemical crystallography to be awarded at the 2002 Congress. Each CCDC Poster Prize will comprise a commemorative item and a monetary prize of US\$350. Further details will be available at the Congress.

COMCIFS Meeting will be held Tuesday, August 13. For further information contact D. Brown, COMCIFS Chairperson (idbrown@mcmaster.ca).

Congratulations to A. Yonath, of The Weizmann Inst. of Science who has been selected to receive the 2002 Israel Prize for Research in Chemistry. Prof. Yonath is speaking at the Congress on August 9 in the Ribosome Symposium.

## Workshops

All workshops will take place on Tuesday, August 6 at the Palexpo Conference Centre. Registration for Workshops is additional to Congress registration and the number of places is limited. Registration is on the basis of 'first-come first-served'.

## Scattering methods for nanoscale structure characterization

This full day workshop organized by J.D. Barnes and sponsored by IUCr Commission on Small Angle Scattering is designed to acquaint researchers who currently do not practice small-angle scattering with the fundamentals of SAS methods as they are applied to the characterization of such diverse structures as synthetic polymer molecules, protein complexes, alloys and ceramics, composite materials, self-organizing molecular structures, engineering plastics, and microphotonic materials. Workshop instructors will describe the principles of small-angle X-ray and small-angle neutron scattering (SAXS and SANS) and will demonstrate how these principles are applied to the practical elucidation of structure on distance scales ranging from nanometers to some tens of micrometers.

## Protein crystal growth

Full day workshop organized by N. Chayen. The aim of this workshop is to present the state of the art in practical methodology for crystal growth of biological macromolecules. Some of the methods are also suitable for the crystallization of small molecules. The workshop will consist of lectures/videos dealing with methods for screening and optimisation of crystallization conditions, including high throughput trials, membrane proteins, new ways of growth in gels, heterogeneous nucleants, etc. It will conclude with a panel of experts who will answer questions from the audience. Questions and comments regarding this workshop should be directed to N. Chayen ([n.chayen@ic.ac.uk](mailto:n.chayen@ic.ac.uk)).

## Twinning and the CRYSTALS program

Full day workshop organized by S. Parsons and D. Watkin. For further information: [www.xtl.ox.ac.uk](http://www.xtl.ox.ac.uk).

## Cambridge Crystallographic Data Centre (CCDC)

Full day workshop organised by F. Allen and K. Lipscomb. The CCDC Workshop will cover all aspects of the Cambridge Structural Database System, including database searching using ConQuest, structure visualisation using Mercury and data analysis using Vista. The Workshop will also cover other CCDC products, including DASH for structure solution from powder diffraction data, the IsoStar knowledge base of intermolecular interactions, SuperStar and GOLD for investigating protein-ligand interactions and for protein-ligand docking, the Relibase+ database system for analysing experimental (PDB) data on protein-ligand complexes, and the developing enCIFer program for editing CIFs for submission to journals and databases.

## Joint open meeting of the commissions on biological macromolecules and journals

A joint meeting of the IUCr Commissions on Biological Macromolecules and Journals has been organized in conjunction with the IUCr Congress to be held in Geneva this coming August. The meeting will be held on Friday August 9 from 12:30 to 14:30 at Palexpo, the principal Congress venue.

The meeting will focus on the challenges macromolecular crystallography faces in the era of high-throughput structure determination resulting from initiatives in a number of countries to fund structural genomics projects. As a result of these and other efforts, the world of macromolecular crystallography faces similar changes to those that confronted chemical 'small molecule' crystallography 25 years ago. These include the verification of structures, deposition of structural data and perhaps most importantly publication of macromolecular structures.

The discussion at the open meeting will be led by short presentations from members of the NIH/ Wellcome Trust task forces for structural genomics who have been dealing with these issues for the past several years. Some of the questions that will be addressed include:

Is there a need for enhanced data capture in a PDB deposition? What additional data should be deposited? How do we ensure that deposition guidelines are enforced?

Can we validate structures automatically? How can we assist referees of publications to assess the quality of structures?

Is there a difference between an enhanced deposition and a short paper? Is there still a need for formal publication for all structures in the era of freely available electronic databases?

The editors of *Acta Crystallographica* will also present their new ideas for publication of macromolecular structures. The meeting will be jointly chaired by John Helliwell, Commission on Journals and Mitchell Guss, Commission on Biological Macromolecules.

The following speakers will make short presentations with generous time for general discussion of the issues raised.

Udo Heinemann. Introduction to 'structural genomics', the ISGO and NIH/Wellcome Trust task forces.

Guy Dodson. 'Short publication' versus 'enhanced deposition' — the pluses and minuses.

Tom Terwilliger. The problems and possible methods for automatic structure validation — the search for a simple indicator of quality.

Helen Berman. Enhancing PDB deposition to capture all the experimental conditions. Automating the deposition process — links with crystallographic software.

Pete Strickland and Jenny Glusker. Managing Editor *Acta Crystallographica* and Editor of *Acta Crystallographica* Section D. Rapid publication and *Acta*.

*Mitchell Guss, M.Guss@mmb.usyd.edu.au*

## FEATURE ARTICLE

# Optical rotation of tartaric acid crystals finally determined

(Editors note: After hearing Bart Kahr's presentation at the XIth Symposium on Organic Crystal Chemistry, I asked him to contribute a brief description of the determination of optical rotation of tartaric acid.)



Bart Kahr hardly ever really hits women.

Crystals of tartaric acid and its salts recur in the story of the development of the sciences of stereochemistry and molecular chirality. Pasteur, in 1848, used the sodium ammonium salt to establish the first link between macroscopic chirality, the shapes of hemihedral crystals, and microscopic chirality, the sign of the optical rotation of molecules in solution.<sup>1</sup> Swapping ammonium for rubidium, Bijvoet established the absolute configuration of a molecule for the first time by exploiting the breakdown of Friedel's Law in the presence of anomalous dispersion.<sup>2</sup> Most recently, in 1997, Mucha, Stadnicka, Kaminsky and Glazer reported the optical rotation tensor of tartaric acid crystals, a measurement that is essential for the interpretation of the optical rotatory power in terms of structure.<sup>3</sup> Appearing nearly a century and a half after Pasteur's experiments on the optical rotation of dissolved tartrate crystals, this last paper, by its tardiness, tells a story in its own right, the unhappy marriage of crystals and chiroptics.

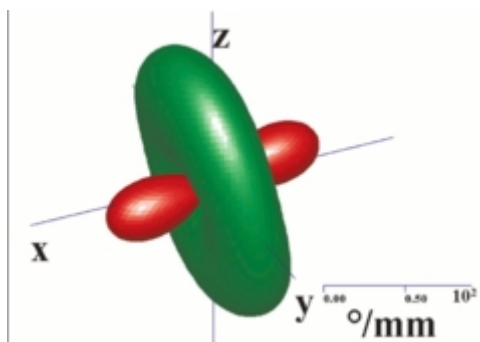


Figure 1. The representation surface of optical rotation in tartaric acid. The distance from a point on the surface to the origin of the Cartesian coordinates  $x$ ,  $y$  and  $z$  is in proportion to the optical rotation measured in that direction. Negative optical rotation is drawn in red, positive optical rotation in green colors. The  $y$ -axis is parallel to the two-fold rotation axis in TA,  $z$  is along the crystallographic  $c$ -axis. Despite the fact that the first measurement of optical rotation was made on a section of quartz by Arago,<sup>4</sup> Pasteur had no hope of measuring the optical rotation of his tartrate crystals because the large linear refractive index anisotropy has a much greater influence on the state of polarization of light passing through the sample than does chirality. As the science of crystal optics progressed throughout the nineteenth century, researchers identified the two optic axes in tartaric acid, those very special directions where the refractive index anisotropy disappears. When optical rotation was measured for light passed along these axes, researchers were struck with the most confounding result; the optical rotation for dextrorotatory tartaric acid in solution was along both optic axes *levorotatory*.<sup>5</sup> Where were the dextrorotatory directions? Did the sign of rotation change upon crystallization? These questions remained unanswered until Mucha and Stadnicka from the Jagiellonian U. brought this problem to the attention of Kaminsky and Glazer, scientists at Oxford U. Building upon advances in chiroptics first

introduced in 1983 by Kobayashi and Uesu<sup>6</sup> at Waseda U. the researchers from Oxford U. introduced refinements<sup>7,8</sup> that ultimately produced a general, robust strategy for measuring optical rotation in low symmetry crystals. Application of these techniques finally revealed the orientational dependence of optical rotation in tartaric acid crystals as shown in Figure 1.

If the Science Citation Index is any indication, the work of Mucha *et al.* has scarcely received the attention it deserves. Few measurements in science are so difficult as to require 150 years. In the case of the optical rotation of tartaric acid crystals, so much time had elapsed since the work of Pasteur that we forgot what we did not know, principally how to measure the orientational dependence of optical rotation in molecules and crystals. Perhaps this note will bring a fine, historic study to the attention of a wider audience.



Attendees at the XIth Symposium on Organic Crystal Chemistry in Rydzyna, Poland  
Bart Kahr, U. of Washington  
Seattle, WA USA

## References

- [1] L. Pasteur, *Comptes Rendus*, 1849, 29, 297.
- [2] J. M. Bijvoet, A. F. Peerdeman, A. J. van Bommel, *Nature (London)*, **1951**, 168, 271.
- [3] D. Mucha, K. Stadnicka, W. Kaminsky, A. M. Glazer, *Journal of Physics, Condensed Matter*, **9**, 10829.
- [4] D.-F. Arago, *Memoire de le Institut Paris*, **1811**, Part I, 93.
- [5] A. V. Shubnikov, *Principles of Optical Crystallography*, Consultants Bureau, New York, 1960, p 141.
- [6] J. Kobayashi, Y. Uesu, *Journal of Applied Crystallography*, **1983**, 16, 204.
- [7] W. Kaminsky, S. Haussuehl, *Z. Kristallogr.*, **1993**, 203, 79-91.
- [8] W. Kaminsky, A.M. Glazer, *Ferroelectrics*, **1996**, 183, 133-141.

## REGIONAL NEWS

# US science adviser



The U.S. National Committee for Crystallographers met Washington, D.C., November 2001.

The US National Committee for Crystallography (USNCCr) represents U.S. crystallographers within the IUCr through the National Research Council. The USNCCr maintains close ties to US professional societies while promoting international scientific cooperation.

A highlight of the November 2001 meeting of the USNCCr was the presence of Jack Marburger, Director of the Office of Science and Technology Policy, and White House Science Adviser. He commented on five questions addressed to him.

1) How will funding and the justification/priorities for funding in the sciences change in light of September 11th?

2) What changes can we anticipate for those who work with 'bio-hazardous' materials?

3) Concerns about support for research in the physical as well as the life sciences.

4) Openness in scientific publication and communication with peers in other countries. What can we expect in terms of restrictions in travel to meetings abroad?

5) Policies regarding patenting of crystal structures (and genes) derived from naturally occurring specimens?

Dr. Marburger impressed the committee with his knowledge of and approach to these issues. He spoke of crystallography as an 'enabling' science at the interface of many exciting fields such as drug development, proteomics, and nanomaterials. He encouraged us to work with his office to create a more informed environment to help the public appreciate how science works and benefits society. He stressed the need to better communicate the importance of not just our findings but also the role of the underlying technologies and national resources that support our successes in research. He expressed concerns about balance in funding and the need to foster the enabling technologies as well as support efforts directed towards the end-products of research. On the 'select agents' issue, he commented that it will be important to develop procedures to control the access to biohazardous materials and urged us to work with our respective institutions to create a dialogue as to how this can best be implemented. He also said that we should not anticipate much change in travel restrictions to other countries. In light of the events of 9/11, we can expect increased scrutiny of foreign visas and improved efforts to track foreign students once they are admitted into the United States. On the patent issue, he noted that it is not a scientific issue other than its possible impact to inhibit science in affected areas.

In other activities, the USNCCr voted to award a minimum of \$20,000 in travel grants for young scientist to attend the Geneva IUCr meeting and allocated \$5,000 in travel assistance for Latin American crystallographers to attend crystallographic schools or workshops in the US. See the website for a list of current members and more information about the USNCCr: [www.sdsc.edu/Xtal/USNCCr/USNCCr.html](http://www.sdsc.edu/Xtal/USNCCr/USNCCr.html).

*Marv Hackert, Chair USNCCr*

## NOTICE

## Canadian Light Source (CLS)

The protein crystallography beamline developer Pawel Grochulski is now resident at the CLS and will continue with the design and construction of the PX beamline for the CLS. A Letter-of-Intent has been submitted for a second PX beamline. Jim Britten from McMaster U. has been organizing a small molecule beamline team, whose task it is to define the scientific goals and operational parameters of the proposed Small Molecule Single Crystal Beamline. The proposal for this beamline is to be reviewed in February 2002. The Danfysik people will start assembling the booster components on October 26 and the commissioning of the booster ring will start at the end of this year. All magnets of the main storage ring have been ordered and will start arriving at the CLS soon. Currently the staff of the CLS consists of 61 people.

*Louis Delbaere*

## NOTICE

# Crystallographic Society of Japan



Noritake Yasouka

## New CrSJ President

Noritake Yasuoka was elected President of the CrSJ in April 2002. Other new members of the Executive Committee include: General Secretary: M. Konno; Treasurer: K. Sugiyama; Chair of the Committee on Meeting and School of Crystallography: Y. Kai, Chair of the Committee on Public Relations: M. Takata; Chair of the Committee on Data Base and Information: H. Uekusa; Chair of the Committee on Journal of the CrSJ: Y. Matsui.

## New logo for CrSJ



The Logotype of CrSJ has been selected. A design by T. Hikone won the contest and has already appeared on the CrSJ home page: [wwwsoc.nacsis.ac.jp/crsj/index-e.html](http://wwwsoc.nacsis.ac.jp/crsj/index-e.html).

## MEETING REPORT

# BCA Winter 2001 meeting reports

## Biological sciences



The winter meeting of the Biological Science Group of the BCA focused on recent results in membrane protein research, and covered expression, crystallization, kinetic crystallography, electron microscopy, single-molecule observations and structural studies. S. Iwata reported the structure of formate dehydrogenase-N at 1.6 Å, the highest resolution for a membrane protein complex obtained so far. More than 200 delegates attended the largest ever BSG winter meeting, which attracted financial support from 10 sponsors.

*So Iwata and Bernadette Byrne*

## Chemical crystallography

'Mesomolecular Crystallography' and structure and bonding in large molecular and supramolecular materials was the topic of the BCA Chemical Crystallography Group.

M. Schroder discussed construction of framework polymers of catenates, helicates and porous materials based on n-connected nets which can arise as a result of metal-metal interactions between organic chains.

Borrowing an idea from synthetic organic chemistry, A. Burrows (Bath) used 'Combinatorial crystallography' to produce supramolecular network formation fashioned from dicarboxylates and thiosemicarbazides in a systematic way, other topics discussed included Hydrogen bonding in Sulfimides (K. Holmes, Loughborough), high nuclearity 3D-Metal cages with unusual magnetic properties (R. Winpenny, Manchester), structures involving large numbers of formula units in the crystallographic asymmetric unit (J. Steed, King's College), the impact of anion size on the structure of polycationic chains in co-ordination polymers (A. Khlobystov, Nottingham), and network structures from the host molecule CTV (M. Hardie, Leeds). Finally, A. Bond (Cambridge) discussed crystal structures of multiporphyrin oligomers and the definition of the term 'mesomolecular crystallography'.

*Harry Powell*

## Industrial group

Pilkington, a company with manufacturing plants in 25 countries, developed float glass in the 1950s. Many Pilkington products are thin films deposited on glass to improve thermal, optical or mechanical properties. At its technical center in Lancashire, powder diffraction is used to check the quality of raw materials, identify the phases in dusts and corrosion products and do troubleshooting on final products. Using X-ray reflectometry, one can obtain information about the film thickness, density and roughness.

The polymorphic form of a drug influences its stability, solubility and hence bioavailability, A. Kavanaugh described how powder diffraction is used to characterize pharmaceuticals at Astra Zeneca where a new system with a point source and a 2-dimensional position sensitive detector is ideal for very small samples and spatially resolved work. M. Abraham (U. of Oxford) described production of nanocrystalline nickel 5 times harder than conventional large grained nickel that is produced by electrodeposition. K. Rogers talked about CdTe-CdS solar cells, synthetic materials that mimic human bone and can be used to repair breaks and make implants, and SAXS on breast tissue with and without cancer.

D. Beveridge (Ilford) discussed silver halide photography, the challenges of trying to identify dyes and pigments in new inkjet products, and how a crystal structure can strongly influence color. I. Slipper described determining glass content in samples of ground granulated blast furnace slag (an additive to cement) and efforts to automate the analysis process.

Many industrial systems cannot be analyzed by classical line profile approaches. Steve Norval (ICI) described a new approach, Linear optimization of a simulated set (LOSS) to handle such problems.

C. Frampton, Chairman of the IG, presented Ian Langford with the Industrial Group Award for his work on profile analysis. Ian has published extensively on zinc oxides which are used in paints, ceramics, catalysts, lubricants, paper, electronic devices, pharmaceuticals and even chemical smoke. Appropriately the award included a Beevers model of zinc oxide.

*Mary Vickers, Cambridge U.*

## Physical crystallography group

A symposium on applications of high-pressure techniques in the study of crystal structures was organized at Daresbury Laboratory. There were talks on the complementarity of Raman spectroscopy and X-ray analysis (A. Jephcoat, Oxford U.), neutron diffraction single-crystal techniques (D. Keen), high-pressure powder-diffraction using synchrotron radiation (M. Mezouar, ESRF), and CCD detectors in high-pressure crystallography (S. Parsons, U. of Edinburgh)

*David Allen*

*BCA Crystallography News, No. 80*

## MEETING REPORT

# Student views down under



Comments from students who attended the 22<sup>nd</sup> meeting of the Society of Crystallographers in Australia and New Zealand (SCANZ) included the following:

Many of the contributions concerned fields of work new to me such as Hirshfeld surfaces and their use in examining intermolecular contacts, quasi-crystals and new aspects of structural biology. The use of powder diffraction to elucidate crystal structures and the loss of water from DNA crystals to give new structures caught my attention at the poster session on Sunday night. (*S. Lorenzo, New South Wales*) Meeting highlights included: Fingerprinting Intermolecular Interaction in Molecular Crystals (*J. McKinnon*), and Practical Aspects of Structural

Genomics (*J. Newman*). The Conference Lecture 'Structural Genomics: A Foundation for Functional Genomics and for 'Fold Phylogeny' given by S.-H. Kim opened my eyes to the immense possibilities and challenges facing science. The overall program was diverse and interesting, and considerable credit should go to the organizing committee for all of their hard work. (*M. Spiniello, Melbourne*)

As an inorganic/supramolecular chemistry PhD student who is learning to use crystallography to determine the structures of metal complexes, the conference was a real eye-opener. The most exciting aspect was hearing about the diversity of areas to which crystallography is applied, including biotechnology, supramolecular chemistry and materials science. (*V. Russell, New South Wales*)

*Taken from SCANZ Newsletter*

## MEETING REPORT

## Protein crystallography in the heart of Europe

What do Walkmuehle near Jena, Luebben near Berlin, Poznan, and Bedrichov in the Czech Republic have in common? They are the sites of past annual Heart of Europe bio-Crystallography (HEC) Meetings, a series, launched in 1998 by Rolf Hilgenfeld and Manfred Weiss. The meetings unite the biocrystallography groups in the region and give young apprentices an opportunity to present and discuss their research. At HEC meetings the podium is reserved for junior participants. Traditionally, there is one invited HEC Lecture. This year, Z. Otwinowski (U. of Texas) spoke about the treatment of errors in processing of X-ray diffraction data. There were 50 participants representing the nine HEC groups (FU Berlin, Charite Berlin, MDC Berlin-Buch, GBF Braunschweig, MLU Halle, IMB Jena, CBB Poznan, IMC Prague, IMG Prague). The HEC family welcomed a new offspring (EMAU Greifswald) led by G. Palm. This year, the First HEC Prize for outstanding presentation (in the form of a book and a certificate) went to Bartholomeus Kuettner (IMB Jena) for his dissection of the structure of alliinase from garlic. The prize, recognized his success as well as his perseverance and determination. The hosts of HEC-4, held September 27-29 in the Jizerske Mountains were J. Sedlacek and his team (R. Stouracova, I. Sieglöva, J. Brynda and P. Rezacova) from the Inst. of Molecular Genetics in Prague. HEC-5 will be organized in Goslar near Braunschweig by Dirk Heinz of the German Research Center for Biotechnology (GBF).

*Mariusz Jaskolski, Poznan*

## MEETING REPORT

# Young people's guide to ACA - LA



The 2001 American Crystallographic Assn meeting in Los Angeles was my first. I found the seminars to be informative and intriguing, and I enjoyed the opportunity to network with my colleagues and peers. My poster presentation allowed me to gain fresh perspectives and to engage in beneficial dialogue about my research. This meeting was one of the highlights in my career and I look forward to furthering my relationships and educational opportunities at the next meeting. (*S. Nadaraia, U. of Missouri, Columbia*)

Monday was the day I found most revealing as it included the Transactions symposium on high throughput crystallography. These talks made me realize for the first time just how much money is going into structural genomics. The automation available, robots which can grow your protein, purify it, crystallize it and mount in on the synchrotron beam line is amazing. Add to this programs like Arp/Warp and, in future, crystallography may be reduced to pressing a button. However, one couldn't help but feel that the most difficult proteins, i.e. those that are insoluble and membrane associated are being neglected by structural genomics. Sometimes I had difficulty choosing between simultaneous sessions, which is better than having no interesting talks to choose from. This is often the situation in meetings where most talks are dedicated to either small molecules and physics or molecular biology. (*V. Tuominen, Turku Centre for Biotechnology*)

The greatest opportunity for me was to present our results and ideas on a new class of metal-organic frameworks we currently explore at the Nat'l Research Council of Canada. What started in 1997 from a single discovery at the Steacie Inst. for Molecular Sciences, has led to dozens of useful host receptors incorporating chelated metal complexes, hundreds of new supramolecular materials and several new ideas for Crystal Engineering. This is why I felt especially honored to receive the Margaret Etter Award. I would be happy to believe that my attendance at the conference was as useful to the society as it was useful to me. (*D.V. Soldatov, Steacie Inst. for Molec. Sci, NRC*)

Challenging crystallographic problems will override the automation of crystal structure determination and require a crystallographers skills. No matter how advanced technology is, an understanding of crystallographic concepts such as the reciprocal lattice, Ewald sphere, space groups, symmetry, twin laws and the phase problem will be required. J.P. Glusker's illustrations helped me a lot her approach to teaching crystallography to the students was the most fascinating part of the meeting. (*Babu A. Manjasetty, U. California, Santa Cruz*)

*From the ACA Newsletter, Winter 2001*

## MEETING REPORT

# High throughput structures



International panel of experts on supramolecular crystallography at the 2001 American Crystallographic meeting in Los Angeles include (first row) R. Tamura, Y. Ohashi, P. Scardi, M. Olmstead, (back row) A. Beatty, J. Lipkowski, I. Huc, G. Gohel, N. Seeman, and M. Fujita.

The CCP4 meeting on 'High Throughput Structure Determination' (January, 2002, York), organized by R. Esnouf (Oxford) and K. Wilson (York), attracted nearly 500 participants.

T. Terwillinger (Los Alamos) described the NIH supported Tuberculosis Structural Genomics Consortium. The consortium has purified 156 of the 4000 gene products of the *Mycobacterium tuberculosis*, crystallized 40 proteins, and determined crystal structures of 22. In a session on high throughput, bioinformatics and optimal target selection, M. Weir (Inpharmatica, UK), described obtaining integrated and interpretable information. J. Gough (Cambridge) explained how the SUPERFAMILY web server (<http://supfam.org>) can assign about half of all new structures to existing superfamilies and J. Peden made a pitch for the uses of Laboratory Information Management Systems (LIMS), P. Alzari (Pasteur Inst., Paris) described optimization of target selection; genomic analysis; functional analysis; proteomics; and comparative genomics. E. de la Fortelle described LIMS that are operational at Structural GenomiX in San Diego. The software tracks highly-automated experiments from the cloning stages through protein expression and purification, crystallization, data collection, structure solution, and 'publication' in the SGX Virtual Journal. Membrane-bound targets are being examined using automated detergent screens. Robotic crystallization for storage/retrieval and image capture allow examination of 1000 plates a day.

A session on techniques included descriptions of recombinant protein expression (I. Jones, Reading), mutant *E. coli* hosts able to overproduce high levels of globular and membrane proteins (F. Hill, Avidis), 96-well plates for the vapor diffusion methods, a multichannel-pipetting robot for drop preparation, a detection system for identification of crystals (L. Nyarsik, Berlin Protein Structure Factory), high-throughput structure determination by NMR (I. Campbell, Oxford) and electron crystallography of very small crystals (J. P. Abrahams).

In a session entitled 'Crystallization/Data Collection' G. Spraggon (GNF) and J. Wilson (York U.) described systems that scan automatically to detect crystals, M. Walsh (ESRF-UK) described robotic devices for mounting crystals developed at ALS, SSRL, APS, and by MSC/Rigaku and A. Thompson (EMBL/ESRF) described developments in beamline automation at ESRF, A. Leslie (Cambridge) reviewed the needs of an 'expert system' to reduce the whole process to pressing a button. We may soon be sending crystals to the synchrotron in steel blocks in a transport Dewar with bar codes. In a session on phasing and software, M. Winn outlined ongoing developments in the CCP4 program package, Y. Jia-Xing described *ab-initio* structure determination of proteins for which atomic resolution data is available with the program ACORN, G. Murshudov talked about recent advances in the REFMAC maximum likelihood refinement program and P. Adams concluded the session with a description of the PHENIX software initiative.

With respect to molecular graphics, D. Turk presented improvements to his Main program for automatic building of maps even at moderate resolution ([www.bmb.ijs.si/doc/](http://www.bmb.ijs.si/doc/)), L. Potterton presented the plans for the CCP4 viewer and demonstrated it in its current rasmol-like state and A. Jones discussed the latest

bells and whistles on O (<http://xray.bmc.uu.se/-alwyn/>). C. Nave reminded us that there are cultural changes on the way in macromolecular crystallography; 'you may be worried by this or excited by it but it will happen'. The volume of the data that worldwide efforts in high-throughput structure determination will yield is daunting and downstream analysis may prove to be the 'real bottleneck' in the future.

*BCA Crystallography News, No. 80*

## MEETING REPORT

# Materials microstructure



Main themes at the Third Size-Strain Conf. in Trento, Italy, (December, 2001) were methodologies for the study of lattice defects, residual stress and texture in thin films and surfaces, line profile fitting/modeling based on fundamental parameters, simulation of materials microstructure, defects related to diffraction profiles, phase analysis with amorphous fractions, highly defective nanocrystalline materials, and residual gradients and stress mapping in thin layers. Conference proceedings are collected in a booklet of extended abstracts (available on request). Abstracts are also displayed in electronic format in the IXAS website ([www.ixas.org](http://www.ixas.org)). A book, containing full chapters of significant contributions is currently being edited (P. Scardi and E. Mittemeijer).

The Barrett Award, established for excellence in the powder diffraction field, was presented to David E. Cox, (Emeritus) Brookhaven Nat'l Lab by P. K. Predecki (U. of Denver). The Jenkins Award, newly established in 2001 to recognize a scientist for lifetime achievement in X-ray analysis of materials, was presented to Ron Jenkins, (Emeritus) ICDD by R.L. Snyder, Ohio State U. Dr. Jenkins also received the Distinguished Fellows award, presented by J. Messick (ICDD). C.R. Hubbard, Oakridge National Labs, presented the 2001 Hanawalt Award to Raymond P. Goehner and Joseph R. Michael, Sandia Nat'l Labs. This award is given in recognition of an important, recent contribution to the field of powder diffraction. The Hanawalt Award lecture, 'Phase identification using electron backscatter diffraction in the SEM: a powerful tool for materials science' was presented at the Plenary Session.

*Paolo Scardi, [paolo.scardi@ing.utitn.it](mailto:paolo.scardi@ing.utitn.it)*

## MEETING REPORT

# ECM20 - Krakow

## Amorphous materials



David Sayre said in his Plenary Lecture, that 'non-periodic objects provide some of the most challenging subjects for crystallographers'. D Cockayne (UK) described the use of energy filtered electron diffraction to obtain structural parameters from small volumes of amorphous materials including samples as small as 2nm on a side. T Weber (Switzerland) discussed the analysis of disordered systems by Monte Carlo methods using algorithms that allow a more extensive search of parameter space compared with traditional approaches. J Cole (UK) showed the power of combining a range of analytical techniques to study the structures of glasses. She analyzed rare-earth phosphate glasses using neutron, X-ray and EXAFS data. A Le Bail (France) stressed the importance of the choice of starting models in refinement algorithms. He compared results from the RDM (Rietveld for Disordered Materials) and the RMC (Reverse Monte Carlo) methods, and raised questions about the optimum approach to take. Y Golubev (Russia) considered supermolecular ordering in some naturally occurring substances, in which globular clusters were detected. An underlying theme of the symposium was the importance of reliable techniques for refining models against structural data, and of obtaining data which can discriminate between alternative models of amorphous structures.

*D Cockayne*

## Quasicrystals



Speakers and chairs in session on Molecular Basis of Disease and Rational Design of Drugs.

M. de Boissieu (France) reported evidence for phason fluctuations detected by high resolution synchrotron X-ray diffraction on single grains of quasicrystals. The I-Cd-Yb phase, the first stable binary icosahedral phase, opens the way for a deeper understanding of quasicrystal structure and formation. Optical conductivity of several intermetallic compounds of the Al-Cr-Fe system in a broad range of frequencies was described by J.M. Dubois (France).

Other topics addressed included stable icosahedral quasicrystals in binary Cd alloys (A.P. Tsai, Japan), a novel method for construction of four-coordinated structures from the Frank-Kasper dense packed systems (V. Dmitrienko, Russia), and the physical and electronic transport properties of quasicrystals determined by their electronic structure (Z. Stadnik, Canada).

*Janusz Wolny*

## Structure determination from powder



Andre Authier introduced Plenary speaker C. Giacovazzo

Two speakers presented the latest results of their work on the global optimisation method using a Genetic Algorithm (K.D.M. Harris, Birmingham) and Simulated Annealing (M.A. Neumann, Accelrys). A new direct space program optimised for non-molecular compounds using object-oriented programming (V. Favre-Nicolin, Geneva), the latest developments of the program EXPO (R. Rizzi, Bari) and a review of achievements of the grid search method in direct space (V.V. Chernyshev, Moscow State U.) were presented. Several oral presentations in other microsymbiosia and plenary lectures by C.J. Gilmore (Maximum Entropy and Structure Solution from Difficult Data) and by C. Giacovazzo (Direct Phasing in Crystallography: from Powder Data to Proteins) dealt with structure solution from powder diffraction. *R. Cerny, Switzerland*

## Minerals



Officers of the ECA 2002: D. Viterbo, C. LeCompte, M. Duarte, M. Jaskolski, G. Filippini, and P. Beurskens. Presentations by representatives from Germany, Denmark, Italy, Switzerland, Russian and Australia described new approaches to the study of minerals including the use of synchrotron radiation and the Rietveld method which has opened a new era in physics and chemistry of minerals and their synthetic analogues. The application of modular theory and the polysomatic concept for the systematization and interpretation of large mineralogical families, namely zeolites, titanosilicates, minerals of heogbemite and eudialite groups, were discussed.

*D. Pushcharovsky, Chairman*

## Physical properties and structural relationships



Alex Wlodawer at the exhibits

Studies of physical properties in organic and inorganic materials were combined with detailed structural investigations in order to identify correlations. J. Cole illustrated the balance between molecular and supramolecular attributes in organic non-linear optical materials designed for potential use in telecommunications. Her structural studies included charge-density experiments, hydrogen-bonding

characterization, bond-length variation and thermal motion analysis. H. Ehrenberg described a type of Morin transition in  $(\text{Co}_{1-x}\text{Mn}_x)_4\text{Nb}_2\text{O}_9$  dependant on the Co: Mn ratio using high-resolution synchrotron powder and single crystal diffraction techniques. For  $x = 0$  a co-linear magnetic structure is observed and for higher Mn content weak ferromagnetism occurs. This transition might find application in new sensor materials. B. Mihailova investigated spatial variation of atomic arrangements and the related strain in ferroelastic W domain walls of lead phosphates using micro-Raman spectroscopy. Using *in situ* high-pressure diffraction experiments, B. Palosz illustrated that the distinctive properties of nanocrystalline materials are critically dependant on the local atomic structure of the constituent crystallites. J. Schreuer demonstrated how resonant ultrasound spectroscopy permits detailed study of the elastic behavior of crystals and how elastic properties can be related to chemical composition.

Ulrich Bismayer and, Katarzyna Stadnicka



## Post closing ceremony pose on the steps of the Lecture Hall with the new ECA banner. Structure prediction

Computational methods for predicting the crystal structures of organic molecules from their chemical diagrams were tested in spring 2001 by the Cambridge Crystallographic Data Centre. Eighteen participants sent predictions for the unpublished crystal structure of each of three organic molecules. Sam Motherwell (CCDC) presented an overview of the results of this test, which enabled nonparticipants to appreciate both the progress and problems in organic crystal structure prediction.

Most successful predictions had been based on searches for the global minimum in the lattice energy. W. Mooij (Accelrys, ex-Utrecht) described how increasingly accurate models for the lattice energy, including atomic multipolar electrostatics and *ab initio* calculation of the intramolecular distortion energy, improved the relative lattice energies of small alcohols and sugars. J. Novoa (Barcelona) demonstrated that dispersion corrected Density Functional calculations predicted that the experimental structure of acetic acid was the global minimum.

This is a significant improvement of the relative energies compared with the GROMOS forcefield. He also described pioneering *ab initio* molecular dynamics simulations, in which crystal structures involving collective proton transfer were seen, emphasizing the limitations of the usual rigid molecular model approximation. J. Breu (Regensburg) emphasized the sensitivity of relative lattice energies to the molecular model, describing calculations on polymorphs in a series of organo-metallic salts. Correcting for the apparent bond shrinkage due to librational motion made a significant difference to the relative lattice energies. Despite the accuracy demanded of lattice energy minimization methods, J. van de Streek (CCDC, ex- Nijmegen), presented the first extensions of such methods to zwitterion and molecular salts, suggesting that the methods may be more widely applicable than previously thought. Although all this work showed that improvements in the computational model increased the reliability with which the known polymorphs would be found at or very close to the global minimum in lattice energy, there often remained rather more energetically feasible crystal structures than known polymorphs. G. Desiraju (Hyderabad) discussed a new approach designed to determine which of the thermodynamically feasible structures were also kinetically favored. He illustrated a method that had successfully re-ranked the low energy structures of one of the molecules in the CCDC test. This was based on identifying crystal structures in the CSD with the supramolecular synthons appropriate to the target molecule, and replacing the parts of the molecular structures which differed.

The microsymposium demonstrated that some organic crystal structures have been successfully predicted, considerable development in the thermodynamic basis of crystal structure prediction is in progress, and fundamental questions about kinetic control of crystallization need to be incorporated into the prediction process.

*Sally Price (UCL) Chairperson*



## U. Shmueli Motion and change in crystals

The dynamics of crystals are usually ignored in diffraction studies, probably because the determination of the static aspects of crystal structures is so sophisticated. Such disregard is not justified! The speakers in this microsymposium illustrated the power of combining diffraction and NMR-methods to reveal motion in deoxycholic acid clathrates (C.K. Prout), to interpret variable-temperature diffraction experiments (C.C. Wilson), to elucidate complex changes in molecular packing within a few degrees of phase transition temperatures (F. Iwasaki), and to distinguish topochemically controlled, organic solid-state reactions from alternative transformation mechanisms, (M. Kaftory), and to classify and understand the phase transitions observed in ionic cyano-elpasolite compounds (D. Chernyshov). A better understanding of the dynamics of phase transitions is relevant to a better understanding of polymorphism. The complex potentials of hydrogen bond dynamics revealed by the atomic displacement parameters of protons may be important for the prediction of structures of biologically relevant molecules.

*H.B. Bürgi, Chair*

## Supramolecular materials



Pierre Becker

Supramolecular systems include discrete complexes, nano-structures, crystal-engineered polymers, and polar molecular crystals. In introductory remarks I. Goldberg (Tel Aviv U.), co-chair of the session, demonstrated successful application of molecular recognition algorithms in the construction of supramolecular porphyrin domains in solution as well as in the solid state. M. Zaworotko (U. of South Florida) discussed the design of hybrid nanoporous solids and discrete infinite structures of nanoscale faceted polyhedra. V. Langer (Göteborg U.) presented a colorful report on efforts to engineer supramolecular hydrogen bonded arrays using organic phosphoric acids as building blocks consisting of layered motifs with architectures that are tunable by chemical modification of the basic unit. S. Bourne (U. of Cape Town) described self-assembly of polynuclear complexes between substituted thioureas and metal ions, showed that the metallomacrocyclic moieties formed in this manner may further combine into polymeric networks, some of which can be useful as chemical sensors for volatile solvents. T. Bartczak (Technical U. of Łódź) addressed the host-guest chemistry of lariat ethers, their conformational flexibility and ability to form supramolecular structures. J. Hulliger (U. of Berne) described polar domain formation in molecular crystals and growth of bipolar macroscopic crystals with an inhomogeneous spatial distribution of polarity by controlled seeding. The phenomenon was studied theoretically and by scanning pyroelectric- and phase-sensitive second harmonic- microscopy.

I. Goldberg

## Cryo electron microscopy



Barbara Oleskyn

The Cryo-EM symposium focused on structural analysis of biological objects that are difficult or impossible to crystallize. Following the plenary lecture by D. Sayre (SUNY, USA) concerning X-ray analysis of a whole cell, E. Orlova (Birkbeck college, UK) began the symposium with a review of the principals of single particle structural analysis and its application on symmetrical (viruses) and non-symmetrical (ribosomes) objects. The resolution alone may not tell much about system functioning since structural fragments could undergo significant conformational changes within the complex. For big complexes, like ribosomes, there is no need to obtain the structure at atomic resolution to confirm that tRNAs have different positions in pre- and post-translocational states. D. Nicastro (MPI fur Biochemie, Martinsried) presented applications of tomography for analysis of cryo-electron images of whole cells and organelles. 3D structures obtained by this technique from a single-axis tilt series of supramolecular assemblies provide new insight into their organization *in situ*. H. Stuhrman (Inst. de Biologie Structurale, Grenoble) described how variation of proton spin polarization can be used for structure determination in a way similar to neutron scattering with various concentrations of D<sub>2</sub>O in crystals. E. Chabriere (U. Henri Poincare, Nancy) demonstrated a direct phasing method, based on topological properties of connectivity of electron density maps, for identification of elements of the protein's secondary structure. J. Bosch (MPI fur Biochemie) combining EM data and X-ray crystallography for structure determination of the Tricorn protease forming hexamers. Finally, A. Urzhumtsev (U. Henri Poincare) discussed modeling bulk solvent in macromolecular crystals.

Elena Orlova

## Enzymes



Henk Schenk

The microsposium on Enzyme Mechanism and Intermediates included reports on the reaction mechanism of urease, a nickel metalloenzyme (S. Ciurli, Bologna), molybdenum and tungsten enzymes (M. Ramao, Lisbon), dehaloperoxidase, a probable descendant of an ancient oxygen carrier (L. Lebioda, South Carolina), ondothiapepsin (J. Cooper, Southampton), intermediate states of thymidilate kinase (E. Fioravanti, ESRF), a novel serine-carboxyl proteinase (A. Wlodawer, NCI Frederick), a bifunctional IMPase/ FBPase enzyme (B. Stec, Rice U.), hyperthermophilic amylase (A. Linden (EMBL Hamburg), an outer membrane protease OmpT (L. Vandeputte-Rutten, Utrecht), and a complex multi-threaded investigation of the mechanism and specificity of L-asparaginase. (J. Lubkowski, NCI Frederick).

Wojciech Rypniewski

## Crystallogenesi



M. Souhassou

R. Hilgenfeld (Jena) discussed developments in crystallization in 13 European groups, the synergy between biology and physics in macromolecular crystal growth, and new crystal kits and methods. Other topics addressed included over expression of proteins in *E. coli* and eukariotic systems (Zou, EMBL), crystallization of membrane proteins, and a semi-rational approach to handling multi-parameter space (J. Zeelen, Frankfurt), control of pH to promote crystallization and act as a cryoprotectant (M. Brzozovski, York), and the importance of the purity in samples of membrane proteins (J. Abramson, Imperial College).  
*Naomi Chayen*

## Theory and experiment



H. Gies and H. Fuess

The 'Wavefunctions and Properties from Experiment' Microsymposium was designed to encompass interactions between theory and experiment, densities other than charge densities and applications of diffraction experiments to theory and chemical properties. D. Jayatilaka reviewed the philosophy behind the extraction of wavefunctions from experimental measurements, described a method for constraining variational quantum mechanical wavefunctions in order to reproduce experimental measurements and outlined applications to three systems from X-ray and polarised neutron diffraction experiments using his TONTO software.



In the central court of the Royal Castle before the banquet at ECM 2001 in Krakow.

B. Dittrich (FU-Berlin) described a straightforward method of space partitioning in the context of transferability of electron density fragments from amino acids and oligopeptides in modelling the electron density of proteins. Hirshfeld surfaces, based on spherical atomic densities for molecules in a crystal, are easy to calculate compared with surfaces obtained from topological analysis of density distribution.

P. Becker (CNRS, Paris) introduced a new approach for computing charge and momentum densities which uses an *ab initio* model in the form of cluster-based calculations and adopts a 1-particle reduced density matrix partitioning scheme to eliminate cluster surface effects. For LiH and MgO crystals the resulting Compton profiles and structure factors compare well with experimental data. The use of Hartree-Fock

and correlated wavefunctions for the clusters enables one to estimate the local correlation effects in ionic crystals. P. Macchi (Milan) showed that the bonding in a series of octahedral metal carbonyl clusters can be characterised according to molecular charges and environments.

This is done in terms of the topology of the electron density, electrostatic properties, and intermolecular interaction energies. Intra- and inter-molecular effects can be distinguished by analysing differences between solid state (experimental) and in vacuo (theoretical) properties. J. M. Raulot (CNRS, Paris) presented an *ab initio* study of two lead-containing perovskite minerals and their ferroelastic and ferroelectric phase transitions. P. Starynowicz (U. of Wroclaw) discussed charge densities in two salts of biologically important phosphate esters.

P. Mallinson

## Prizes



Mike Zaworotko

The ECM 20 Cambridge Crystallographic Data Center (CCDC) Poster Prizes prizes were awarded to:  
L. Dobrzycki, Warsaw (*YAG Crystals Substituted with Erbium and Ytterbium*);

G. Paliwoda, Jagiellonian, Krakow (*Mutual Recognition Between Diastereoisomers, Quinine and Quinidine, in the Solid State*);

M.U. Schmidt, Clariant GmbH (*Ternary Mixed Crystal Structure Solved by Predictions and Powder Diffraction*);

The Prizes (amethyst geodes and \$250 checks) were presented at the Closing Ceremony by CCDC Scientific Director, Frank Allen.

## Protein Crystallography Beyond 2000 (PCB2k) - Satellite meeting on macromolecules



M. Dutheil

High throughput and high quality protein crystallography in the post genomics era brought 60 young scientists and experts together to Krynica, Poland, immediately after ECM20. The PCB2k conference, organized by the Jagiellonian U. (Krakow), the U. of York, and A. Mickiewicz U. (Poznan) with support from the MAX-INF network of European crystallography laboratories and synchrotron sites was divided into four sections. In a section on protein expression and crystallization, T. Wilkinson's (York) introduction to protein production was followed by M. Brzozowski's (York) lecture on crystallogenesis and P. Umbach's presentation of the Protein Structure Factory in Berlin. A session on bioinformatics and structural genomics, included lectures on predicting protein interactions (R. Russell, Heidelberg), analysis of information flow in structural genomics (W. Minor, Charlottesville), crystallographic probing of enzymatic mechanisms (B. Stec, Huston), and presentations from structural genomics centers at Argonne (A. Joachimiak) and Orsay (A. Bentley). X-ray sources and data acquisition strategies were discussed by S. McSweeney (Grenoble) and S. Popov (Hamburg). The phasing and refinement session featured lectures on S/I/Br phasing (Z. Dauter, Brookhaven), automated molecular replacement (C. Kissinger, San Diego), multi crystal averaging (E. Dodson, York), NCS averaging (D. Turk, Ljubljana), maximum likelihood (G.

Marshudow, York), and high resolution structure refinement (K. Wilson, York). The meeting ended with a lecture by G. Dodson (Mill Hill) who summarized the awesome past achievements of macromolecular crystallography and emerging challenges to understanding of the molecular clockwork of the living cell. There were tutorial sessions on HKL2000 (W. Minor), Main (D. Turk), and CCP4 (M. Winn). Discussions continued at a bonfire, with folk music and dancing, that lasted long into the night. The meeting was held concurrently with an ECM20 Satellite on synchrotron radiation organized by J. Grochowski (Krakow). Participants could attend the lectures of both programs, fostering exchange between the biological and physical worlds. We are indebted to the organizational skills of S. Krzywda (York and Poznan) and K. Lewinski (Krakow).

*Mariusz Jaskolski, Poznan*

## AWARDS AND PRIZES

## Honors

The \$35,000 Minister's Prize for Achievement in Life Sciences has been awarded to **Bostjan Kobe** (U. of Queensland) for research in exploring the shape of basic building blocks-proteins. The Prime Minister and Minister for Industry, Science and Resources presented the 2001 Science Prizes during a dinner in the Great Hall of Parliament House on September 25, 2001.

**Chick Wilson** has been awarded the first BTM Willis Prize, from the Neutron Scattering Group of the Inst. of Physics and the Royal Society of Chemistry, for outstanding contributions to neutron scattering science.

**Richard Nelves** was made an OBE, **Andrew Leslie**, **J.A.K Howard**, and **George Sheldrick** have been elected Fellows of the Royal Society, and **Julia Higgins** was made a Dame in the Queen's Birthday Honors in 2001. **Jack Dunitz** was made an Honorary fellow of the Royal Society of Chemistry, **Jane Brown** was awarded the 2001 Walter Hargraves Prize. **Dorothy Hodgkin** was honored by the presentation of a Royal Society of Chemistry Landmark in Oxford.

**Gabor A. Somorjai**, professor of chemistry at the U. of California, Berkeley received the US National Medal of Science.

NOTICE

## In the news

Dr. Richard Walker, who spent 13 years in the Accelerator Physics Section at Daresbury Laboratory, has been appointed Technical Director for Diamond, the synchrotron due to be built at the CLRC Rutherford Appleton Laboratory

*BCA Crystallography News, No. 80*

**NOTICE**

## The Chatt lecture 2002

The second Chatt lecture was presented by Tom Blundell (Cambridge) on January 25<sup>th</sup> at the John Innes Center in Norwich, UK. The lecture is held in honor of Joe Chatt, Director of the Nitrogen Fixation Unit from 1962 until 1980. In his talk entitled 'The post genomic challenge: from sequence, to structure, to function and therapeutic intervention', Blundell presented the thesis that the process can be automated by using homology modeling to trace evolutionary relationships between protein molecules.

## NOTICE

## A Critical Assessment of Predicted Interactions (CAPRI)

CAPRI is a blind test of the ability of protein docking algorithms to predict the mode of association of two proteins based on their three-dimensional structures. The prediction starts whenever an experimentalist offers an adequate target, and ends six to eight weeks later with the submission of predicted structures.

The Management Group of CAPRI calls upon all structural biologists who have just completed, or hope to complete soon, the X-ray or NMR structure of a protein-protein complex, to provide new targets. If both components of the complex are already in the Protein Data Bank, predictors will be given the two ID codes. Alternatively, only one component structure may be available. The other is then given as atomic coordinates carved from the complex and communicated by the authors on a confidential basis. Six to eight weeks later, a complete set of coordinates should be forwarded to the member of the Management Group in charge of evaluation, also on a confidential basis.

We hope that CAPRI will attract crystallographers and structural biologists who reckon that the predicted modes of association can be useful guides for genetic and biochemical experiments, but the prediction methods and the algorithms must first be extensively tested and their validity assessed.

*The CAPRI Management Group:* K. Henrick (Hinxton, UK), J. Janin (Gif-sur-Yvette, France), J. Moult (Rockville, MD), L. Ten Eyck (San Diego, CA), M. Sternberg (London, UK), S. Vajda (Boston, MA), S. Wodak (Brussels, Belgium).

For information on submitting targets, visit <http://capri.ebi.ac.uk> or contact J. Janin ([janin@lebs.cnrs-gif.fr](mailto:janin@lebs.cnrs-gif.fr))

## BOOK REVIEW

## BOOKS

✓ **Forensic Science: Every Contact Leaves a Trace, in Industrial Applications of X-Ray**

**Diffraction**, Eds. F.H. Chung & D.K. Smith, Marcel Dekker Inc., New York/Basel, pp. 659-675. D.F. Rendle (2000).

✓ **Dynamical Theory of X-ray Diffraction** by André Authier. This is the first comprehensive book on the dynamical diffraction of x-rays since the development of synchrotron radiation. Authier begins with an introduction to the subject, presenting early developments and the basic results, followed by a development of the diffraction and propagation properties of x-rays in perfect crystals and by an extension of the theory to the case of slightly and highly deformed crystals. The last section presents three applications of the theory: x-ray optics for synchrotron radiation, locations of atoms at surfaces, and x-ray diffraction topography. The book is well illustrated and contains a wide range of references to the literature.

## AWARDS AND PRIZES

# Mineralogical Society awards



Peter J. Wyllie

The eighty-second annual awards luncheon of the Mineralogical Society of America (MSA) was held on November 6, 2001, during the 2001 Geological Society of America meeting in Boston, MA. **Peter J. Wyllie**, was awarded the Roebling Medal for lifetime scientific Achievement. The Distinguished Public Service Award was presented to **Jeffrey E. Post** for his work as lead curator of the Smithsonian's new permanent exhibition 'Geology, Gems and Minerals'.



Jeffrey E. Post

**Peter C. Burns** received the MSA Award for outstanding early career research. He was promoted to Associate Professor of geology at the U. of Notre Dame in 1999, and became the Henry Masman Chair in Civil Engineering and Geological Sciences in 2000. He directs the Environmental Mineralogy and Crystal Structures research laboratory, and has research interests in low temperature mineralogy, especially the mineralogy of actinides.



Peter C. Burns

The Mineralogical Society's website continues to expand and develop thanks to Gordon Nord. In October there were 138,000 hits. The website includes new additions, funded in part by the NSF, including 'Mineralogy 4-Kids' developed by the K-12 Outreach Coordinator, N. McMillan and the Crystal Structure Database managed by B. Downs and P. Heese. The MSA Lecture Program, coordinated by Helen Land, has been expanded to include tours outside of North America. Next year three lecturers, B. Bodnar, R. Rudnick and C. McCammon, will visit 35 institutions. The membership has increased to just over 2100 members. Over half of the several hundred member increase is from student memberships. Pressing questions from the society include: How will we interact with other Societies in arranging meeting and related publications? Are there other societies in materials and environmental science communities that should be included?

Grants for Research in Crystallography from the Edward H. Kraus Crystallographic Research Fund were increased to \$5000 starting in 2002.

*The Lattice, Volume 17, No. 4*

## MISCELLANY

## Rietveld on Rietveld

Thirty-five years ago in the search for mechanically stable fuel element for nuclear reactors, the structure of some uranates had to be determined. Because of the small crystal size only powder diffraction data were available. This restriction was an immense obstacle, because in those days only single crystal diffraction data could lead to a successful refinement. Powder diffraction was regarded to be obsolete for refining structures, because of the problem of overlap with low symmetry compounds and at high diffraction angles. Step scanning yielded a powder diagram that showed definite detail in the profile of these overlapping peaks. The information contained in this detail could however not be extracted by conventional means and one had to resort to taking the sum of these overlapping peaks as data for the least squares refinement. It was therefore clear that full use was not made of the information contained in the powder diagram.

My experience with computers, built up over the years doing single crystal diffraction work, gave me a head start in tackling this problem of extracting the maximum amount of information from a powder diagram. My efforts ultimately led to what is now known as the Rietveld Method. When the method was first reported in Moscow in 1966 at the IUCr Congress, there was hardly any response. A few years later, when I wrote a more comprehensive computer program, first in Algol 60 and later in Fortran IV, the demand for the program and its subsequent use increased, and the popularity of the Rietveld Method grew. I already had foreseen that it could be used for X-ray data, but due to the lack of an actual problem, I did not pursue it any further.

I am totally amazed looking at the ever-increasing use that is being made of the method. Yearly, hundreds of publications use or refer to the method. What began as a solution for a particular problem, turned out to be a tool of much broader value. Now it is not only applied to structure refinement, but also to such diverse fields as quantitative phase analysis, measurement of strain and size and the analysis of time-resolved data. I am deeply gratified that I could have been instrumental in reviving the powder diffraction method. This in itself would have given me enough satisfaction. Receiving the Gregori Aminoff Prize in 1995 from The Royal Swedish Academy of Sciences for my work gave an added luster.

*Hugo Rietveld*

*Thirty Five Years Ago, Newsletter of the  
Commission on Powder Diffraction, (No. 26, Dec. 2001)*

## OBITUARY

**Don C. Wiley (1944-2001)**

The accidental death of Don C. Wiley, Harvard U., on November 16, 2001, has deeply saddened the scientific community worldwide. Don went to Tufts U. as an under graduate, and was a graduate student in biophysics at Harvard U. with William Lipscomb. Don became an assistant professor in the department of biochemistry and molecular biophysics at Harvard and spent a sabbatical at the medical research council (MRC) Cambridge and the National Inst. for Medical Research, Mill Hill London, in 1976 pursuing crystallization and diffraction studies of the Hong Kong 1968 influenza virus hemagglutinin with Joan Skehel. I became Don's first postdoctoral fellow in 1977. Those years were to be as exciting as one could ever imagine in a scientific venture. We received monthly shipments of the HA protein from Skehel shipped in hand-blown glass vials lovingly cradled in fluffy white cotton wool. Countless oscillation photographs of both native and heavy atom derivatives of HA were collected on an Elliott X-ray GX-6 machine. Only one suitable heavy atom derivative was found, which necessitated averaging and solvent flattening concepts that had only been used in cases of extensive non-crystallographic symmetry. Don adapted the Bricogne Program that Steve Harrison had used for tomato bushy stunt virus (TBSV), provoking a great deal of skepticism even from Bricogne who questioned whether three-fold averaging of data phased on a single derivative with no anomalous information could work. It did! Cycle by cycle, the map improved culminating with a 75% phase difference from beginning to end – one could now visualize the outline of the long trimer of the HA stacked like Lincoln logs head to tail around a four-fold screw axis. The structure was one of the first to be built on the computer, rather than in a Richard's box, using the BILDER program of Bob Diamond, as modified by Bob Ladner at Harvard. The structure was amazing with its globular head and long helical coiled-coil system. Don mapped the antigenic variations of the influenza virus from 1968 to 1977 onto the HA structure. The results were astounding as the mutations mapped into four discrete areas on the HA structure – it appeared that for a new viral epidemic strain to emerge, mutations were required in four regions on the surface. It was immediately apparent that carbohydrate could mask the surface and help render the virus invisible to the immune system, whereas the few highly exposed regions accommodated most of the amino acid variation and acted as a decoy to avert the immune response away from the conserved receptor binding site. The impact of these structure on the virology and immunology communities was profound. The HA was to become the model for how the enveloped viruses fuse their membranes with the host cell. Don followed up that work with the structures of fusion domains of HIV-1 gp41 and Ebola virus. In 1987, the major histocompatibility (MHC) complex class molecule, HLA-A2 was unmasked by Don, Pamela Bjorkman, and Jack Strominger and another historic milestone was achieved. The HLA structure revealed a completely new fold, now known as the MHC fold. Between the  $\alpha$ -helices and the  $\beta$ -sheet floor was a long, narrow groove in which extra density was seen that could not be accounted for by atoms of the MHC. The density was a mixture of bound short peptides that are derived from digestion of intact protein antigens by the proteasome. The polymorphic residues of the class I MHC mapped beautifully onto the walls and floor of the groove exactly where the peptide contacted the MHC. At last, one could visualize how the MHC was able to present peptides to the T cell receptor. It would take another five years to untangle the details of the peptide interaction due to the difficulty of making single peptide MHC complexes. It is hard to capture the vastness of the contributions that Don made to virology, immunology, structural biology, molecular biology, cell biology, and biochemistry. His legacy is monumental. It epitomizes how structural work can facilitate a deep understanding of complex biological processes. Don was awarded the Gairdner Foundation Award (1994), the Lasker Award (1995) and Japan Prize (1999). he became a Howard Hughes

Medical Ins. investigator in 1987 and was elected to the national academy of sciences in 1991. Don was a captivating speaker whose reasoning was painstaking and thorough. He was the consummate scientist that most aspire to be. In our sorrow over this terrible tragedy, we celebrate and pay tribute to the tremendous career that brought so many insights into really important scientific problems.

*Ian A. Wilson, Nature Structural Biology, Mar. 2002, Vol. 9, No. 33*

**OBITUARY**

## **Norio Kato (1923-2002)**

We are saddened to learn of the death of Professor Norio Kato, an exceptional crystallographer and President of the IUCr from 1978-1981. He died at his home in Nagoya from heart failure.

*Chris Gilmore*

## OBITUARY

## Jim Graham (1929-2001)

Jim Graham, UWA, received a Hackett Research Scholarship in 1953 to study for a PhD at the U. of Birmingham. He completed his PhD in Physical Metallurgy, under the legendary Gilbert V. Raynor, Professor of Physical Metallurgy.

He returned from Australia to work as a Research Officer in the Cement and Refractories Laboratories of the CSIRO Division of the Industrial Chemistry, Melbourne and to Perth in 1964 to set up microprobe, micro analysis and X-ray diffraction (XRD) facilities in the new Secondary Industry laboratories of the Div. of Applied Mineralogy.

He published over 100 papers and technical reports, in crystallography, solid state physics and chemistry of minerals, particularly those hosting the nickel, tantalum and titanium deposits of WA, applied mineralogy, physical methods of analysis and characterization of minerals, including XRD, electron beam and magnetic methods, quantitative analysis by XRD, and trace analysis using the electron microprobe analysis.

He was a Founding Member of the Society of Crystallographers in Australia and a member of the Committee that organized the IUCr Congress and General Assembly (1987).

With his long academic and industrial research experience, quick brain, good nature and judgment and calm temperament, he was a wonderful mentor to students, colleagues and industry collaborators.

*Frank Lincoln, SCANZ Newsletter June 2001*

## OBITUARY

## Ryoichi Sadanaga (1920-2002)



With profound regrets we send the sad announcement that Emeritus Professor Ryoichi Sadanaga, having struggled against cancer for the last few years, passed away on January 17, 2002. He was born in 1920 in Osaka Japan. After he graduated from the U. of Tokyo in 1943, he remained there first as a Research Assoc., then Lecturer and Assoc. Professor. He worked with the late. K. Lonsdale at the U. of London for two years starting in 1951. From 1954 to 1981 he taught and did research on X-ray crystallography and theoretical crystallography as Professor of Mineralogical Inst., Faculty of Science, U. of Tokyo. He successively held the posts of President of the Crystallographic Society of Japan and President of the Mineralogical Society of Japan. The crystallographic community of Japan has appreciated his great contributions to the promotion of crystallography in Japan not only in mineral science but also in material science. He successfully organized the IMA-Kyoto meeting in 1970 and the IUCr-Kyoto conference in 1972. After his retirement he became an honorable member of the Japanese Academy of Science. For many years he served on the Editorial Board of the Proceedings of the Japan Academy and made great efforts to publish papers relating to crystallography. During his career, he mentored many young Japanese crystallographers. His theoretical works on 'Diffraction Enhancement of Symmetry' and 'Space Groupoids' were acknowledged in the International Tables for X-ray Crystallography, Vol. A (1983). We, his pupils, cannot adequately express our grief and sorrow at his passing.

*Takamisu Yamanaka*

## MISCELLANY

# The very model of a protein crystallographer

I am the very model of a protein crystallographer  
Not just a biologist but density cartographer  
I know the space group symmetries triclinic and tetragonal  
And cubic, monoclinic not to mention the hexagonal

I'm very good at FFT's and series termination flaws  
And the corresponding ripples that they too often cause  
Jokes about P1 bar leave me doubled up in laughter  
As I am the very model of a protein crystal(lo)grapher

I can tell a  $\beta$ -sheet from helix or a random coil  
And to Ramachandram plots I am currently immensely loy'l  
I know when a protein comes from *S. typhermurium*  
And I have read the scientific works of Dr. Kuriyan

I can write coordinates in formats for the PDB  
And often have to pay a large proprietary software fee  
I know of EJ Dodson and sometimes I talk with 'er  
As I am the very model of a protein crystallographer!

*Severely abridged from Janet Newman's rendition of Gilbert and Sullivan's 'A Model of a Modern Major General' forwarded by Mitchell Guss.*