

INTERNATIONAL UNION OF CRYSTALLOGRAPHY

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# IUCr Newsletter

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Original article text and available illustrations

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## LETTER FROM THE PRESIDENT

# Letter from the President



William L. Duax

Since becoming president of the IUCr, I have had the opportunity to visit Moldova, Germany, Russia, Algeria, Brazil, Denmark, Italy, and Canada. In each country I met with crystallographers to discuss their strengths, goals, and needs. Brief reports on my visits to Moldova and Novosibirsk appear in this issue. I would like to visit crystallographers in all countries that adhere to the Union, but that is not possible. I have written letters to each of the members of the Executive Committee asking for their help in reporting on the activities of the Union in the 38 countries that currently belong to the Union. I have also asked for their help not only to expand Union activities in these countries, but to extend our services to the dozens of countries that are not presently members. I have asked them to take every opportunity when traveling abroad to offer to meet with crystallographers, as an official representative of the IUCr, and to discuss their needs. The Executive Committee has members in the three Regional Affiliate domains, AsCA (Y. Ohashi and Z. Zhang), ECA (L. Aslanov, M. Carrondo, D. Viterbo, G. Heger, S. Larsen, and H. Schenk) and ACA (I. Torriani and W. Duax).

I attended the biannual meeting of the Brazilian Crystallographic Soc. (BCO) in São Paulo, Brazil, where I was extremely impressed with the vibrancy of their crystallographic activities. Iris Torriani, Executive Committee member from Latin America is gathering material for an issue of the IUCr Newsletter that will highlight Crystallography in Brazil. The issue will include a report on the biannual meeting, a survey of crystallographic laboratories in Brazil, the structure, officers, by-laws and programs of the BCO and the Brazilian Nat'l Committee for Crystallography, a detailed report on the history and development of one laboratory, a report on the only synchrotron facility in the southern hemisphere and a brief summary of Iris Torriani's current research activities and responsibilities.

I went to Florence to meet with Carlo Mealli, (program chair) and other members of the local committee for the 2005 IUCr Congress. While there I also had extended discussions with Italian representatives on IUCr Commissions and with Davide Viterbo, a newly elected member of the IUCr Executive Committee. The Italian Crystallographic Assn will be meeting in Trieste in May 2003. Davide has agreed to prepare a report on Crystallography in Italy having the same form and content as the report on Brazil.

I hope that these will be the first in a series of IUCr reports that will eventually cover all countries in the Union. I will be asking each member of the Executive Committee to take responsibility for developing such reports from the countries in their regional affiliate. Sine Larsen and Henk Schenk will see to it that reports on upcoming meetings of the Danish and Dutch Crystallographic Assn will be submitted to the IUCr. I urge Brazilian and Italian crystallographers to lend their support to Iris and Davide when they write their articles. I would be most happy to see crystallographers everywhere contact members of the executive committee and offer to assist them in preparing reports on crystallography detailing activities in their home countries.

At a meeting of the Finance Committee, we learned that authors submitting papers to Union journals currently come from 70 countries indicating that there is interest and activity in at least 20 countries that are not presently members of the IUCr.

*Bill Duax*

*duax@hwi.buffalo.edu*

## EDITORIAL

# Guest editorial - John R Helliwell

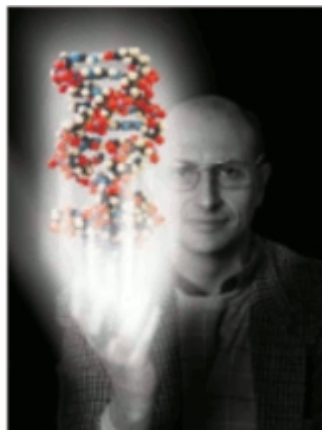


Image: J. R. Helliwell 'holding infinity in the palm of his hand' (William Blake)

Interviewed by the U. of Manchester magazine recently for a personal profile article, in the end entitled 'John's Journey', I responded to the question 'Why did I decide to concentrate on science at age 16?' with the reply 'For no good reason, but I do recall having had excellent science teachers at my school'. On reading this in the cold light of day of the printed copy I felt slightly shocked ie where was the flash of insight and passionate call to science. Fortunately, as well as '...no good reason...', I did mention my vivid memory of using the prism spectrometer in the school physics lab; the awe inspiring moment when you see for the first time the discrete emission lines from a sodium vapour lamp...that it is indeed not a continuum emission of light....that the periodic table of the elements, indeed all of chemistry and life itself, rests on the electronic discrete energy level structure of the atom seen through that eyepiece. But clearly my recollection was that my teachers were the most important factor in inspiring me into science. I had, in that interview, re-realised the importance of being a good teacher. Within this theme of re-inspiration something else important happened for me recently. Whilst I was amidst tortuous budget wrangles and seemingly endless centrally imposed audits, I found myself listening to a cassette tape of Sir Aaron Klug's Rosalind Franklin Lecture given in 1999 at The Royal Society. In fact I have listened to this tape several times over. Sir Aaron's lecture truly gripped me with its clear and lucid exposition of Rosalind Franklin's work. I felt inspired, actually my point in this Guest Editorial is that I felt re-inspired, by hearing afresh the details of Rosalind Franklin's work. The truly beautiful work of the physical chemist turned diffractionist achieving the careful humidity controlled isolation of the diffraction patterns from distinct A and B form DNA structures; 'humidity-resolved' structural intermediates. Of course DNA is very much on our minds this year with the 50<sup>th</sup> Anniversary celebration of the double helix structure model from the X-ray fibre diffraction work by the 'networked' research groups of Cambridge and Kings' College London. The magic of those three papers in *Nature* in 1953 from the teams of researchers involved, along with the breakthrough helical diffraction theory paper published in 1952 in *Acta Crystallographica*, changed the face of science in so many fields. Today, fifty years on, as crystallographers and diffractionists, we have the privilege to live daily the beauty and importance of, in Sir Lawrence Bragg's words, 'seeing atoms'. Currently for me this means the understanding of the intricacies of the colouration mechanism of the lobster carapace, neutron protein crystallography studies, and also my Lab's starting structural studies of our protein targets within the global project on *Mycobacterium tuberculosis* led by Los Alamos and U. of California, Los Angeles, USA as well as helping with the bringing on-line of the new MPW-MAD10 beamline at Daresbury SRS.

## LETTER TO THE EDITOR

## MAD about identification

Dear Judith,

Yesterday I got my copy of the IUCr Newsletter, Vol 10 # 3. I must say I'm rather puzzled by the illustration you have chosen for the paragraph 'MAD, Sad and difficult phasing' on pag. 11. I don't see any madness, sadness and certainly not difficult phasing in the picture. Maybe you did not want the people on the photographs to be identified easily, so both names were misspelled intentionally.

*Sybolt Harkema*

Dear Sybolt,

The photograph you refer to in your letter was not intended to be part of the 'Mad, Sad and Difficult Phasing' article. It was just a nice photo from the IUCr Congress that we used to insert some color and to provide a break in the text for that page. I apologize for the typos in the spelling of the names. I think the problem here was that they are so easily identified just by looking that we didn't pay enough attention to the figure legend.

*Judy*

LETTER TO THE EDITOR

## Magazines available

Dear Judy,

I am just reading your note in the current number of the IUC Newsletter. I have 40 years (almost complete but unbound) of the Scientific American (1960-2001) to give away to anyone who may bring a truck to the door (in North London) after giving me notice of time and date.

*Alan L. Mackay*

## LETTER TO THE EDITOR

# Large crystals!

Dear Editor:

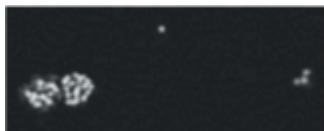
I was excited to see the article on the Singapore Crystal Growth Challenge in IUCr Newsletter Volume 10(3). As we grow crystals of chrome alum in one of our freshman laboratories here at Illinois State, it was nice to show the students just how large some of these crystals can grow! However, my students and I have to wonder about the caption for the 'prize-winning crystal' displayed. Certainly we can not be the only ones in the crystallographic community who would notice that those units must be  $\text{cm}^3$  not  $\text{mm}^3$ ! A quick check of the referenced SNIC website reveals the truth. I guess no one ran checkCIF on that one!

*Craig C. McLauchlan*

## IUCR JOURNALS NEWS

# Experimental lensless soft-X-ray imaging using iterative algorithms: phasing diffuse scattering

***Acta Cryst.* (2003). A59, 143-152**



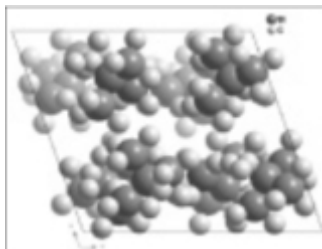
Clusters of gold balls, 50 nm diameter, imaged using soft x-rays. Image obtained using iterative algorithm to solve the phase problem. Resolution about 10 nm.

Phase information is encoded in diffuse x-ray scattering from nonperiodic objects if it is sampled finely enough. The Fienup HiO iterative algorithm has proven the most successful method of extracting it. We record soft x-ray ( $\lambda = 2.1$  nm) transmission speckle patterns from clusters of 50 nm diameter gold balls lying on a transparent substrate. We use the HiO algorithm to solve the phase problem and so reconstruct images of the balls. The presence of an isolated ball also produces a faithful image in the Patterson map. A reconstructed image is shown to the right. Beam stops, absorption filters, density modification and Fourier transform holography are also discussed.

*H. He, S. Marchesini, M. Howells, U. Weierstall, G. Hembree and J.C.H. Spence*

# Influence of the molecular structures on the high-pressure and low-temperature phase transitions of plastic crystals

***Acta Cryst.* (2003). B59, 60-71**



The unit cell and the molecular packing of the low-temperature structure of  $\text{Si}[\text{C}(\text{CH}_3)_3][\text{Si}(\text{CH}_3)_3]_3$  viewed along the monoclinic axis. Only the most probable orientations of the molecules are shown. The compounds *tert*-butyl-tris(trimethylsilyl)silane,  $\text{Si}[\text{C}(\text{CH}_3)_3][\text{Si}(\text{CH}_3)_3]_3$  (Bu1), and  $\text{Si}[\text{C}(\text{CH}_3)_3]_2[\text{Si}(\text{CH}_3)_3]_2$  (Bu2) belong to a class of crystalline molecular compounds with orientationally disordered, quasi-spherical molecules in a cubic closest packed (ccp) arrangement. Solid-state NMR studies have shown that the molecules undergo rapid (kHz scale) reorientational jumps about fixed centers of mass forming so-called 'rotator-phases' or 'plastic' crystals. X-ray powder diffraction with synchrotron radiation is used to characterize the order-disorder phase transitions at low temperatures and high pressures. The structure at 105 K corresponds to a monoclinically distorted ccp arrangement with partial orientational order of the molecules. At room temperature the same structures are found at 0.3 GPa, but additional phase transitions are found at still higher pressures, up to 5 GPa, that are tentatively interpreted as due to further orderings of the molecules.

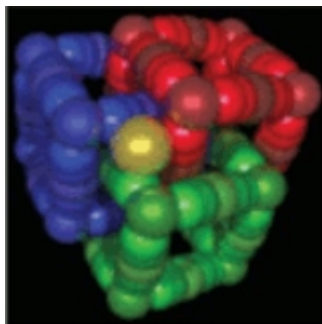
*Markus Wunschel, Robert E. Dinnebier, Stefan Carlson, Piotr Bernatowicz and Sander van Smaalen*

## IUCR JOURNALS NEWS

# KMnAg<sub>3</sub>(CN)<sub>6</sub>, a new triply interpenetrating network solid

KMnAg<sub>3</sub>(CN)<sub>6</sub>, a new triply interpenetrating network solid

*Acta Cryst.* (2003). C59, i21-i23



The designers of open-frame network crystals face the age-old conundrum that nature abhors the void, i.e., the network distorts to a denser form unless special precautions are taken during the crystal growth. However, if the bridging ligand has a strong propensity for staying straight, the system has yet another possibility: it can grow in the form of interpenetrating networks, such as in the title compound. This particular triply interpenetrating net has been seen in a few other salts, but never before with paramagnetic manganese(II) in the lattice. The exceptionally precise structure determination ( $R_1 = 1.2\%$ ,  $wR_2 = 3.2\%$ ) allowed for the unequivocal assignment of carbon vs. nitrogen atoms and the resolution of a symmetry ambiguity.

*Urs Geiser and John A. Schlueter*

## IUCR JOURNALS NEWS

# Sheldrick's 1.2 Å rule and beyond

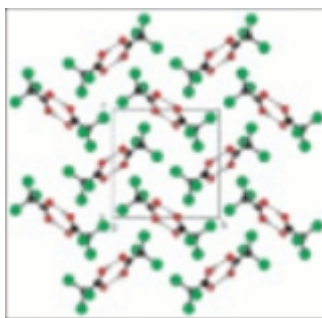
## ***Acta Cryst.* (2003). D59, 615-617**

In 1990 George Sheldrick summarised his experience in solving crystal structures of small organic molecules by the rule that at least half the number of possible reflections between 1.1 and 1.2 Å resolution had to be well measured [ $F > 4\sigma(F)$ ] for direct methods to succeed (*Acta Cryst.* A**46**, 467–473). The present authors investigate the expectation value  $|E|^2$  of the squared normalized structure-factor amplitude as a function of resolution for numerous organic molecules, including 700 proteins. Direct methods assume that atoms are statistically independent and predict  $|E|^2 = 1$  at all resolutions. However, the authors observe a consistent peak with a value of about 1.3 around a resolution of 1.1 Å, and trace its origin to not only the existence of individual bonding distances, but to the occurrence in these molecules of numerous families of inter-atomic distances which *differ* by 1.1–1.2 Å. They conclude that incorporating data in this critical resolution range contributes not only to resolving atoms, but also to introducing some of the structural information that is missing from the stereochemistry-free foundations of direct methods. Finally, they argue that a 'stereochemically aware' extension of direct methods proposed by the senior author should significantly relax the data resolution requirements embodied in Sheldrick's rule.

*Richard J. Morris and Gérard Bricogne*

# Trichloroacetic acid at 105 K

***Acta Cryst.* (2003). E59, o316-o318**



Packing of the molecules, viewed down the *a* axis.

Crystal structures of a number of simple compounds remain unknown for a variety of reasons. The answer to 'Why has the crystal structure of trichloroacetic acid, a simple and yet an important compound, not been reported until now?' lies perhaps in its highly deliquescent nature. This low-temperature x-ray study reveals that the molecules form centrosymmetric pairs leading to hydrogen-bonded dimers. In the absence of 'scope' for other strong intermolecular interactions, Cl...O and Cl...Cl interactions presumably play a role in stabilizing the crystal structure. Interestingly, there is another dimension to simple crystal structures of these types: trichloroacetic acid represents a class of simple organic molecules of the type R-COOH and accurate x-ray crystallographic investigations on such molecules may prove to be useful in the design of crystals, assuming a 'direct' relationship between the nature of R and the difficulty of design.

*K. Rajagopal, A. Mostad, R. V. Krishnakumar, M. Subha Nandhini and S. Natarajan*

## IUCR JOURNALS NEWS

# Polycapillary focusing optic for small-sample neutron crystallography

*J. Appl. Cryst.* (2002). 35, 677–683



The image of the focused beam using a tapered monolithic lens with cold neutrons. The focal spot at the center is about 100  $\mu\text{m}$  wide. Both the shadow of the hexagonal cross section of the optic and the background halo of neutrons passing through the optic and inside the collimator are concentric around the focus when the optic is aligned with the incident beam. Photos of the lens interior entrance cross section and exterior are also shown.

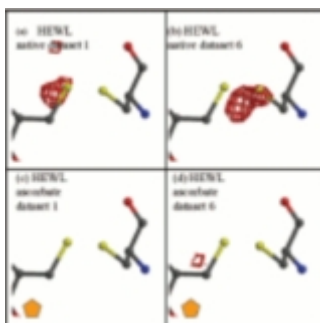
The relatively low flux from neutron sources means that structural analysis using neutron diffraction requires large crystals that are often unavailable. Recent demonstrations of convergent beam electron and x-ray diffraction have motivated the use of polycapillary optics for small-sample crystallography using convergent neutron beams. We have examined the use of a focusing optic for diffraction of both monochromatic neutrons at the NIST research reactor and for time-of-flight polychromatic neutrons at the Intense Pulsed Neutron Source (IPNS) at Argonne National Laboratory. The convergent beam method (CBM) promises advances for crystallography on small samples (less than 500  $\mu\text{m}$ ) of small- to medium-size molecules at extreme pressures and temperatures, for proteins (as demonstrated for x-rays), and for strain and texture mapping of polycrystalline samples.

*W. M. Gibson, A. J. Schultz, H. H. Chen-Mayer, D. F. R. Mildner, T. Gnäupel-Herold, M. E. Miller, H. J. Prask, R. Vitt, R. Youngman and J. M. Carpenter*

## IUCR JOURNALS NEWS

# Papers from Second International Workshop on X-ray Damage to Crystalline Biological Samples

*J. Synchrotron Rad.* (2002). **9**, 327–381



Electron density  $F_o - F_c$  maps of the Cys76-Cys94 disulphide bond in HEWL crystals. (a) and (b) (top left, right) for the first (left) and sixth (right) datasets from a native HEWL crystal, (c) and (d) (top left, right) for the first (left) and sixth (right) datasets from a crystal grown in the presence of 0.5 M ascorbate. Macromolecular crystallographers are now actively investigating radiation damage processes in cryo-cooled (around 100 K) crystals. The aim is to understand them well enough to design minimization and/or mitigation strategies so that intense undulator-produced synchrotron beams can be fully utilized.

The November 2002 issue of the *Journal of Synchrotron Radiation* contains a collection of eight papers on this topic, with an introduction summarising the current status (Garman and Nave). Among the reported experimental results is evidence, provided by reduced specific structural damage and absorption spectra collected with a microspectrophotometer, that the introduction of a radical scavenger (0.5 M ascorbate co-crystallised with HEWL) can prolong the crystal lifetime in the x-ray beam (Murray and Garman). Physical and chemical processes relevant to the damage process are also discussed (O'Neill, Stevens and Garman).

## IUCR ACTIVITIES

# Final report of the Inter-Union Bioinformatics Group



H. J. C. Berendsen

The Inter-Union Bioinformatics Group (IUBG) is a Joint Initiative of the Int'l Union for Pure and Applied Biophysics (IUPAB), the Int'l Union of Biochemistry and Molecular Biology (IUBMB), the Int'l Union of Crystallography (IUCr), the Int'l Union of Pure and Applied Chemistry (IUPAC) and the Committee on Data for Science and Technology (CODATA). The IUBG seeks overlap with the nomenclature committees of IUCr, IUBMB, IUPAC, and CODATA. The IUBG has received support from the ICSU (Int'l Council for Science) Grants Programme and UNESCO (United Nations Educational, Scientific and Cultural Organization).

## Summary statements

**The safeguarding of biological data:** It is the obligation of the scientists and legislators of all nations to archive and support primary (i.e., fundamental experimental) scientific data, including, but not exclusive to, nucleotide sequences of biological organisms, aminoacid sequences of proteins, three-dimensional structures of biological molecules, as well as other primary data produced by genomics and proteomics studies. These data must be validated, stored, made publicly accessible, and safeguarded for future availability and access. Access must be public and unrestricted and no organization should have a monopoly on these data. These primary scientific data are crucial for the development of science and its applications.

**The obligations of data generators:** It has always been the practice that those who claim scientific advances by publication of their work should support their claim by making openly available the objective data on which their claim is based. Thus it is the obligation of scientists who generate primary biological data in the course of publicly funded research to preserve these data for present and future reference and unrestricted access. Regardless of whether publication in journals is appropriate, such data must be deposited into the archival databases to guarantee their availability. Primary data producers in the private sector are also urged to conserve and eventually deposit their primary data.

**Right to fair use of data:** Scientific advances rely on full and open access to data. Primary data that are accessible through the archival databases should not be subjected to any restrictions that would limit fair use of those data. Fair use includes the use for teaching and research purposes.

**Standardization issues:** here are four different aspects associated with primary data for which standardization should be considered: *content*, *nomenclature*, *data format*, and *data exchange protocol*. Standardization is an ongoing activity requiring high-level agreement among scientists of various fields in order to ensure understanding and knowledge exchange across borders of scientific disciplines.

**Education:** Considering the skills required for archiving, validation and dissemination of data, educational institutions should recognize the need for specific education in (bio)molecular informatics.

## Recommendations

**To international unions and scientific societies:**

- (a) It is recommended that each Union, on a regular and ongoing basis, identifies and publicizes a list of key archival data bases.
- (b) It is recommended that Int'l Unions and other scientific societies actively encourage their membership to deposit primary data in recognized data repositories which provide unrestricted access to these data.
- (c) It is recommended that journals of these Unions and societies ensure that these requirements are met before accepting publications in their journals.
- (d) It is recommended that Int'l Unions, specifically IUPAB, address the general issue of education in the field of (bio)molecular informatics.

***To funding agencies:***

- (a) It is recommended that funding agencies insist that all primary data produced by grants that they fund be deposited in recognized data repositories which provide unrestricted access to these data. Int'l Unions and scientific societies should work with funding agencies to create guidelines for this purpose.
- (b) It is recommended that funding agencies actively encourage and adequately support existing and newly funded primary data repositories, including their updating and annotation, to provide the mechanism to preserve in perpetuity the data deposited therein in a form which is fully recoverable by future generations of researchers.

***To for-profit organizations:*** It is recommended that for-profit organizations deposit their data as early as possible in public archival databases.

***To publishers and authors:*** It is recommended that journal publishers make the primary data on which a publication is based available under the same conditions as they make the printed article available, and - if applicable - require that such data are deposited in a recognized key archival database. Authors are encouraged not to publish in journals that do not conform to these rules.

***To legislators:*** Following the recommendations of the ICSU/CODATA Ad Hoc Group on Data and Information, it is recommended that legislators take into account the impact of intellectual property laws on research and education, in order to allow fair use for scientific and educational purposes.

***To scientific committees for nomenclature and standardization:*** It is recommended that Int'l Unions and scientific societies play an active role in the definition of standards in the fields they represent. This should be done through nomenclature and data standardization committees. They should be conversant with both the content and the technologies needed for a full definition of the field, in order to ensure the exchange of data without loss of information.

***To educational institutions:*** It is recommended that bioinformatics curricula should include specific education in the creation and curation of databases, as well as in their use. Life sciences curricula should include courses and training in bioinformatics.

Steering Committee: H.J.C. Berendsen (IUPAB), H.M. Berman (IUCr), R. Cammack (IUBMB), C. Cantor (IUPAB), J. Garnier, (IUPAB), chairman, A. Lesk, (CODATA), A. McNaught, (IUPAC), R. Roberts, (ICSU), M. Vijayan (IUPAB, IUCr).

The full report can be found at <http://md.chem.rug.nl/~berends/IUBG-FinalReport.html>.

*H.J.C. Berendsen, Secretary*

## REGIONAL NEWS

# Science and crystallography in Novosibirsk



Students and mentors from Research Institutes in Novosibirsk.

The Inst. of Science of the Siberian Branch of the Russian Academy of Science (RAS) in Novosibirsk continues to pursue world-class science. Visits to four of the Institutes (Nuclear Physics, Solid State Physics, Bioorganic Chemistry, Microbiology and Cytology) revealed the presence of cutting edge research involving a team of local scientists working closely with outside collaborators around the globe. The Nuclear Physics Inst., the largest Institute of the RAS, houses one of the oldest synchrotron facilities in the world. They manufacture and market detectors, insertion and storage devices that are in use at SPring 8, the Photon Factory, Argonne and CHESS. B.P. Tolochko, the head of the Synchrotron Radiation Instrument Lab, described the 3D detectors as being tailored to applications on powder diffraction and materials studies that require higher sensitivity than other detectors can deliver. They are exploring the potential of bringing the same kind of sensitivity to macromolecular applications. Among ongoing studies in the Institute is the detection of the formation of diamond in explosive chamber reactions at 20 to 30 k volts. Among their consultants and collaborator are M. Kovalchuk (Moscow), Y Amemura (Japan) and J. Hendrix (Germany).

At the Solid State Inst., which was revitalized by Vladimir Boldyreva in the 1960's, new organic compounds are extracted from plants using environmentally friendly and economically advantageous techniques. A major focus is the extraction of natural steroids that are nutrients and growth promoters for livestock. [One of Dorothy Hodgkin's first steroid structures was such a plant extract with estrogenic properties.] The compounds isolated from seeds, flowers, stalks, and roots are being partially characterized by HPLC. There is the potential to extend analysis to the determination of the biological properties of the new compounds. Newly isolated and identified steroids are potential candidates for drug development or as starting materials for partial synthesis of steroid hormones. The lab of E. Boldyreva, at the U. of Novosibirsk, is fully equipped with instruments to measure the effect of pressure, temperature and atmospheric changes on single crystals and powders of organic and bioorganic materials. Solid state Raman, infrared, Mass Spectroscopic and NMR capabilities exist in other institutions of the Academy. The various institutes are interconnected by meandering paths through majestic forests of evergreens and white bark birch trees.

The Inst. of Bioorganic Chemistry has a major program in antisense technology, in studies of tRNA synthetases, and in comparative structural and functional analysis of human and bacterial ribosomes. Investigators there are isolating large quantities of the human ribosome and supply samples to D. Moras in France for crystallization.

Half of the 900 scientists of the Inst. of Microbiology and Cytology are engaged in a broad spectrum of Bioinformatics projects including analysis of 35 protein networks, (HSP-70's, redox regulators, and signaling proteins), RNA folding and nanotechnological design, covariance and cluster analysis of protein sequences, substituent identification and characterization by combining comparative analyses, structure and dynamic calculations, and elaboration of a mammoth database of transcriptional regulatory regions. There are currently 1460 genes, 2242 regulators, 4955 publications, and 6868 transcriptions factors and

binding sites in the largest curated database of its kind in the world that they are developing. [There is a January 2002 publication in Nucleic Acid Research describing this.]

In 2001, the Institute hosted a major international conference on Bioinformatics. There is great potential for combining the wealth of information on the functions and interactions of proteins contained in the databank and the structure data present in the PDB and CSD databases. The Internet could bring together laboratories from all over the world to develop innovative new research initiatives.

E. and V. Boldyreva, a father-daughter team of solid-state chemists have established a Center of Molecular Design and Ecologically Safe Technology in Novosibirsk that has attracted support from international sources. The many excellent Academy of Science institutes and the U. of Novosibirsk combine to give this imaginative program truly interdisciplinary character. The diverse backgrounds and insatiable curiosity of the Boldyreva's are the driving forces that make it work. If you're looking for collaboration in the area of solid state physics, Novosibirsk might suit your needs.

*William L. Duax*

## MEETING REPORT

# Symposia in Spain



The XIII Annual Symposium of the Spanish Group of Crystallography (GEC) was held in Oviedo (Asturias, Spain) July 3-6, 2002, at the 'Príncipe Felipe' Auditorium. It was attended by 80 crystallographers and included 9 plenary lectures, 10 oral presentations, 34 poster communications, a workshop, and exhibitions from three industrial companies.

The main topic was '*New Technologies for the Characterization of Materials: Instrumentation, Detectors, and Radiation Sources*', and its main goal was to show to the Spanish crystallographic community the state of the art in data collection techniques such as methods based on synchrotron radiation, neutron diffraction, area detectors, etc. Plenary lectures included: *SR Crystallography instrumentation from the facility and user point of view; monochromators, mirrors and detectors* (J.R. Helliwell, UK), *SR Bio-crystallography instrumentation, methods and application case studies; anomalous scattering, ultra-high resolution and time-resolved* (J.R. Helliwell), *SpLine: The Spanish line for material sciences at the ESRF. Experimental capacities and timing* (G.R. Castro, France), *The Spanish synchrotron of El Vallès: history, current status and opportunities for the future* (J. Bordas, Spain), *The Spallation Neutron Source: new opportunities in material sciences* (I. Anderson, USA), and *Future opportunities for Crystallography: ESS!* (F. Carsughi, Italy).

The symposium also covered crystal growth, structure determination and data analysis, with lectures like *High-throughput crystal growth for Molecular Biology and Medicine* (J.M. García-Ruiz, Spain), *Sorption of toxic metals by precipitation of solid solutions on mineral surfaces* (M. Prieto, Spain), and *The WinGX Program System - Crystallography made easy* (L.J. Farrugia, UK).

The meeting was sponsored by the Spanish Ministry of Science and Technology (MCyT), the Asturian Foundation for Research in Science and Technology (FICYT), the Spanish Royal Society of Chemistry (RSEQ), the U. of Oviedo, the Spanish Group of Crystallography Association (GEC), the Oviedo Town Hall, Bruker Nonius, Philips, and Dismed. An award for the best poster presentation was given to M.I. Aroyo (Spain) at the gala dinner, and a total of 11 young PhD students were given a grant that covered the registration fee.



Participants of the XIII Annual Symposium of the Spanish Group of Crystallography in July, 2002. Further information, including photographs, is available at [www11.uniovi.es/gec/13simposio/main.html](http://www11.uniovi.es/gec/13simposio/main.html).

*Juan F. Van der Maelen Uría, President, XIII GEC Organizing Committee*

## MEETING REPORT

# Supramolecules in Moldova



Invited speakers, attendees and organizers of the Moldova conference gathered in the home of Yuri Semenov, standing in the center of the photo behind his wife (striped blouse). Janusz Lipkowski and his wife are at the far right.

The Moldovian Chemistry Inst. hosted an Int'l Conference on Supramolecular Structure that brought together leaders in the field from throughout the world with expertise in synthesis, crystal structure determination and analysis, and solid-state chemistry. Over the course of the past 20 years, scientists in Moldova have established innovative international interdisciplinary collaborations. Despite economic setbacks that have accompanied major political change in Eastern Europe, these international collaborations continue to thrive. The conference included exciting reports on the latest developments in design of molecular magnets based on compounds first synthesized in Moldova. P. Christian and G. Timso collaborated on the study of structures of metal-clusters that can be induced to polymerize. They began with a series of fixed valency complexes of cobalt having different oxidation states of the same ion in the same cluster. Increasingly powerful oxidizing agents led to more complex clusters including a  $\text{Co}_7$  cluster with a cubic configuration, and even more complex clusters of  $\text{Co}_{16}$ ,  $\text{Co}_{14}$ , etc. Among their ultimate targets are diamagnetic solids and molecular magnets and the determination of the effects of solvent, oxidizing agents, and other metals and combinations of metals upon form and function. J. R. Helliwell participated in x-ray studies critical to the work. B. Moulton substituting for collaborators M. Zaworotko and L. Morales, gave two eloquent talks and defined and defended the field of supramolecular structure when K. Wieghart challenged the legitimacy of the term asking, 'Is Supramolecular Structure merely chemistry wearing the Emperors new Clothes?' Brian performed so brilliantly that at the next conference he is scheduled to give all the talks.

*William L. Duax*

## MEETING REPORT

# Structural Genomics, Berlin, Germany



The Int'l Conference on Structural Genomics in October, 2002, brought together leaders on the cutting edge of high throughput cloning, isolation, purification and crystallization of protein and NMR, x-ray crystallography, and bioinformatics investigations of the structure and function of gene products in a remarkably productive format. Lectures by Nobel Laureates crystallographer Robert Huber (1990) and NMR Spectroscopist Kurt Wuthrich (2002) set the bar very high but dozens of the speakers met the challenge. Of particular interest were presentations by A. Savchenko on techniques to solubilize many proteins that are expressed in insoluble forms, by C. Lang on protein expression as a function of variation in yeast expression systems, a new significantly different conformation for a tRNA in complex with its cognate tRNA synthetase (S. Yokoyama), further development of powerful algorithms for protein sequence alignment conducive to reliable prediction of fold and function (L. Holm), corroborative evidence of gene prediction in *C. elegans* provided by high throughput protein expression (M. Vidal), and significant progress in defining catalytic substrate sites by covariance analysis of families of proteins (O. Lichtarge and J. Thornton). W. Hol ended his progress report on structural genomics of tropical diseases with an appeal for major funding of a facility for high throughput production of macro quantities of candidates to expedite the drug delivery process. Other talks addressed detection of protein interactions and S. Wiemann presented moving pictures of labeled protein shuttling between the plasma membrane and the Golgi. The Governing Board of the association for the next four years will be composed of U. Heinemann (Germany), T. Terwilliger (USA), and S. Yokoyama (Japan) and newly elected S. Kuramitsu (Japan), D. Stewart (UK) and I. Wilson (USA). G. Montelione has accepted responsibility for planning and organizing the third meeting in the series in late fall 2004 or early spring 2005. Further information is available at [www.isgo.org](http://www.isgo.org).

*William L. Duax*

MEETING REPORT

# XIX Congress and General Assembly



## Reports continued from Volume 10#4

### Amorphous materials and glasses

Speakers at the microsymposium on amorphous materials and glasses demonstrated that, despite not being able to use many of the powerful tools of crystallography, it is possible to gain new, useful and important insights into the structure of non-crystalline materials.

E. Bychkov (France) discussed the change in the structure of silica glass when subjected to laser irradiation. High energy x-ray diffraction and SANS measurements reveal that laser irradiation induces a permanent 2-3% densification.

S. Kohara (Japan) described how high energy x-ray diffraction at SPring8 can provide 'neutron-like' data. High real-space resolution data were presented for  $\text{SiO}_2$ ,  $\text{GeO}_2$  and  $\text{GeS}_2$  glasses, and the results were simulated using the Reverse Monte Carlo (RMC) technique. Evidence was found for three-membered rings in  $\text{SiO}_2$  and  $\text{GeO}_2$ , and for an edge-sharing pair plus near neighbour configuration in  $\text{GeS}_2$ .

A. Hannon (UK) showed neutron diffraction data for lead gallate, thallium containing bismuth gallate and calcium aluminate glasses, and recommended that expanded use be made of information from chemical crystallography in examining glass diffraction results. The concepts of electrostatic bond strength and bond-valence are both of great value in making sense of diffraction studies of glass structure.

L. Pusztai (Hungary) discussed how RMC techniques can be used to assess the quality of non-crystalline diffraction data. A RMC simulation of earlier neutron diffraction data on  $\text{D}_2\text{O}$  deviated from the experimental result, but was subsequently found to be consistent with later more reliable measurements. RMC analysis was shown to be much more resilient to a lack of high momentum transfer information than is the direct Fourier transform analysis.

*Alex C. Hannon*

### Non-ambient diffraction and kinetic studies

The microsymposium emphasized the range of timescales, materials, and problems being addressed using non-ambient crystallography. Applications described ranged from proteins to glasses and ceramics, studied at timescales from milliseconds to hours, using both constant wavelength and white beam synchrotron and neutron diffraction methods.

P. Barnes (UK) showed a range of elegant experimental set-ups to study  $\text{ZrO}_2$  formation, reduction of metal oxides, zeolite dehydration, diffusion of environmentally relevant species into minerals and spatial resolution of the growth of zeolites in gels and on substrates.

E. Kisi (Australia) then gave a fascinating talk on how the new generation of high-flux neutron diffractometers (here D20 at the ILL) can allow the kinetics of even extremely rapid combustion syntheses to be followed, with Rietveld-quality data being collected in time slices down to 0.38 seconds.

J. Wright (France) described high resolution powder x-ray studies using synchrotron diffractometers that have revealed a number of new phase transitions observed on cooling myoglobin. He gave a thoughtful assessment of both the potential benefits and inevitable difficulties of studying such complex, though hugely important, samples by powder methods. C. Benmore (USA) showed how extremes of temperature ( $\sim 2000^\circ\text{C}$ ) can be achieved on levitated droplets of liquid oxides allowing complementary x-ray and neutron scattering studies to be performed.

C. Howard (Australia) presented a detailed ('the final word'?) study of the many high temperature phases of  $\text{WO}_3$  and their symmetry relationships. This elegant methodology prompted an enthusiastic general debate about the group theoretical aspects of phase transitions. The presence of the likes of J. Jorgensen,

T. Hahn, H. Stokes and M. Glazer in the session ensured that firm opinions were expressed, and discussions spilled over into Palexpo's corridors when we were forced to vacate the hall for the next meeting.

*John Evans*

## **Free electron lasers and other pulsed sources**

3<sup>rd</sup> Generation Light Sources (3GLS) presently dominate synchrotron radiation science. Taking prospective demands into account, we perceive a serious limit in storage-ring-based sources where the typical pulse length of SR is in picoseconds, much longer than that of short pulse lasers currently available. SR is obtained when electrons move in the magnetic field. This emission process is the origin of long pulse characteristic of SR. Generally, SR increases the bunch length, energy spread and emittance of electron beam. Therefore, we need so called 4<sup>th</sup> Generation Light Sources (4GLS) based on special accelerators without any SR emission. This was the main topic of the microsymposium.

T. Shintake (Japan) gave a tutorial on SASE FEL, one of 4GLSs. He described an operation mechanism of SASE FEL and special characteristics of the x-ray beam available from it, and showed Japanese activities in this field, especially on the new soft x-ray SASE FEL project at SPring-8. S. Gruner (USA) gave a tutorial on Energy Recovery Linacs, the other kind of 4GLSs, which allows the production of SR beams of exceptional brilliance and flux with very short x-ray bursts. T. Moeller (Germany) described the first scientific results obtained by using the TTF Free Electron Laser at DESY and demonstrated that the high intensity radiation from FELs allows the study of multiphoton processes. J. Arthur (USA) presented a scientific program to be performed in the Sub-Picosecond Photon Source project (SPPS) as well as in the Linac Coherent Light Source project (LCLS), including expected capabilities for performing experiments in various scientific fields. D. Boschetto (France) presented femtosecond x-ray diffraction applications based on x-ray laser-plasma sources, and proposed a new x-ray geometry compatible with the features of 4GLSs.

*Hideo Kitamura*

## **Methods for the characterization of layered structures**

This microsymposium focused on experimental techniques and theoretical approaches used to investigate the structure, microstructural properties, and chemical composition of low-dimensional systems. V. Holy (Czech Republic) showed how surface/interface sensitive x-ray methods (grazing-incidence small angle scattering and diffraction) can be used to investigate shape, position, and chemical composition of buried nanostructured species. Q. Shen (USA) spoke about applications of high-resolution x-ray diffraction for the determination of elastic strain tensor and strain gradients in quantum structures. A. Boulle (France) documented the capability of reciprocal space mapping and diffraction pattern modeling for studies of structural faulting, mosaicity, and strain gradients in highly mismatched oxide thin films. S. Zheludeva (Russia) reported on the generation of standing waves by multilayers, combining high structure sensitivity from x-ray scattering with spectroscopic selectivity. A. Belger (Germany) emphasized a complementarity of several methods for studies of structural and mechanical properties of hard multilayers, and reported on observed superlattice hardening at nanoscale levels upon heat treatment.

*Davor Balzar and David Rafaja*

## **Novel materials and physical properties at high pressure**

Due to scientific and technical advances, high pressure variability is becoming increasingly important in the study of amorphous materials and the synthesis and design of new technological materials. This

interdisciplinary session opened with a presentation by J. Tse (Canada) on the role of computational studies to predict and understand new and hypothetical high-pressure structures and physical phenomena. T. Sekine (Japan) described the latest shock-wave methods for high-throughput synthesis of high-pressure nitride and oxynitride spinels and N. Serebryanaya (Russia) presented studies of new super-hard carbon materials based on high pressure-high temperature treatment of fullerenes and C-nanotubes. K. Shimizu (Japan) showed the latest techniques for electrical and magnetic properties measurements under high-P and cryogenic conditions, and showed that the 'superconducting periodic table' now extends to all classes of elements under megabar pressures. C. Bull (UK) described results of 'pressure-tuning' IR absorption properties of electronic perovskites, and M. Somayazulu (USA) gave new insights into the comparative 'mineralogical' structural chemistry of CO<sub>2</sub> and N<sub>2</sub>O/NO<sub>2</sub> solids. A. Zerr (Germany) ended the session describing the structure and physical properties of the newly-discovered family of high-pressure nitride spinels and post-spinel materials.

*Paul F. McMillan*

## **Liquids and amorphous materials at high pressure**

C. Tulk (USA) gave a lively introduction to the session on the fundamental complexities of the phase diagram of ice. He presented neutron and x-ray results clearly showing the formation of several new distinct meta-stable amorphous forms of ice at ambient pressure, between the well known high and low density forms. These were obtained by annealing and subsequent relaxation of the high density form. S. Klotz (France) continued the high density ice theme with high quality *in-situ* neutron diffraction data at 2.2GPa that was interpreted using the EPSR Monte Carlo technique to reveal the collapse of the second nearest neighbour shell. Klotz suggested that the local structure resembled that of crystalline ice VII. S. Sampath (USA) presented neutron and high energy x-ray diffraction data on permanently densified GeO<sub>2</sub> glass (recovered from 10GPa). The two measurements were combined to extract detailed structural information. The next nearest neighbour oxygen atoms determine the high pressure phase of the glass, which appeared as a rotation and distortion of the GeO<sub>4</sub> tetrahedra. T. Hattori (Japan) discussed the structure of liquid group III-V compounds measured using synchrotron techniques. InSb was studied up to 20GPa and temperatures up to 1300°C, and showed a clear discontinuity at around 10GPa. The data appeared to be a mixture of two configurations (beta-tin and the bcc phase) which was most stable in equal proportions. P. McMillan (UK) gave an inspirational talk on amorphous Si, negative melting slopes and enthalpic signatures. Above 6GPa he showed a high density amorphous form of Silicon which relaxes on decompression, and suggested this amorphous-amorphous phase transition may be linked to an underlying phase transition in the liquid state.

*Chris Benmore*

## **Diffuse scattering**

The papers presented in this session reflected the great diversity of different systems and types of disorder and diffuse scattering that are of current interest. The topics discussed included measurement of phonon dispersion curves from thermal diffuse scattering in silicon and niobium (with possible future application to plutonium!); diffuse scattering due to stacking faults in the zeolite mordenite; diffuse scattering associated with phase transitions in relaxor ferroelectric materials; magnetic diffuse scattering in icosahedral quasicrystals; magnetic diffuse scattering in CMR manganite materials and diffuse scattering due to orientational ordering in C<sub>70</sub> single crystals.

It is clear that with increasing use of synchrotron radiation and area detectors many more people are seeing diffuse scattering and there appears to be a burgeoning interest in the field.

*Richard Welberry*

## Crystals for pharmaceutical applications: high-throughput and combinatorial techniques

The pharmaceutical industry is concerned with reliable and reproducible crystallization methods to guarantee consistent production of a specific solid forms. In addition to monitoring many crystallization parameters during scale-up and production particular emphasis is put towards discovery of polymorphs, with the ultimate aim to know all polymorphs of a given drug. The empirical nature of the phenomenon of polymorphism enforces a systematic search via crystallization experiments in order to discover as many polymorphs as possible. These prerequisites render the combinatorial high throughput approach extremely suitable for polymorph discovery.

R. Storey (UK) illustrated the knowledge-based approach followed by Pfizer UK. High throughput crystallization together with adequate characterization methods were given equal importance to detailed studies of individual polymorphs using various physical chemistry and theoretical techniques. C.W. Lehmann (Germany) presented a development from the non-industrial sector, which focuses on the problem of x-ray diffractometric analysis of potentially different polymorphs, crystallized in a multi-well plate. A fully automated solution, including computational design of the crystallization library, crystallization experiments using robotics, characterization the solids with different analytical techniques, and the statistical analysis of crystal forms versus experimental conditions, was offered by P. Desrosiers (USA). A. van Langevelde (Netherlands) described a proprietary crystallization plate and x-ray diffraction system used for statistical evaluation and single crystal structure elucidation. A completely different experimental approach developed at Solid State Characterization Services was presented by P. Stahly (USA). Crystals of meta-stable forms are grown in capillaries, either from the melt or from highly concentrated solutions, whereby supersaturations exceeding those of larger volume experiments by at least an order of magnitude are achieved. Direct XRD analysis of the capillaries is possible and yields a unique characterization.

Lively discussion followed the talks, this was a rare opportunity for those involved in polymorph discovery to collect information about the state of the art.

*C. W. Lehmann*

## Hot structures I

The papers in the Hot Structures Microsymposia give a snapshot of exciting new macromolecular structures across the whole breadth of biological crystallography. Although it is perhaps unfair to single out any one contribution as the highlight of a fascinating session, D. Vassylyev's (Japan) presentation of the structure of a bacterial RNA polymerase, complete with its bound sigma factor snaking its way over and through the core enzyme represented a spectacular crystallographic achievement on an enzyme of extreme biological importance. Also focused on transcription, A. Roll-Mecak (USA) described the intriguing chalice-shaped structure of the translation initiation factor IF2/eIF5B, which facilitates the Met-tRNA binding to ribosomes, and in which a small conformational change is translated and amplified over 90 Å. Also on the theme of transcription, X. Cheng (USA) described the structures of enzymes from a family of methyltransferases that modify lysine and arginine side chains and are critically important in the role of histones in regulating access to chromatin during transcription. Surprisingly, these enzymes have a completely different fold from other SAM-dependent methyltransferases. Other cellular processes were not forgotten. T. Garrett (Australia) presented structures of the extracellular regions of two members of the EGF receptor family, mutations which are associated with many cancers. The structures revealed elongated, multidomain molecules in which ligand binding and dimerisation are linked by quite novel mechanisms. P. Haebel (Switzerland) described a complex that is critical to correct disulfide bond formation and folding in the bacterial periplasm. In this complex, in which redox state is vital, a modified Ig domain from a membrane-bound electron transporter DsbD binds to the Y-shaped dimer of the

periplasmic isomerase DsbC. Finally J. Emsley (UK) described another use for leucine-rich repeat proteins, with the beautiful structure of the LRR domain from the platelet receptor GPIb, leading to a model for the way in which this protein may mediate the aggregation of platelets at sites of vascular damage.

*Ted Baker and Andrea Mattevi*

## Twins, disorders and other demons

There is a growing awareness that twinned crystals and structural disorders occur frequently and present major obstacles to the correct determination of crystal structures. The microsymposium centered on twinning according to the classical twin laws, and on planar polytypic disorder as a frequently encountered mechanism of disorder. S. Parsons (UK) presented his program ROTAX which proposes possible twin orientations by examining poorly fitting data after refinement of the structure. From zones showing a systematic tendency of  $|F_{\text{obs}}|^2 > |F_{\text{calc}}|^2$ , twin matrices are proposed which often give dramatically improved refinement results. Use of the program is highly recommended. R. D. Gilardi (USA) presented several case studies of difficult structures of multiple polymorphs in energetic organic materials. Vastly improved results were obtained once a structure was recognized to be twinned. One compound presented six polymorphs with asymmetric units containing between 3 and 18 molecules; the figures presented may suggest different stacking variants of a planar structure. H. Birkedal (Switzerland) presented heavily stacking faulted structures of orange  $\text{HgI}_2$  and of an organic molecule assembling in hexagonal layers, both exhibiting rods of diffuse intensity. **He showed for both compounds, that two very different stacking sequences result in exactly the same observable intensities**, even in the limit where the stacking faults result in equi-volume macroscopic twinning. A.D. Rae (Australia) uses the symmetry of the so-called parent structure, defined by a subset of structure factors, e.g. those of a polytypic family invariant of the stacking order, to enumerate the symmetries of the possible ordered structures agreeing with observed unit cells. He also desymmetrizes parent structures by interpreting superstructure reflections as commensurate modulations. E. Estevez-Rams (Cuba and Germany) quantitatively derives from x-ray powder patterns pair correlation functions between layers of polytypic structures, e.g.  $\text{RE}_2\text{Co}_{17}$ . From this, the depth of interaction between layers may be derived. Stacking-faulted layer structures occur very frequently, and clearer presentations on some aspects ought to be foreseen for future meetings.

*Dieter Schwarzenbach*

## Macromolecular neutron scattering and sources

The development of the neutron imaging plate (NIP) produced a breakthrough in neutron protein crystallography. The first application of the NIP was realized on the Laue type diffractometer, LADI at ILL. In Japan the NIP has been constructed on high-resolution neutron diffractometers that use a monochromatized neutron beam and are dedicated to biological macromolecules (BIX-type). Hydrogens and hydration in Myoglobin, Rubredoxin (wild type and mutant) are observed by a BIX-type diffractometer at 1.5 Å resolution, and those in Lysozyme, Pyrophosphatase and Endothiapepsin have been observed by LADI. Neutron diffractometers equipped with NIPs open a new field of structural biology that will include locating hydrogen atoms and water of hydration.

*Nobuo Niimura*

## X-ray microdiffraction

With the advent of high brilliance 3<sup>rd</sup> generation synchrotron sources and progress in x-ray focusing optics, very intense small x-ray beams in the micron and submicron range are now routinely produced at synchrotron beamlines around the world. While very small monochromatic beams are extensively used

for imaging techniques such as x-ray microscopy and tomography, x-ray microdiffraction using either monochromatic or white beam is expected to become an increasingly important tool with many applications in soft material physics, thin film mechanics and earth sciences. It allows for the structure determination from very small crystals, and texture studies of fiber only a few micrometers in diameter (C. Riekell, France). Combined with other microprobe techniques, such as scanning x-ray microfluorescence and micro-EXAFS, it becomes a powerful tool to study the speciation of trace elements in soils (A. Manceau, USA). Orientation imaging and strain/stress mapping obtained by white beam scanning x-ray microdiffraction allows the study of thin film mechanical properties at a granular and subgranular level (R. Spolenak, USA). The development of 3D x-ray microdiffraction using either monochromatic (H. Poulsen, France) or white radiation (B. Larson, USA) allows dynamical studies of grain deformation and plasticity in polycrystalline bulk materials during *in-situ* loading conditions.

*Nobumichi Tamura*

## Visualization of macromolecules

The microsymposium concerned algorithms, software development, and novel user interfaces. H. Bernstein (USA) discussed advances in the widely used molecular visualization program RasMol. He described his approach to displaying molecular surface representations with adequate performance on computers that do not necessarily have the power of today's hardware.

C. Bajaj, (USA) discussed new algorithms useful for the display and analysis of molecular properties, including rapid interactive recontouring of volumetric data sets such as electron density maps or electrostatic potential maps, techniques for finding the most informative contour levels for visualization and an extension to conventional volume rendering, for visualizing functions in 4, 5 or higher dimensions. Much of his software is available at his website ([www.cs.utexas.edu/users/bajaj/](http://www.cs.utexas.edu/users/bajaj/)).

M. Sanner, (USA), discussed his strategy for design and implementation of software for biomolecular visualization and analysis, including the Python programming language to develop re-useable software components to enable rapid evolution of useful molecular modelling tools, Viper a visual programming network editor, for developing new applications without the need for writing new code, the Bajaj rapid isocontouring algorithm, and a graphically programmable symmetry generation network.

A. Olson (USA) described 'Tangible Interfaces for Molecular Biology.' He discussed the evolution of computer graphics from physical models to computer graphics, and now back to physical models produced as 'solid prints' by computer autofabrication, including output from his new full color solid printer, a Zcorp 406. Using Augmented Reality technologies, the physical model can be tracked by a video camera, and computer graphics representations and other computer stored data can be superimposed on the physical model using video see-through glasses. He showed an example of manipulating a drug molecule into the active site of an enzyme, using physical models combined with computer graphics.

*Arthur J. Olson*

## Structures and phase transitions at high pressure

E. Gregoryanz (France) described recent work on the high pressure phase diagram of nitrogen. Over the past 2 years he and co-workers at the Geophysical Lab of the Carnegie Inst. of Washington have discovered remarkable complexity in the megabar region including the first evidence for the long-sought after non-molecular phase. J. Chen (USA) described a translating image plate detector and its use for real time kinetic studies of olivine to spinel phase transition. P. McGregor (UK) discussed high-pressure structures of alcohols illustrating the structural complexity which can now be handled at high pressure and the remarkable range of conformations which the pressure variable can produce.

S. Redfern (UK) described the development of a high-temperature/high-pressure cell for neutron diffraction and recent experiments in structural studies of hydrous minerals and of order-disorder phase transitions. N. Ashcroft (USA) explored the implications of the complex structures recently discovered in elemental metals at high pressure. These high density metallic systems have a very different balance of length-scales from that which operates in 'normal' metals at ambient pressure and offer new insights into the general problem of electrons in metals.

*John Loveday and Serge Desgreniers*

## MEETING REPORT

# Fundamentals of modern methods in biocrystallography



Participants at the course on Fundamentals of Modern Methods in Biocrystallography, Oeiras, Portugal. The first BioCrys-Course on Fundamentals of Modern Methods in Biocrystallography, organized by M. Arménia Carrondo (ITQB Oeiras, Portugal) and T. Schneider (U. of Göttingen, Germany) took place at the Inst. de Tecnologia Química e Biológica in Oeiras, Portugal in October, 2002 with support from the European Union, MAXINF network ([www.maxinf.org](http://www.maxinf.org)) and Astra Zeneca. It brought together 30 students and 20 tutors from 18 different countries.

The course presented fundamental theoretical concepts of macromolecular crystallography to scientists in early stages of their crystallographic careers. This is particularly important due to the rapid development of the field and also due to the fact that many young researchers do not receive a formal education in crystallography. Additionally, with the introduction of high-throughput methods, the need to understand and grasp the theory behind modern methods will certainly be critical to tackle the difficult problems that will not be solved by the automated procedures.

Lectures and tutorials covered topics from the cooling of crystals to the validation of the final structural model. Lectures were held in the morning and interactive practicals and tutorials in the afternoon. A cluster of 16 Linux-computers were set up for the course by P. Matias, F. Enguita and D. Aragão (all from ITQB, Portugal). Tutors or invited speakers reported about a current topic in structural biology in an evening lecture.

J. Drenth (U. Groningen, The Netherlands) laid out the basics of crystallography in real and reciprocal space. C. Hermes (EMBL Hamburg, D) gave an overview of the principles of x-ray sources and detectors and E. Garman (Oxford U., UK) lectured and demonstrated about the practical side of crystal cooling and data collection. A tour of crystallographic resources on the web collected was presented by F. Enguita (ITQB Oeiras, Portugal).

Strategic questions of data collection and the principles of data processing were subsequently addressed by Z. Dauter (Brookhaven Nat'l Lab, USA) and A. Leslie (MRC Cambridge, UK). This included a 2 hour tutorial on 'How to read (and understand ...) the Int'l Tables' given by Z. Dauter and an overview about the various statistical descriptors in use for crystallographic data by C. Frazão (ITQB Oeiras, Portugal).

The MIR-method was first discussed and later practised in a tutorial by C. Vonrhein (GlobalPhasing Cambridge, UK). The substructure solution process and MAD-phasing were covered by T. Schneider (U. Göttingen, Denmark); the theoretical basis and recent successful applications of SAD-phasing were described by Z. Dauter. Rag de Graaf (U. Leiden, The Netherlands) reported about new matrix-based methods for solving substructures in an evening lecture. K. Cowtan (U. York, U.K.) discussed the principles of the different density modification techniques used for phase improvement and guided the students through the world of structure factors in his web-based tutorial ([www.yorvic.york.ac.uk/](http://www.yorvic.york.ac.uk/))

~cowtan/sfapplet/sfintro.html). R. Read (U. Cambridge, UK) described the phasing process in the framework of structure factor probabilities and maximum likelihood.

Lectures and practicals on molecular replacement and the self rotation function were given by R. Read, P. Matias, and M. Archer (ITQB Oeiras, P), and P. Lindley (ITQB Oeiras, Portugal) gave an overview of the past, present, and future of synchrotron radiation sources.

After taking the students from crystals to an interpretable electron density map in six very dense days, the first part of the course finished with a dinner in the Fabrica de Pólvora, to which the City Council of Oeiras had generously invited all course participants. The following day was the very much earned free day, which most participants enjoyed during a visit to Lisboa.

The course continued with instruction on methodologies used in the determination of ribosomal structures (D. Brodersen, MRC Cambridge, UK), the use of the Cambridge Structural Database (F. Allen and G. Battle, CSD Cambridge, UK), crystallographic model-building was practiced in a tutorial run (F. Enguita), structure refinement (P. Gross, U. Univ, The Netherlands), the ideas behind automatization of crystallographic model-building (A. Perrakis, NKI Amsterdam, The Netherlands), dealing with twinned crystals (C. Frazão). Tutorials run by P. Matias and A. Perrakis revealed how both classical and automated methods were used in practice.

The course ended with lectures and tutorials on how the quality of models resulting from crystal structure determinations can be critically assessed. T. Schneider introduced different measures of coordinate precision. G. Kleywegt (U. Uppsala, SE) discussed the various indicators that can be used to judge the correctness of a structure and illustrated these by alarming examples from the literature.

During the entire course, a box to which specific 'burning questions' about crystallography could be submitted anonymously was available. These questions were later answered by the tutors in a special session. This system proved to be very popular and gave valuable feedback to the tutors.

We thank the European Union and our industrial sponsors for the generous support, the staff of ITQB, and M. João Santos and H. Cordeiro for very efficient administration.

*Maria Arménia Carrondo and T.R. Schneider*

## MEETING REPORT

# 2002 CrSJ Annual Meeting



Sumio Iijima (honorary member of CrSJ)

The Annual Meeting and General Assembly of the Crystallographic Soc. of Japan was held in Tokyo, Japan, in December 2002. It was attended by 423 people and included 2 symposiums, 82 oral presentations and 145 poster presentations covering all aspects of crystallography. There was also an industrial exhibition.

The symposia were on 'Recent development in the crystallographic studies of the structures of crystals and their functions' and 'Recent development of structural biology in the genome era by crystallography'. The lectures 'Carbon nano tube: The Science and application' (S. Iijima, Meijyo U.), 'Determination of the structure of molecular crystals on the level of the electron densities using x-ray powder diffraction method' (E. Nishibori, Nagoya U.), 'Control of the structure of the organic superconductor by uni-axial compression' (T. Kondo, U. Tokyo), 'Crystal structure of molecule-based chiral magnet--structure near magnetic phase transition point' (K. Inoue, IMS) were included in the former symposium, and 'Structural biology of biological machineries' (M. Tanokura, U. Tokyo), 'Promotion of protein 3000 project, and protein crystallography of the near future' (T. Tsukihara, Osaka U.), 'High-throughput technology of RIKEN High-throughput Factory at the SPring-8' (M. Miyano, RIKEN), and 'X-ray crystallography in genomic drug discovery' (T. Hata, Sankyo Co., Ltd.) were in the latter.



Awardees at the 2002 Annual Meeting and president of CrSJ. A. Kita, M. Tanaka, N.Yasuoka (President), T. Ishikawa, Y. Sugawara, Y. Takahashi

At the annual CrSJ Awards Ceremony, the S. Nishikawa Award was presented to M. Tanaka (Tohoku U.), Research Awards were given to T. Ishikawa (RIKEN) and Y. Sugawara (Kitazato U.); and the Young Crystallographer Awards went to A. Kita (Kyoto U.) and Y. Takahashi (JSPS). A full detail of the meeting program can be viewed at CrSJ homepage [wwwsoc.nii.ac.jp/crsj/index-e.html](http://wwwsoc.nii.ac.jp/crsj/index-e.html).

*Nobuhisa Watanabe*

## MEETING REPORT

# Supramolecular chemistry, Israel

The 12<sup>th</sup> Int'l Symposium on Supramolecular Chemistry (ISSC-XII) was held in October, 2002 in the resort city of Eilat, Israel. The unique sights of the Red Sea, the surrounding desert and the red-colored ore-rich mountains, enhanced a romantic welcome reception by the swimming pool of the Magic Palace Hotel (the Symposium venue). ISSC-XII was attended by senior and junior scientists from Asia (Japan, South Korea, India, China & Hong Kong), Europe (Moldova, Russia, Poland, Czech Republic, Germany, The Netherlands, Switzerland, France, Italy, UK), Africa (Ghana) and North America (Canada, US), as well as from Israel. A number of travel grants sponsored by the Vigevani Foundation and the IUCr, were awarded to young participants. The Symposium focused on recent advances in both basic as well as applied research of supramolecular chemistry and materials, encompassing a wide spectrum of subjects from nano-science, through structural and functional chemistry, to biomaterials.

The session on the self-assembly and function of nano-structures. Its highlights included lectures by J. Sagiv (Israel) on a hierarchical fabrication of organic-inorganic nano-composite architectures in thin films, as a potentially useful technology for the construction of functional nano-devices, and by S. Stupp (USA) on the self-assembly of organic nano-fibers with interesting mechanical properties which could be used in bone repair in medicine. M. Rampi (Italy) showed self-assembled monolayers with transistor-type functionality in the context of molecular electronics, while E. Joselevich (Israel) focused on carbon nanotubes as building blocks. Very colorful presentations on supramolecular materials with unique optical properties were delivered by M. Hollingsworth (USA) on ferroelastic and ferroelectric domain switching in solid inclusion complexes of urea and calixarenes, and by P. de Silva (Northern Ireland) on the application of luminescent compounds as information processors and their utility in medical treatment. De Silva and S. Speiser (Israel) showed how binary logic operations could be implemented at the molecular scale.

Advances in the syntheses and characterization of new supramolecularly ordered compounds, which can be used in electronic devices, were highlighted by P. Bäuerle (Germany) and M. Drain (USA) who referred to conjugated macrocyclic oligothiophene oligomers and porphyrin-array-based functional photonic materials, respectively. I. Willner (Israel) explored nanoparticle architectures, composed of organic moieties and either gold or cadmium sulfide nanoparticles, which have photonic, electronic and sensoric functionalities. J. Fuhrhop (Germany) described controlled synthesis of porphyrin-based nano-assemblies on gold and silicate substrates/particles. D. Schlüter (Germany) described the elegant synthesis of fourth and fifth generation dendronized polymers and their behavior on solid interfaces. These polymers, when positively charged on their surface, can be wrapped by DNA strands to yield poly-electrolyte aggregates. T. Aida (Japan) reported the beautiful design of light-harvesting dendritic macromolecules and their application to materials science. His systems consist of gigantic porphyrin dendrimers that can effectively capture visible photons. Design of smaller multiporphyrin assemblies for artificial photosynthesis was presented by Y. Kobuke (Japan). J. Miller (USA) added an enlightening review of supramolecular organometallic materials exhibiting the technological important property of bulk magnetism.

S. Zimmerman (USA) led the discussion on molecular recognition, illustrating the construction of supramolecular polymers from 'sticky' monomeric entities that associate strongly in a predictable manner. Molecular tectonics, which relates to the design by self-assembly of molecular networks with pre-programmed structures, was further dealt with by W. Hosseini (France). He showed that the formation of molecular networks may be achieved through an iterative self-assembling process by using programmed building blocks which contain both recognition and iteration information. Related presentations by N. Kobayashi (Japan), I. Williams (Hong Kong) and D. Soldatov (Canada), focused on the designed construction of new hybrid organic-inorganic supramolecular complexes and coordination

polymers. Structure, properties and functionality studies of inclusion host-guest chemistry based on a wide variety of organic and inorganic host systems were then addressed by K. Komatsu (Japan) - fullerene-based nanomaterials, R. Ungaro (Italy) - multivalent calixarene ligands as specific molecular delivery systems potentially useful in environmental chemistry, P. Lhoták (Czech Republic), K. Suwinska (Poland), Y. Inoue (Osaka, Japan), W. Saenger (Germany), J. Lipkowski (Poland), H. Gies (Germany) - zeolites, and T. Iwamoto (Japan).

J. Sessler (USA) discussed a large variety of polypyrrole-based anion binding agents. Stereoid-based receptors for inorganic anions as well as for carboxylates were presented by A. Davis (UK) and B. Smith (USA). These and related receptors were found effective in transport experiments through the interior of non-polar membranes. Anion-controlled assembling of porphyrin-guanidine-, porphyrin-alkaloid- and porphyrin-guanosine-conjugates were described by V. Kral (Czech Republic). U. Maitra (India) spoke on self-assembled fibrillar networks formed from bile acid analogs.

J. Sanders (UK), envisaged new opportunities for molecular recognition and catalysis by applying the methodology of dynamic combinatorial chemistry. Z. Gross (Israel) highlighted the unique catalytic properties of the corrole macrocycles. L. Mandolini (Italy) described new organometallic ditopic catalysts based on various functionalized platforms (calixarenes, pyridines and azacrownethers) with high substrate selectivity features. Dendrimer-based reaction catalysts were also discussed by M. Portnoy (Israel). In the biological area, F. Diederich (Switzerland) evaluated on molecular recognition features at enzyme active sites, highlighting the successful design of *de novo* nonpeptidic enzyme inhibitors. These studies were based on detailed crystallographic characterization of the enzyme structures.

The Symposium was concluded by sessions devoted to biological systems. R. Nolte (The Netherlands) described methodologies to construct supramolecular assemblages from building blocks which contain the desired information encoded within them for a stepwise, hierarchical assembly process. G. von Kiedrowski (Germany) discussed design principles used to generate noncovalent 3D-nanoobjects in which both the topology and the geometry is well defined by complementary molecular recognition algorithms. Turning oligopeptides into molecular machines (receptors and catalysts) was also the theme of P. Scrimin's (Italy) lecture. G. Gokel (USA) described a synthetic heptapeptide system as an effective transporting agent of chloride ions through membranes. New artificial receptors based on aminopyrazole nuclei for protein recognition were designed by T. Schrader (Germany). A. Coleman (France) described the construction of organized and active assemblies based on protein (Bovine Serum Albumin or Fibrin)/ salt mixtures prepared in the form of thin film gels, which exhibit electrical conductivity, frequency dependent switching capacity and differential conductivity paths along and across the dendritic architectures.

Poster contributions were displayed throughout the Symposium, their themes paralleling the range of topics encompassed by the oral program.

*Israel Goldberg*

## AWARDS AND PRIZES

## L'ORÉAL-UNESCO science award



Karimat El-Sayed

The 2003 L'ORÉAL-UNESCO Award Laureates include Karimat El-Sayed (Egypt), professor of solid state physics, Ain Shams U. Cairo, who has specialized in the detection of impurities in materials relevant to industrial metallurgy and semi-conducting materials; and Fanghua Li (China), professor, Inst. of Physics, Chinese Academy of Sciences, Beijing, who has specialized in electron microscopy. Her work has pushed back the limits of observation of crystalline structures through the elimination of interference.



Fanghua Li

These awards, presented by the Chief Executive Officer of L'ORÉAL, L. Owen-Jones, and Director-General of UNESCO, K. Matsuura, recognize women working in the field of the material sciences. Five laureates in the material sciences, in addition to fifteen fellowships in the life sciences, were honored at the event. This year's awards bring to 71 the number of women, from 45 countries, who have been honored by the program.

The L'ORÉAL-UNESCO 'For Women in Science' programme aims to improve the position of women in science by recognizing outstanding women researchers who have contributed to scientific progress (L'ORÉAL-UNESCO awards of \$100,000 each), and young women scientists engaged in exemplary and promising projects (UNESCO- L'ORÉAL fellowships of \$20,000 each).

The awards distinguish five remarkable women researchers representing the five continents: Africa, Asia-Pacific, Europe, Latin America and North America. Often, these women's exceptional careers have opened up new and revolutionary ways of improving conditions of life and well-being. Pierre-Gilles de Gennes, Nobel Prize in Physics 1991, presided over an international selection committee of ten eminent scientists.

## AWARDS AND PRIZES

## Struchkov prize 2002



From left to right: Mikhail Antipin, Leokadia Zorina, and her adviser Rimma Shibaeva.

In December, 2002, the sixth Struchkov Prize (\$800) was awarded to Leokadia Zorina, a young scientist from the Inst. of Solid State Physics, Chernogolovka, Russia, for her research 'The structure of low-dimensional organic conductors on the basis of cation-radical salts possessing photochromic and magnetic properties'. She recently received her PhD degree for this work.

The Struchkov Prize Society (SPS) was founded in 1997 by the two former deputy directors of the X-Ray Structural Center, Russian Academy of Sciences (RAS), M. Antipin (Inst. of Organoelement Compounds, RAS, Moscow) and A. Yanovsky (Pfizer, San Diego, USA). The goal of this Society is to support young crystallographers in all independent States of the former Soviet Union. The Society was established to memorialize Professor Yuri Struchkov (1926-1995), Corresponding member of the Russian Academy of Sciences and former Vice President of the IUCr. During its first two years the SPS was financially supported by Antipin and Yanovsky. In 1999 on the initiative of I. Dubchak (Lawrence Berkeley Lab, USA), almost all former members of Struchkov's Lab who worked with him earlier in Russia and subsequently moved abroad, joined the SPS. Several of Struchkov's coworkers in Russia, international coworkers, and IUCr members also joined the Society in 1999. Their donations allowed for a significant increase of the main award and permitted for the addition of several supplementary awards. In 2002 seven young scientists from Moscow, Chernogolovka, Kazan', Novosibirsk, Samara, and Petrozavodsk were honored with supplementary awards (\$150). The SPS is very grateful for the active moral and financial support of K. Caulton and W. Duax (USA), T. Workman (USA), L. Dong-Cai (China), and J.A.K. Howard (UK).

*Tatiana Timofeeva (New Mexico Highlands U.)*

## NOTICE

## Visa alert

There have been reports indicating that some foreign scientists are having difficulty getting their visas processed in time to assure attendance at scientific meetings in the US. As a precaution, we suggest that member societies include the following information on websites, calls for abstracts and other conference related communications. US scientists going overseas are also encouraged to check with their respective universities for resources relating to travel and visa issues abroad **EARLY IN THE PLANNING PROCESS**, in the event of reciprocal delays.

As part of new security procedures, many visa applications are being sent to the State Dept. in Washington, DC, for review by a variety of federal agencies. Due to the number of visas being processed and heightened security concerns, this review can take as long as six to eight weeks, or longer, depending on the applicant's country of origin. Therefore, scientists intending to come to the U.S. should apply for their visa **AS EARLY AS POSSIBLE** and to pay attention to US State Dept guidance on this matter. The US Nat'l Academies has a website containing information about this situation (<http://national-academies.org/visas>).

The most frequent reason that visitor visas are denied is because the applicant was unable to provide enough evidence, in the opinion of the consular officer, that he or she was not intending to immigrate to the US (per Section 214(b) of the Immigration and Nationality Act). Therefore, we encourage you to pay particular attention to State Dept. advice on how to deal with this type of denial. For more information, see <http://travel.state.gov/visadenials.html>.

**AWARDS AND PRIZES**

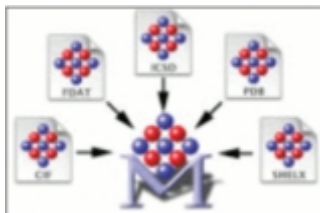
## **PDB announces new poster prize**

The Protein Data Bank (PDB) is pleased to announce the establishment of the PDB Poster Prize. Beginning this summer, a prize will be awarded for the best student poster involving macromolecular crystallography at each of the meetings of the IUCr Regional Associates (ACA, ECM and AsCA) as well as at the IUCr Congress itself. This year's prizes will consist of two signed texts – Biochemistry - Vol I by Donald and Judith G. Voet and Introduction to Macromolecular Crystallography by Alexander McPherson. Details on how undergraduates and graduate students can 'label' their posters for review will be made available at the PDB website ([www.pdb.org](http://www.pdb.org)) and at the registration desk for all three meetings.

Questions may be sent to [info@rcsb.org](mailto:info@rcsb.org).

## NOTICE

## CrystalMaker 6.0 for Mac OS X



CrystalMaker Software announced the release of a new Mac OSX version of their CrystalMaker crystal and molecular structures visualization program.

CrystalMaker is an interactive program for building, displaying and manipulating crystal and molecular structures featuring real-time photo-realistic graphics with 'out-of-the-screen' 3D (stereo) display, digital video and virtual reality output, plus analysis and diffraction tools. It includes new data editors and a symmetry browser with search capability.

Educational and multi-user discounts are available, with tiered upgrade schemes for existing users. A demonstration version, with examples files, can be downloaded from [www.crystallmaker.com/crystallmaker/download.html](http://www.crystallmaker.com/crystallmaker/download.html)

For further information, please refer to [www.crystallmaker.com](http://www.crystallmaker.com) or e-mail: [info@crystallmaker.co.uk](mailto:info@crystallmaker.co.uk).

*David Palmer*

## NOTICE

## New generation of confocal X-ray multilayer mirror systems

Xenocs has developed a new generation of confocal x-ray multilayer mirror systems. Installations show major flux-on-sample increases from x-ray rotating anode generators, enabling efficient protein structure determination in the lab. In addition, the system is particularly suited for high throughput screening of small weakly diffracting protein crystals. The system features patent pending advanced mirror technology, including a gradient period multilayer and vacuum enclosure to ensure long lifetime. The new design is easy to adjust for optimal flux using the compact alignment system provided and interfaces with any port of all rotating anode x-ray generators, both as an upgrade or with new systems.

For information contact [daniel.brau@xenocs.com](mailto:daniel.brau@xenocs.com) or visit [www.xenocs.com](http://www.xenocs.com).

## BOOK REVIEW

# Crystal Growth Technology

**Byrappa & Ohachi (eds.)****[www.williamandrew.com/titles/1453.html](http://www.williamandrew.com/titles/1453.html)**

Advances in many modern technologies depend greatly on the availability of suitable single crystals, whether for lasers, semiconductors, magnetic devices, optical devices, superconductors, etc. Unless the science of growing these crystals is understood precisely, it is impossible to grow several types (i.e. diamond, silicon carbide, PZT) for application in industry. This book fills in the blanks, through the writings of the most senior engineers in the industry.

## NOTICE

## The first drug design courseware

Molecular Conceptor is the most comprehensive, detailed, and lavishly illustrated guide to Molecular Modeling & Drug Design ever published. This CD-ROM is the equivalent of 50 hours of lectures; it contains 1500 pages and features more than 1200 3D illustrations. It has the scientific advantage of being a teaching device and a research instrument for both academia and industry. Visit [www.molecular-conceptor.com](http://www.molecular-conceptor.com) to receive your free Demo CD.

*Ouri Fischel*

## OBITUARY

# Jürg Waser (1916-2002)



Jürg Waser, who was president of the ACA from 1960 to 1961 (vice-president, 1959-1960), died at his home in La Jolla on August 16, 2002, at the age of 86. He is survived by his wife Plüdi, children Nicki, Peter and Kathy, grandson Andrew Waser, and stepson Roy Weiss.

Jürg was born in Zurich and attended the U. of Zurich. He went to Caltech on a one-year graduate exchange program in 1939 but remained because of World War II, receiving his PhD (chemistry) in 1944 under the supervision of Linus Pauling. He continued at Caltech as an Instructor in Mathematics and a Research Fellow in Chemistry until 1948, when he returned to the U. of Zurich. He soon came back to the United States as Professor of Chemistry at Rice U. in Houston, and returned to Caltech as Professor of Chemistry in 1958. He retired in 1975.

Jürg's primary responsibility at Caltech was to teach the introductory chemistry course required of essentially all undergraduates. He taught it meticulously; meticulous in his preparations for lectures, meticulous in his insistence that he thoroughly understand the subjects himself, meticulous in his supervision of the Teaching Assistants. He was famous for his 'pop qwisses' (pronounced with his native Swiss accent), and for his stern yet sympathetic mien. In effect, he ruled the course with an iron hand - well hidden under a soft glove, for he was always willing to give help to any student who sought it. When he could find no satisfactory textbook for the Analytical Chemistry portion of the laboratory work, he wrote one; it went through two editions and was used in several other colleges. He also wrote a slim volume on 'Basic Chemical Thermodynamics', to help the students (and TA's) understand these concepts. His thoughtful lectures and his close interaction with his Teaching Assistants surely inspired many students, both undergraduate and graduate, to become more disciplined and more understanding - as well as far more knowledgeable in their pursuit of a scientific career.

Although most of his time at Caltech was spent with his teaching duties, he carried out extensive research in the field of structural chemistry, using the experimental methods of x-ray diffraction and his thorough knowledge of mathematics; he particularly enjoyed the concepts and notations of dyadics. He was one of the first to include 'restraints' in the least-squares refinement process. After his retirement he turned more and more to questions involving basic thermodynamics, and often collaborated on this subject with his close friend, the late Verner Schomaker (also a past president of the ACA) and with Hans Kuhn of the Max Planck Inst. at Goettingen, Germany on theories concerning the origin of life.

Jürg was tall and stately, and an excellent dancer - particularly enjoying Viennese waltzes. He also enjoyed camping and the outdoors, He returned to Switzerland most summers, and it is easy to visualize him striding along with an alpenstock and a red-feathered hat, planning in his mind a lecture on chemical equilibrium.

*Dick Marsh, ACA Newsletter, Winter 2002*

## OBITUARY

**Tadeusz Glowiak (1935-2003)**

Tadeusz Glowiak, Polish crystallographer and chemist, passed away in his home on February 25, 2003, at the age of 68. Born in 1935 in Luka (presently the Ukraine) and as a child he witnessed the cruelty of the Second World War. His entire academic career was associated with the Wrocław U., starting in 1959, when he joined the group of Bogusława Jeowska-Trzebiatowska. In 1961/1962 he visited the Moscow U. to study crystallography in the group of Mikhail A. Porai-Koshits. Having returned to Wrocław he obtained his PhD in 1967 and next his DSc in 1978. His early works pioneered the application of x-ray single crystal analysis to problems of co-ordination chemistry in Poland. In the 60's and 70's he organized the Polish Schools of Crystallography with the most prominent crystallographers in the world as lecturers. At this time, especially in 60's, this was the only way to maintain a contact with modern methods and developments in crystallography. In 1973 he obtained the first four-circle diffractometer (Syntex P2<sub>1</sub>) in Central Europe. From 1978 until his death he was head of the Crystallography Dept in the Inst. of Chemistry and then the Faculty of Chemistry of our University. In his group, six PhD students completed their theses. The laboratory directed by him was eagerly opened for international collaboration. Scientists from Vietnam, Ukraine, Slovakia and Bohemia took advantage of his ample hospitality. From 1987-1993 he was a vice-director of the Inst. of Chemistry. For several years he was a member of Committee of Crystallography of the Polish Academy of Sciences. Prof. Glowiak published more than 360 original papers. Most of them presented results of studies on co-ordination compounds. The latest issue of the Cambridge Crystallographic Database contains 395 structures associated with his name. These numbers will be even greater because Prof. Glowiak left many more results to be published. He received important Polish honours and awards and in 2002 the National U. of Lviv (Ukraine) conferred upon him the title of Doctor Honoris Causa.

With Prof. Glowiak's untimely death, the Polish community of crystallographers and chemists suffers the loss of not only an experienced and eminent scientist but also a man with great spirit and rich personality.

*Z. Ciunik, L. Jerzykiewicz, A. Kochel, M. Kubiak, T. Lis, Z. Olejnik, W. Sawka-Dobrowolska, P. Starynowicz*

## OBITUARY

## John H. Robertson (1923-2003)

Born in China in 1923 to missionary parents, Dr. Robertson had a distinguished undergraduate career at the U. of Edinburgh, being Class Medallist in Chemistry for three consecutive years and graduating with First Class Honours in that subject in 1944. He spent three years in industry with the ICI Explosives Div., Ayrshire, before returning to Edinburgh as the holder of a Senior Carnegie Scholarship to complete a PhD on the X-ray structure determination of strychnine hydrobromide. This work rapidly achieved an established place in chemical literature. Post-doctoral research at Pennsylvania State, USA (1950-51) and a fruitful period as Research Assistant to Dorothy Hodgkin at Oxford (1951-54), working on a structure of vitamin B-12, preceded his appointment as Brotherton Lecturer in the Dept of Inorganic and Structural Chemistry at Leeds in October 1954. He was appointed a full Lecturer in the following year, being promoted to Senior Lecturer in 1968.

Dr. Robertson was an influential, enormously liked and respected figure within the Dept of Chemistry. A clear and thoughtful lecturer, he was unfailingly approachable and courteous to students. As one of a prestigious team of X-ray crystallographers, his research work was central to the development of modern crystallographic techniques. He was responsible for the solution of several crystal structures and published extensively in the field, his output being characterized by the quality of his work and his attention to minute detail. A Chartered Chemist, Fellow of the Royal Soc. of Chemistry and Fellow of the Inst. of Physics, he was at various times Honorary Secretary of the Crystallography Group of the Inst. of Physics, Honorary Secretary of the UK Crystallographic Council and a member of the British Nat'l Committee for Crystallography. He was also instrumental in setting up the British Crystallographic Assn. Between 1964 and 1968, he served as Chair of Chemistry at the Dar-es-Salaam College of the U. of East Africa, where he was responsible for establishing new laboratories and a new curriculum, gaining a fine reputation as a teacher and administrator in the process. At Leeds, Dr. Robertson served on a number of University bodies and was an active member of the AUT and the University Staff Society.

Dr. Robertson retired from the University in September 1988. In his appreciation for the University Review at the time, John Lydon described him as a 'kindly, caring man...meticulous in those civilities we all intend, but do not always get round to... He took pains to make contact with newly arrived research students from abroad and worked hard to make them feel at home... at a deeper level, John Robertson was of the same mold and generation as other crystallographic social crusaders like Katy Lonsdale and J.D. Bernal and in his own quiet way was no less determined that the universities should be centers of tolerance and social progress... For over three decades, he was more than anyone else, the human face of the School of Chemistry.'

It was characteristic of Dr. Robertson's generosity of spirit that, in retirement, he should have continued to look after the Departments Colvin Library, relinquishing this role only shortly before his death in January, 2003.

*J. R. Gair*