

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



Henk Schenk

My last letter - it is amazing how three years have flown by! Last time I wrote about the days before our Congress in Geneva. I can tell you now that it has been a great success. Excellent science and almost perfect organisation. My congratulations to the organising and programme committees and to everybody who played a part in it; in particular to the key persons, Joel Bernstein and Menahem Kaftory

We had a successful General Assembly (GA) as well. New members for the Executive Committee (EC) and the Commissions have been elected and, in particular, the election for the EC was exciting. The GA had a very good discussion about the payment of dues of member countries with very weak economies. Other Adhering Bodies are initiating actions, which will enable us to keep them on board. The EC welcomes these initiatives, as it has to abide by the statutes in its decisions. We are very happy that our members feel so much loyalty. At the next GA we should have at least one more Adhering Body. Thailand has a strong and growing crystallographic community and will apply for membership of the IUCr in the coming year.

The EC meetings and the closed meetings of the Commissions also went very well. This is crucial for the IUCr as the plans for the future are developed at the time of the Congress. I believe all of this will place us in a very good position for the next triennium. There is a great enthusiasm for our Union!

The Commission on Journals met in Villigen three days before the Congress.

The journals are doing very well and also their rankings. We think that the availability of all back issues on line is important in this respect. But, of course, the enthusiasm and knowledgeability of our commission with its chair John Helliwell is the driving force, and last but not least our loyal and competent staff in Chester.

Isn't it strange how a successful research project in general ends? After spending a lot of salaries and other costs to realize the project and to write an article, the copyright must finally be transferred to a scientific journal. In fact, transferred to industry, as the majority of journals are in commercial hands. So, the only product of a research project, the paper, is almost given away. However, crystallographers are in a much better position, as in our field the community itself owns the leading Journals. So in this way it is much easier for us to get permission for re-use of our material. Let us be happy that the IUCr owns our copyrights and treasure our Journals!

I want to thank you for the fantastic years I have had as President of our Union. So many people have made my job interesting, enjoyable and easier. In fact a list of their names could easily fill this page. All these fantastic visits all around the world with so many great hosts. All these volunteers, devoted to the work of our Union, organising meetings, arranging special projects. All these lively email-discussions with so many of you. And so on. Thank you all very much.

I also want to thank a few people in person: Sine Larsen, so nice and efficient to work with, Michiyoshi Tanaka, very wise and pleasant in his advice, Ted Baker for helping me to take over. And from the staff in Chester in particular Mike Dacombe, main node in our network, but also Anne Cawley, Jane Robinson, Andrea Sharpe, Brian McMahon and Peter Strickland.

Finally I wish our new president Bill Duax and his EC and all other IUCr workers, volunteers and professionals, a very successful triennium 2002-2005.

*Henk Schenk*  
*Schenk@science.uva.nl*

## EDITORIAL

# Editorial



This is the last issue of the IUCr Newsletter of which I will be the Editor. I am very pleased to be able to leave this newsletter in the capable hands of Judith Flippen-Anderson.

I want to thank all who have submitted materials to the Newsletter during the ten years of its existence. Jane Griffin, who did her best to catch and correct my errors (I always outwitted her) and especially, Patti Coley and Tammy Colley in the Buffalo Editorial office, who will continue to work with the new editor on the future production of the Newsletter.

Thanks to all session chairs who have already sent reports on the XIX IUCr Congress and general Assembly in Geneva. This issue contains some of those reports and many others will appear in upcoming issues. Therefore, if you haven't done it yet, there is still time to submit your report and see it in a future issue of the Newsletter,

Also in this issue is a copy of the four page Call for Papers for the 21st European Crystallographic Meeting in Durban, South Africa, August 24-29, 2003. In order to assist the Regional Affiliates of the IUCr (ACA, AsCA, and ECA) in promoting their annual meetings, the Newsletter will henceforth make its pages available for the publication of an abbreviated Call for Papers.

Exerpts from the reports of session chairs at the spring meeting of the ACA in San Antonio are also included in this issue (pages 18-19). The complete set of reports appears in the Fall issue of the ACA Newsletter ([www.hwi.buffalo.edu/ACA/](http://www.hwi.buffalo.edu/ACA/)).

## LETTER TO THE EDITOR

# Franklin Medal

Dear Bill

I was astonished to read in Paul Guinnessy's note in *IUCr Newsletter* Vol 10, No.2, page 17 that the Royal Society's Rosalind Franklin medal 'will be bestowed next year to coincide with the 50<sup>th</sup> Anniversary of the publication of Crick and Watson's *Nature* article on DNA'. In my innocence I thought it was to coincide with the 50<sup>th</sup> Anniversary of the publication of Franklin and Gosling's *Nature* letter 'Molecular Configuration in Sodium Thymonucleate'. It is true that in the same issue of *Nature* there were also letters from Watson & Crick and from Wilkins, Stokes & Wilson but the medal is neither a Watson nor a Wilkins one.

*Geoff King*

## LETTER TO THE EDITOR

## Basic crystallography in the PC era

The recent XIX IUCr Congress in Geneva featured the 'rediscovery' of twins by molecular crystallographers. The number of communications concerning polytypes in organic and inorganic compounds is constantly increasing, although some authors improperly call them 'polymorphs'. And allotwins (twins of polytypes recently defined) are attracting attention (e.g. the poster No. 46 in the second poster session). The data on these topics is seldom accompanied by crystallographic knowledge. This ignorance comes from the fact that the basic texts on the topic are not in English (ex. Friedel's classic French texts on twins, and Dornberger-Schiff's lectures in German on OD and polytypism). Twins and polytypes were gathered in a microsymposium under the ironic category of 'demons'. Nowadays courses of basic crystallography are rarely offered to future crystallographers except at universities where a mineralogical influence is still present. Consequently the solution of 'demon' structures is entrusted to 'blackbox' software packages requiring just a bit of experience in using a computer. The user is untutored in the process of recognition and treatment of twinning. This is not surprising when viewed in the context of the transformation of the crystallographerscientist into a technician-button-pusher. But it has additional costs. Use of a polarizing microscope and critical analysis of space-group absences to detect twinning should precede data collection and structure determination rather than be a post-solution procedure. The user uncritically accepts the robotic post-solution analysis. Analysis of polytypes is even worse, because streaks accompanying families of reflections are usually ignored resulting in loss of vital information, because the OD theory could easily offer an explanation and even reveal undiscovered polytypes (incorrectly termed 'polymorphs'). Some contributions at crystallographic meetings are characterized by arbitrary, ambiguous, confusing, and contradictory nomenclature. These reports often fail to document the analysis strategy that was followed. Despite this dark landscape, the symposia, workshop and satellites about 'software usage' flourish. While nobody can deny the assistance these packages offer the crystallographer, the time has come to question whether one also needs schools for basic crystallography, to insure informed use of the programs. Some comprehensive textbooks dealing with basic crystallography have been published recently, and should be popularized more extensively. Finally, the education of a knowledgeable crystallographer should be considered a task of primary importance for the IUCr. Before it is too late . . .

*Massimo Nespolo and Giovanni Ferraris*

LETTER TO THE EDITOR

## Equipment and journals available

Dear Bill

I am willing to donate two precession cameras (Nonius and Huber) if someone will cover shipping costs.

I also have a fairly complete holding of Acta Cryst from 1968 to 1999 that I would donate to a 3rd world school if someone can cover the cost of shipping.

*Edgar Meyer, Texas A&M U., e-meyer@tamu.edu*

## IUCr ACTIVITIES

# New !... Mexican mirror site of the IUCr WWW



A new Mexican mirror site (MxMS) of the IUCr WWW services was fully operational on August 2, a few days before the opening ceremony of the Int'l Congress and General Meeting in Geneva. Thanks to the efforts of David López, manager of the MxMS, Brian McMahon, the Research and Development Officer of the IUCr, José Luis Boldú, President of the Mexican Society of Crystallography (SMCr) and Secretary of the Mexican Committee for Crystallography, and Michael H. Dacombe, Executive Secretary of the IUCr, the Mexican Delegates in Geneva were able to announce the news about the existence of this site ([www.mx.iucr.org](http://www.mx.iucr.org)) to the international community attending the event. This mirror site was created by taking advantage of the fact that the SMCr was recently able to up-date the computer facility currently used to support their site ([www.smcr.fisica.unam.mx](http://www.smcr.fisica.unam.mx)) on the web, and it was set up to serve especially the Latin American community of crystallographers who frequently find a slowness of transmission of information across the internet due to both the technical features of the local and international network and the excessive visitors flux at the primary electronic site. The MxMS is updated once every 24 hours from Chester at a time when network traffic is low and it supplies information on the Union, its Commissions and Regional Associates, its journals and other publications and on crystallography and crystallographers in general. It was developed under the auspices of the SMCr and the IUCr, and it is running by courtesy of the Inst. de Física of the U. Nacional Autónoma de México.

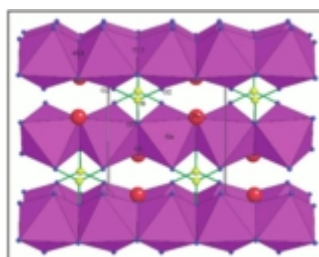
*A. E. Cordero-Borboa, Inst. de Física, UNAM,  
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## IUCR JOURNALS NEWS

# PbGaBO<sub>4</sub>, an orthoborate with new structure type

## PbGaBO<sub>4</sub>, an orthoborate with new structure type

Hyunsoo Park and Jacques Barbier, *Acta Cryst.* (2001). E57, i82-i84



View of the PbGaBO<sub>4</sub> structure approximately along the [100] direction. Strong angular distortions are associated with the bridging borate groups.

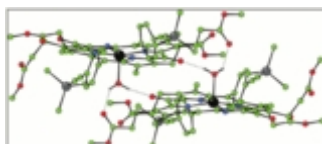
Binary compounds have simple structures with relatively uninteresting properties. Ternary compounds, such as the perovskites, have more complex structures with more interesting properties such as ferroelectricity. Recently, inorganic crystallographers have been studying compounds with four or more elements whose structures are even more complex and continue to stay one step ahead of the ability of theory to predict them or their properties. PbGaBO<sub>4</sub> is a good example. It consists of chains of edge-sharing GaO<sub>6</sub> octahedra linked by PbO<sub>4</sub> and BO<sub>3</sub> groups. Because the BO<sub>3</sub> groups share corners with two different GaO<sub>6</sub> octahedra in the same chain, they cause the octahedra to twist (see the figure). One consequence is that the bonds to O<sub>3</sub> are stretched leaving O<sub>3</sub> underbonded (bond valence sum = 1.79). To compensate, the Ga–O1 bond is shortened, leaving it overbonded (bond valence = 2.23). Although it would be difficult to predict this structure *a priori*, one can at least understand the twists in the chains and the distortions of the GaO<sub>6</sub> octahedra.

Reviewed by I. David Brown, Brockhouse Inst., McMaster U. Canada

## IUCR JOURNALS NEWS

# Aqua{5,15-bis[4-(2-trimethylsilylacetylene)phenyl]-2,8,12,18-tetrakis(2-methoxycarbonyl-ethyl)-3,7,13,17-tetramethyl-10,20-dioxoporphyrinato} zinc(II)

**Andrew D. Bond, Neil Feeder, Simon J. Teat, Zoe Clyde-Watson, Nick Bampos and Jeremy K.M. Sanders, *Acta Cryst.* (2001). E57, m454-m456**



Molecules of the title compound linked into dimers via hydrogen bonds.

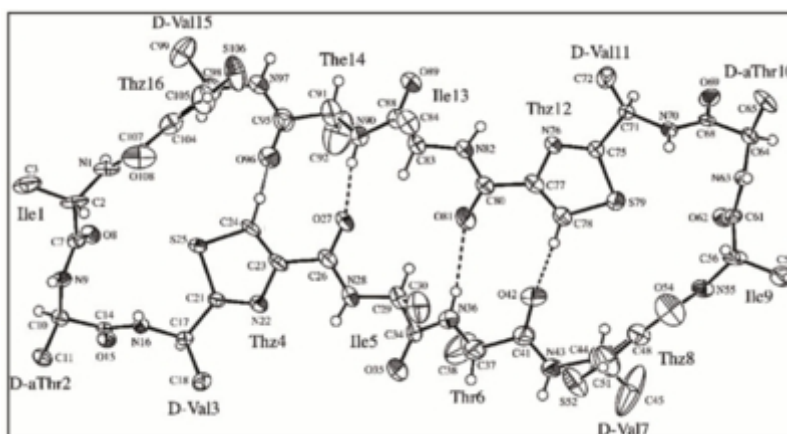
A group from the Cambridge Centre for Molecular Recognition and CLRC Daresbury Laboratory reported the structure of a *trans*-zinc dioxoporphyrin with the other two *meso* positions occupied by the electron-withdrawing group 4-(2-trimethylsilylacetylene). There is a molecule of water occupying an axial site that hydrogen bonds to the carbonyl oxygen of a 2-methoxycarbonyl-ethyl side chain of another molecule to form a centrosymmetric dimer (see figure). The porphyrin adopts a saddle conformation. Adjacent dimers are stacked via laterally shifted porphyrin planes with a Zn...Zn1' distance of 5.719(1) Å. In adjacent molecules there are edge-to-face interactions. This large structure has 80 non-hydrogen atoms in the asymmetric unit. A small crystal of dimensions 0.02 × 0.06 × 0.07 mm was used to collect a data set at Station 9.8, Daresbury SRS. The radiation employed had  $\lambda = 0.6879$  Å. An excellent solution and refinement was obtained, illustrating the utility of synchrotron radiation in such instances.

*Reviewed by Marilyn Olmstead, U. of California, Davis, USA*

# A $\beta$ -sheet structure formed by C-H...O hydrogen bonds between the thiazole rings and amide bonds of a dimeric desoxazoline ascidiacyclamide analogue

A  $\beta$ -sheet structure formed by C-H...O hydrogen bonds between the thiazole rings and amide bonds of a dimeric desoxazoline ascidiacyclamide analogue

Akiko Asano, Taizo Taniguchi, Masahiro Sasaki, Hiroshi Hasegawa, Yoshio Katsuya and Mitsunobu Doi, *Acta Cryst.* (2001). E57, o834-o838



Top view of the peptide backbone. Dashed lines represent hydrogen bonds.

This interesting and valuable paper illustrates how much novel information can be derived from one crystal structure and compressed into a small package. The investigators have introduced a non-standard amino acid into a cyclic antibiotic in order to probe the structural determinants of protein folding. In the process, they have elucidated the conformational flexibility of the unusual peptide as well as the cyclic structure, and demonstrated an important role for CH...O hydrogen bonding in the structure. Although the amino acid introduced in the cyclic peptide has not been detected in ribosomally encoded proteins, the recent identification of the occurrence of pyrrolysine in ribosomally encoded peptides in the Archaea *Methanosarcina barkeri* [*Science*, **296**, 1459 (2002)] and its consequent characterization as the '22nd Amino Acid', raises the possibility that in some species (of the 500,000 or more for which the genetic code has not been unequivocally determined) unusual amino acids such as this may actually be ribosomally encoded in proteins. The CH...O hydrogen bond remains controversial despite numerous observations. This structure presents a very good example of a strong CH...O hydrogen bond involved in defining conformation. Recent observations of such hydrogen bonds in protein structures include cases of stabilization of protein fold, and participation in cofactor binding and protein function.

Reviewed by William L. Duax

Hauptman-Woodward Medical Research Inst., USA

## IUCR ACTIVITIES

## Israeli scholars: statement by ICSU



Since its inception in 1931, the International Council for Science (ICSU) has affirmed and vigorously upheld the principle of universality of scientific activity without any discrimination on the grounds of citizenship, religion, creed, political stance, ethnic origin, race, color, age or gender. It has argued that the processes of academic research and scholarship, and the unfettered pursuit of knowledge, are of benefit to mankind as a whole. Moreover, they are dependent for their advance upon the freedom of scholars to converse, to make contact, to travel to conferences, to publish their results and to proffer advice. It is, therefore, in the interests of governments, institutions and above all individuals – whether themselves scholars or not – to support this principle of nondiscrimination. Bona fide scholars pursuing academic activities should be free to do so without hindrance.

Recent moves to foster an academic boycott of Israeli scientists and the dismissal of two Israeli scholars from their roles on the editorial boards of two journals published in the United Kingdom are a flagrant breach of this profoundly important principle and have rightly drawn substantial adverse comment from scientists, newspaper columnists and human rights activists in the United Kingdom.

On behalf of the Executive Board of ICSU, we draw attention to these events to remind all our national member academies and research councils and our scientific unions and associates of the critical importance of the principle of non-discrimination and of the need for constant vigil in securing its continuing adoption.

We urge all scholarly communities and not least those in science and technology, to heed the words of the Leader in the London Evening Standard on July 10, 2002: 'intellectual communities world-wide are in the business of fostering international understanding and co-operation not of penalizing each other for the shortcomings of their governments'.

*James C.I. Dooge, Chairman and Peter Schindler, Executive Secretary  
ICSU Standing Committee on Freedom in the Conduct of Science*

## MEETING REPORT

# Keynote reports



## Computer predictions of organic crystal structures and properties

S.L.Price, probably the most knowledgeable person in the field of crystal structure prediction of organic compounds by theoretical methods, gave a concise presentation of methods, problems and results in this highly promising and exciting enterprise. Although trained as a theoretical chemist, her understanding of crystallography made the lecture especially appropriate to the occasion and the audience. After an introduction of the theory of intermolecular interactions and their simulation, Price gave an overview of some of the impressive successes of the procedures, as well as a clear account of the problems that remain. The results of a blind test organized by the Cambridge Crystallographic Data Centre showed that all proposed compounds, except one, had been correctly predicted by at least one research group. Price also described how her group complements the comparison of lattice energies with an appreciation of other physical properties, like attachment energies, lattice vibrations and bulk moduli, in the selection of promising candidates.

*A.Gavezzotti*

## MEETING REPORT

# Symposium reports



## Soft matter studied by small-angle scattering



### Speakers in the Soft Matter Studied by Small-angle Scattering symposium

The symposium covered aggregates of surfactants, liquid crystals, polyelectrolyte polymers and semicrystalline polymers. B. Demé (ILL) showed how various techniques can be used to study aggregates formed in water-rich, salt-free mixtures of anionic and cationic surfactants. Small-angle neutron scattering was used to obtain quantitative information on icosahedral shells, large stiff discs and lamellar phases. P.S. Clegg (U. of Toronto) presented a study of liquid crystal-aerosil mixtures, where the aerosil works as a random field influencing the ordering of the liquid-crystal molecules. The system was studied by x-ray diffraction and its behavior was found to be in agreement with one of the available theories and in clear disagreement with others. J. van der Maarel (The Netherlands) described a small-angle neutron contrast variation study of micelles formed by block copolymers with a polyelectrolyte block. The scattering was separated into basic contributions and modeling of these revealed complex behavior when the charge density of the polymer and the salt concentration of the solution were varied. J. D. Barnes (Maryland) talked about SAXS and SANS studies of semicrystalline polymers with lamellar structures of amorphous and crystalline regions. In some of the systems, the difference in scattering length density of the amorphous and the crystalline regions vary strongly with temperature and there is even a temperature, where the contrast vanishes. For the samples which had been exposed to various forms of processing, a strong orientation of the lamellar structure was present and a proper analysis of the structure required that 2D scattering data be recorded for all principal orientations of the samples.

*Thomas Zemb, Andrew Allen and Jan Skov Pedersen*

## Nanostructural characterization by small-angle scattering



### Speakers in the Nanostructural Characterization by Small-angle Scattering symposium

The talks focused on recent developments, the possibilities these developments foster and new results. B. Chu (USA) described templating mesostructures of spontaneously formed block copolymer micelles of polyoxymolybdates. The work revealed that the formation of a mesoporous structure did not depend on the presence of the micelles, but could be achieved also by homopolymers in solution. O. Paris (Austria) described the application of the scanning-SAXS method to determining the local structure of

inhomogeneous biological materials at one micrometer, with synchrotron radiation. A.J. Allen described characterization of multi-component systems of industrial interest using the multiple SANS technique. R. Gilles discussed *in situ* high-temperature SANS results for Ni-based superalloys that are used in turbines and jet engines. The modeled microstructure provides information needed for improved materials production. N. Ibraimov described the use of Kumakhov capillary optics to increase the flux and reduce the background of an X-ray reflectivity study of the surface structure of samples of relevance for microelectronics. K. Sakurai extended the discussion to include off-specular measurements on multilayers with the same composition as those used in x-ray monochromators. The measurements provide additional information on lateral correlations in the surface layers.

*Iris L. Torriani and Jan Skov Pedersen*

## Molecular and crystal properties from charge and spin densities



Ewald Prize winner Michael Woolfson with Herb Hauptman

This microsymposium demonstrated the practical impact that theoretical and experimental density studies have on biology, crystal engineering and materials science. C. Lecomte demonstrated the transferability of electron densities in a multipolar refinement of a protein using models derived from previous charge density studies of a series of polypeptides. The application of the MOPRO refinement strategy to ultra high resolution data on Aldose Reductase ( $d_{\min} = 0.64 \text{ \AA}$ ) revealed for the first time the electrostatic complementarity between the protein and the ligand. The era of electrostatic, rather than of purely geometrical, interpretation of the 'lock and key' mechanism is thus opened.

M. Spackman reviewed Hirshfeld surfaces (HSs) as a way of exploring packing modes and fingerprinting intermolecular interactions in molecular crystals using a very simple and efficient partitioning of crystal space. Since HSs encode information about all intermolecular interactions simultaneously, a 2D mapping of these surfaces was recently devised. The mapping plots the fraction of points on the surface as a function of the closest distances from the point to nuclei inside and outside the surface. In this manner all types of interactions (hydrogen bonding, H...H contacts, C-H... $\pi$  interactions,  $\pi$ - $\pi$  stacking, etc.) are readily identifiable as are the similarities and differences of packing modes in related molecular crystals. These visually stunning plots are unique for a given crystal structure and polymorph. Their practical impact on crystal engineering was highlighted. Recent applications showed that partitioning using ionic electron densities yields a remarkably diverse range of shapes, especially for anions. The resulting basins are similar to those obtained through Bader's partitioning of an *ab-initio* periodic Hartree-Fock electron density.

Lectures by Cooper and Paolasini revealed how combined studies of the spin and charge densities of inorganic crystals enables one to understand their material properties. M. Cooper discussed magnetization in ferromagnets with polarized x-rays. The crucial role of complementary Compton and diffraction studies to understand physical properties was illustrated by the study of  $\text{Sm}_{0.98}\text{Gd}_{0.02}\text{Al}_2$  in which gadolinium doping produces a zero total magnetization at temperatures near the boiling point of liquid nitrogen. The results show that it is the small gadolinium itinerant electron spin contribution that preserves the magnetic order of this material above the magnetization compensation point.

Paolasini described Non-Resonant and Resonant X-ray Scattering (NRXS and RXS) studies at ESRF, of the magnetic and orbital ordering in the pseudocubic perovskite  $\text{KCuF}_3$ . RXS has its origin from processes in which photons are virtually adsorbed by exciting core electrons to empty states and subsequently re-emitted when the excited electrons and the core holes recombine. Structurally forbidden reflections,

corresponding to magnetic and 3d-orbital long-range order, have been observed by Paolasini and coworkers. It appears that the orbital and magnetic orderings are closely related (even though the associated energy scales differ by more than a factor of 20) and with a definite interplay between magnetic and orbital order parameters as revealed by an increase in the intensity of orbital Bragg peaks in the temperature range close to the Neél point.

K. Tanaka discussed a multi-temperature measurement of electron density distributions (EDD) in crystals of  $\text{CeB}_6$ . In this rare-earth complex crystal 4f-electrons spontaneously flow from Ce to  $\text{B}_6$  with a decrease in temperature, which starts above room temperature and ultimately leads to an anomalous resistivity increase below 2K. Research on the EDD in rare-earth compounds is a frontier field in X-ray diffraction.

*Carlo Gatti and Malcolm Cooper*

## Nanocrystalline materials



### Delegates Reception

The symposium addressed the design and applications of nanocrystalline materials. R. Nesper (Zurich) described metal oxide nanotubes obtained by controlled scrolling of layered structures and the collapse of nanotubes into nanorods. Applications included cation selectivity, anisotropic NLO materials and potential sensors. M. Remskar (Ljubljana) described the growth of metal disulfide nanotubes, the self-assembly of multi-walled nanotubes, rotation of nanotubes at elevated temperatures, and the rapid migration of  $\text{Cs}^+$  ions along  $\text{WS}_2$  nanotubes. Finally, the role of  $\text{C}_{60}$  was explored as a templating agent in the nucleation of crystals, which contain molybdenum sulfide nanotubes with iodine between them. M. Green (Oxford) described the growth of inorganic crystals within the confines of single-walled carbon nanotubes and the changes in ion coordination number arising from confinement. Crystals of potassium iodide only two or three ions in diameter were characterized by electron microscopy techniques. A. Eichöfer (Karlsruhe) described the synthesis of cadmium chalcogenide based nanoclusters with sizes ranging from 0.8 - 2.0 nm in diameter and containing from 4 - 32 cadmium atoms that exhibit interesting photoluminescent properties. Z. Somogyvari (Budapest), described neutron diffraction studies of transition metal oxides important as magnetic recording materials. In barium hexaferrite (Co, Ti doped) neutron diffraction was crucial to determining the cation distribution, taking full advantage of the substantial differences in scattering lengths between Fe, Co and Ti. The effect of crystal size (nanocrystals vs. microcrystals) on magnetic properties was also explored.

*Lee Brammer*

## Diffraction and symmetry of aperiodic crystals



Microtomography and High Resolution Imaging Session Speakers

This symposium featured recent theoretical and experimental studies of aperiodic crystals. H. Takakura reported on applications of the low electron density elimination (LDE) method to the phase reconstruction of X-ray single crystal data of quasicrystals (i-Al-Pd-Mn). He indicated that the location, sizes and shapes of the occupation domains in the  $n$ -dimensional unit cells are obtained without model structures. M. Honal examined the refined characteristic diffuse scattering observed in the diffraction patterns of decagonal AlCoNi. Features of the scattering are similar to the 'atomic size effect' scattering common in crystalline alloys. Monte Carlo techniques were applied to study the phenomena based on the size effect of the constituent atoms. A. Cervellino compared the structures of the decagonal  $\text{Al}_{71}\text{Co}_7\text{Ni}_{22}$  phase and the related decagonal Edagawa superstructure ( $\text{Al}_{71}\text{Co}_{13}\text{Ni}_{16}$ ). The former is stable over  $950^\circ\text{C}$ , has a low density ( $3.9 \text{ Mg/m}^3$ ) and high structural occupational disorder, the latter is stable between  $500\text{--}850^\circ\text{C}$  is denser ( $4.1\text{--}4.2 \text{ Mg/m}^3$ ) and presents lower occupational disorder. Orientational disorder was measured by diffuse scattering. G. Chapuis described a molecular dynamics simulation of the incommensurate structure in hexamethylenetetramine solved previously with single crystal X-ray data and a superspace approach. The simulation was carried out in the temperature range from 15 K to 580 K with a time step of one femto-second. A unique compensating pressure tensor was applied in order to get lattice parameters close to the experimental ones. The current MD simulation reproduces the experimental diffraction results well. M. Ohmura showed that the two-dimensionally modulated structure of  $\text{Ca}_2\text{CoSi}_2\text{O}_7$  is stable below 489K and the component  $q$  of the primary modulation wave-vector, varies from 0.286 to  $1/3$  with temperature change. The variation of the long-range order in the modulated structure can be derived from the structure parameters determined at room temperature.

Masaaki Ohmura and Marc de Boissieu

## Imaging



This symposium brought together leaders in high resolution X-ray imaging, microtomography and phase-contrast imaging. A variety of techniques were described including those using an objective lens [e.g. *Fresnel Zone Plate* (FZP) or *Compound Refractive Lens* (CRL)] to provide 'full-field' imaging and propagation-based techniques where mathematical methods are used to correct for 'defocus' of the imaging system.

P. Cloetens described how quantitative information can be extracted from high resolution absorption and phase-contrast images and micro-CT obtained via multi-distance phase retrieval methods from holographic data. He finds that phase-retrieved images become preferred as X-ray energy increases. Y. Kagoshima reported on 8 - 12 keV imaging from an undulator at SPring-8 using a Zernike-type phase-contrast microscope. Both positive ( $\pi/2$ ) and negative ( $3\pi/2$ ) phase plates were used to obtain images approaching 60 nm resolution for line pairs. Somewhat inexplicably, the negative phase plate regularly gave considerably better quality images, e.g. of diatoms and *conidia* even in water. G. Tromba presented images obtained using a PDI/DEI-type technique which includes processing of multiple images to obtain separate absorptive and refractive components.

Other topics addressed included: projection-based methods of phase-contrast imaging including high resolution microscopy and tomography of semiconductor devices (S. Wilkins, CSIRO); high energy full-field X-ray microscope with a current resolution of 0.3 microns (C. Schroer); soft- and hard-tissue images using a Bonse-Hart interferometer with micro-CT and projection-based images obtained at DESY (F.

Beckman); and the application of dark-field ('Owl') methods to phase-contrast imaging using monolithic multi-crystal systems (M. Ando).

*Steve Wilkins (CSIRO)*

## Horizons in hydrogen bonding



Henk Shenk and Sine Larson

Advances in fundamental and applied aspects of hydrogen bonding in small molecule and macromolecular structures were combined in this session. Lee Brammer (Sheffield U.) discussed weak hydrogen bonds  $D-H\cdots X-C$  ( $D = C, N, O$ ;  $X = F, Cl, Br, I$ ) and compared them with their stronger cousins  $D-H\cdots X-M$  ( $M =$  transition or main group metal). The use of directional halogen-mediated interactions in the design of ionic hydrogen bonded network solids was illustrated. Bing Gong (SUNY Buffalo) showed bifurcated three-center  $N-H\cdots O$  hydrogen bonds characterized by X-ray diffraction that are stable in solution (NMR). It is possible to tune the cavity size of helical nanotubes (15–30 Å diameter) in folded oligomers through the choice of carbon backbones and the conformation of the hydrogen bonding groups. I. Olovsson (Uppsala U.) discussed the refinement of the hydrogen atom position in a short hydrogen bond in KHdichloromaleate determined by low temperature neutron diffraction. Interestingly, when the heavy atoms are refined in P-1 and the protons are refined in P1, the non-hydrogen structure is still centrosymmetric but the hydrogen atoms are off-centered! The details of this unconventional structure refinement procedure continued to be debated well after the formal session was over. P. Chakrabarti (Bose Inst.) presented results on the significance of aromatic–aromatic and charged polar interactions between Phe, Tyr, Trp and His residues in protein structures. The geometry of recognition motifs (face-to-face, offset-facestacked, edge-to face) and their occurrence in proteins with greater than predicted probability may be explained through specific interactions ( $N-H\cdots O$ ,  $N-H\cdots \pi$ ,  $C-H\cdots \pi$ ). According to P. Auffinger (IBMC, CNRS) hydration in RNA, bifurcated hydrogen bonds, stability of  $C-H\cdots O$  H-bonds, and the processes of melting and crystallization may be better understood through the use of molecular dynamics simulations. With a better understanding of the hydrogen bond phenomenon it is possible to design and analyze complex structures, thus providing a continuum from fundamental to applied and biological studies.

*Ashwini Nangia (Hyderabad U.)*

## Detectors



Speakers in the Workshop on Protein Crystal Growth

The microsymposium focused on X-ray area detectors for use with synchrotron radiation. H. Graafsma (ESRF), gave a comprehensive overview of the role and importance of detectors in the field of synchrotron radiation. E. Eikenberry (SLS) described pixel arrayed detectors with extremely high counting rates. The development and application of an imaging plate scanner with a large format (400 mm x 2000 mm) for automated protein crystallography, was discussed by N. Sakabe (Japan). The final talk was on the development of a phosphor screen with improved efficiency based on a new concept. *Yoshiyuki Amemiya (U. of Tokyo) and Heinz Graafsma (ESRF)*

## MAD, SAD and difficult phasing

The role of selenium in MAD phasing is now well-established but, as G. Leonard demonstrated, other elements and softer X-rays should not be neglected. For instance, if the technical difficulties were overcome, a single uranium atom would give an rms  $\Delta F/F$  signal of 6.9% for the whole ribosome at a wavelength of 3.5Å. Even at a wavelength of 1.7Å, a SAD experiment exploiting intrinsic sulfur atoms is sufficient to solve many protein structures. SAD experiments have become more popular recently because problems of radiation damage are reduced compared to multi-wavelength approaches. R. Pannu showed that it is possible to get better phases from such experiments by using a new SAD likelihood function. This new target takes full account of correlations ignored by previous methods, such as errors in anomalous scattering predicted for the two members of the Friedel pair. G. Bricogne straddled the theoretical and experimental by describing improvements in the speed and performance of the popular SHARP phasing program, and new ideas for introducing anomalous scatterers by soaking in tri-iodide or combinations of salts. Z. Otwinowski ended with a philosophical discussion of considerations in processing data to preserve small anomalous differences, as a prelude to using such differences to exploit radiation damage for phasing.

Case histories illustrated what can be learned from difficult structures that would have been impossible a few years ago. The structure of KPHMT was solved by Se-Met MAD, setting a record for the size of the anomalous substructure: 160 seleniums. In describing this work, Frank von Delft showed that greater redundancy is not always better. Finally, Gabby Rudenko showed how persistence paid off in solving the extracellular domain of the LDL receptor where iterative improvement of the phases from tungsten clusters led to an interpretable 3.7Å map.

*Randy Read and Andy Thompson*

## Molecular dynamics of crystals and phase transitions

Chairperson, A. Gavezzotti, described the application of modern molecular dynamics simulation techniques, to the study of the properties of crystals and of their transformations. Cochair, L.R. Nassimbeni, commented on experimental problems in phase transitions of inclusion compounds.

These preliminary statements elicited a lively discussion. F. Herbststein (Haifa) gave a masterly description to the main thermodynamic features of phase transitions, with examples taken from real-life crystallography. J. Scott (Melbourne) reported on her exciting results in experimental synthetic solid-state chemistry on compounds of interest to agricultural applications. J. van de Streek (Nijmegen) described the dynamics of the complex phase behavior of nalkanes, highlighting the importance of the inclusion of kinetic energies and temperature in theoretical simulations.

*A. Gavezzotti*

## MEETING REPORT

# Open commission reports



## Commission on crystallographic nomenclature

The Commission on Crystallographic Nomenclature comprises an elected Chairperson and ex officio members, namely the editors of the Union's journals and International Tables, the Chairman of the IUCr/OUP Book series Committee, the Chairman of the Teaching Commission, the Chairman of the Committee for the Maintenance of the Crystallographic Information File Standard, the President and the General Secretary of the IUCr. After the retirement of its past Chairman, Sidney Abrahams, André Authier was elected as the new Chairman.

Nomenclature problems arising in specific fields of crystallography are studied by *ad hoc* committees of experts appointed by the Commission.

The Second Report of the Subcommittee on the Nomenclature of *n*-Dimensional Crystallography, chaired by T. Janssen, has been accepted by the Commission, and will shortly be printed in *Acta Crystallographica, Section A*.



Members of the Commission on Crystallographic Nomenclature (left to right: Å. Kvik (France), G. Ferguson (Canada), D. Mills (USA), K. El Sayed (Egypt), T. Hahn (Germany), D. Litvin (USA), F. Allen (USA), S.R. Hall (Australia), C.P. Brock (USA), B. McMahon (UK), I.D. Brown (Canada), D. Schwarzenbach (Switzerland), W. Clegg (UK), J.P. Glusker (USA), U. Shmueli (Israel), A. Authier (France)).

The present working groups are:

- 'Working group on the definition of crystalline phase identifiers', chaired by I.D. Brown, charged with generating machine-readable forms of identifiers suitable to uniquely characterise crystalline phases reported in electronic databases, in line with the IUPAC/CODATA/ICSTI project to standardise the representation of physicochemical properties led by H. Kehiaian. An early conclusion of the working group is that it is useful to work with multiple-component identifiers (in the spirit of the recommendations of the Phase Transition Nomenclature subcommittee). Early proposals are defining possible components by the use of data fields in CIF notation. The final form of an identifier will not necessarily be a collection of CIF data items, and alternative but equivalent representations might be appropriate for different purposes.
- 'Working group on co-crystal nomenclature' chaired by F. Allen. This group arose from an observation by Professor J. Dunitz that there is no systematic nomenclature in general for the large variety of multi-component solid-state systems. A nomenclature to differentiate and define such systems could be applied to examples as diverse as inclusion compounds, supramolecular

complexes, addition compounds, zeolites, solvates, racemic compounds etc. The working group will study any existing IUPAC recommendations and practices, and will work closely with IUPAC on this topic.

- 'Working group on synchrotron radiation nomenclature' chaired by D. Mills. An example of nomenclature problems is given by the existing confusion between the uses of the terms 'brilliance' and 'brightness'.
- Crystallographers are invited to bring additional nomenclature problems to the attention of any Commission member.

The Nomenclature Commission web page is currently being revised. The draft new web page can be consulted at <http://www.iucr.org/iucr-top/comm/cnom/index.html>.

*André Authier*

MEETING REPORT

## XIX IUCr congress and general assembly





The Assembly of Delegates to the XIX Congress. *Photo courtesy of Caroline Duax.*

## MEETING REPORT

## ACA 2002

## Electron crystallography



Electron diffraction and imaging has a fascinating history in both biology and materials science. A special session on the topic was organized in conjunction with the presentation of the Patterson Award to Doug Dorset at the San Antonio, Texas ACA meeting. Doug provided an overview of the field, with emphasis on electron crystallography of organic crystals, as discussed in his comprehensive book. The symposia included talks by K. Downing on tubulin, B. Jap on two-dimensional crystallization techniques, C. Gilmore on the phase problem, J. Fryer on electron crystallography generally, and J. Spence and L. Marks on new methods. Application in the field of materials included mesoporous material (O. Terasaki), charge-density measurements by CBED imaging (Y. Zhu), electron nano-crystallography (J.M. Zuo), electron imaging from glasses (M. Treacy), and energy-filtered diffraction patterns from diatom frustules (Y. Kim). Two things are driving this growth in electron diffraction and imaging methods - in biology, the urgent need to determine the shape of large macromolecules, at sub-nanometer resolution, which cannot be crystallised, and in materials science, the boom in nanoscience, for which the electron microscope provides the ideal probe.

*John Spence*

## Electron microscopy of biological macromolecules



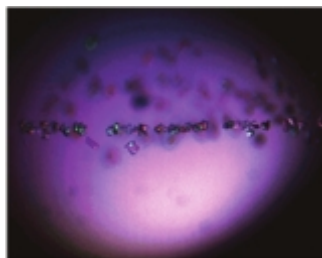
Transactions Symposium 'Crystal Structure Determination' speakers

In addition to the day-long Symposium on Electron Crystallography that was organized in conjunction with this year's Patterson Award to Doug Dorset, the Spring 2002 meeting featured three half-day sessions on Electron Microscopy of Biological Macromolecules. Electron microscopy of samples embedded in vitreous ice ('cryo-EM') has recently developed as a powerful way to visualize the three-dimensional assembly of macromolecules into various complexes and machines, and thus it is regarded as providing an important bridge between structural genomics and cell biology. A session focused on the quantitative interpretation of cryo-EM density maps included K. Namba's presentation of a comprehensive and stunning survey of the bacterial flagellar apparatus and H. Li's description of tubulin assembly. The second session moved on to report technology-developments that aim to automate many of the steps in cryo-EM that must currently be done 'by hand' and application to the pyruvate dehydrogenase complex from *B. stearothermophilus*, an 11 megadalton 'catalytic machine' by J. Milne and the changes in structure of GroEL chaperonin during its biochemical cycle by H. Saibil. The final session concerned work in which 2-D crystals are used in order to obtain 3-D density maps at high enough resolution to allow *de novo* modeling of the structure at atomic resolution. Other structures reported were: the membrane protein, bacteriorhodopsin (Y. Fujiyoshi), a bacterial oxylate (S.

Subramaniam), and an aquaporin (A. Philippsen).

Bob Glaeser

## Crystal structure determination



Streak seeding crystals from Allan D'Arcy

The Transactions Symposium dealt with *Crystal Structure Determinations from Powder Diffraction*.

Powder patterns contain an enormous amount of information. However, a stumbling block to obtaining structural data was the lack of mathematical methods of peak shape duplication. It was not until the early 1980s that software began to appear that would allow for decomposition of the powder pattern to obtain accurate intensities. Since then, there has been great progress in both hardware and software for all aspects of structure determination and refinement. This symposium was convened to highlight these advances.

L. Cranswick and R. Shirley discussed methods of indexing the powder pattern. C. Giacovazzo described his EXPO, a much used program for *ab initio* structure solutions. Powder patterns with low angular resolution (H. Toraya), organic crystals affected by preferred orientation (M. Tremayne), metal terephthalates (J. Kaduk), and the use of high brightness synchrotron x-ray and high flux neutron sources to study powder samples under high pressure (J. Parise) were all addressed in the symposium. C. Hubbard discussed the use of the Powder Diffraction File (PDF) published by the Int'l Center for Diffraction Data (ICDD) to help establish phase identification, corrosion and decomposition products in the varied fields of mineralogy, materials science, manufacturing and pharmaceuticals. The solution of organic structures from powder data becomes very difficult when molecules are flexible or three or more are present in the asymmetric unit. Complex structures with poor resolution were addressed by C. Gilmore. P. Stephens discussed his use of the public domain Powder Structure Solution Program for the solution of structures of drugs. M. Deem described a Monte Carlo scheme to determine the crystal structure of all known zeolites. R. Grothe is developing a program for structure determination from anisotropic powder diffraction data collected on an area detector. By combining high-resolution synchrotron X-ray powder diffraction data and stereochemical restraints, it has been demonstrated that the Rietveld refinement of protein crystal structures is feasible (R. Von Dreel and P. Stephens).

Abraham Clearfield

## New macromolecular crystals

In the microsymposium *New Macromolecular Crystals, Techniques and Hardware*, A. D'Arcy demonstrated that microbatch minimizes sample oxidation, makes temperature variation easier and allows increased reagent and sample concentrations by incorporating Si oil in the experiment. He modifies the protein by complexation (adding an inhibitor), proteolysis, deglycosylation, and site directed mutagenesis. T. Tisone (Cartesian Technologies) described the use of non contact microfluidics and automation for protein crystallization. B. Haushalter (Parallel Synthesis Technologies) discussed nanoengineered surfaces for the epitaxial nucleation of protein crystals.

J. Jancarik discussed sparse matrix crystallization screens centrifugal filter devices for concentration and detection of monodispersity by dynamic light scattering (DLS). A. Hassell designed constructs using homologous models limited proteolysis, and the use of 'seeding' with good results, especially cross-seeding with apo forms to grow kinase-ligand complex crystals.

*Bob Cudney*

## Protein folding and design

J. Richardson taught us a lesson in the importance of hydrogens in sidechain packing and introduced her new, interactive MAGE tools for evaluating and correcting mistakes in crystal structures (<http://kinemage.biochem.d-uke.edu/molprobuty/>).

*Chris Bystrof*

## New methods in macromolecular crystallography

A number of groups are developing detectors that employ discrete semiconductor devices. Thin film transistor (TFT) technology produces a single, monolithic detective surface relatively inexpensively. E. Merritt described a procedure for comparing the validity of different techniques for modeling anisotropy in protein structure, which he applied to several refinements of anisotropic displacement parameters (ADP), translational, librational, and screw (TLS) motions at resolutions between 1 and 2Å. He concluded that the TLS method works well over this entire resolution range. The ADP method becomes preferable to TLS at resolutions higher than 1.6Å, but the precise resolution at which this happens is structure dependant. Both the ADP and TLS methods performed better than purely isotropic refinement. Several groups have tried to work at temperatures in the low teens (Kelvin) rather than at the ~100K accessible with liquid nitrogen. One successful method uses a cryostat that directs a fine, high-velocity stream of gaseous helium on the specimen.

*Jim Fait*

## Scattering in nanoscience and nanotechnology

This symposium ranged from the fundamental to the applied and from purely inorganic to biological. Topics covered included research to understand the novel electronic properties of complex transition metal oxides (R. Osborn, Argonne), studies of nanoporous glassy materials in the encapsulation of radioactive waste (P. Thiyagarajan, Argonne), the characterization of the perfection of photolithographically created nanostructures (R. Jones, NIST), and videos of scattering from dancing nano-scale oil drops under shear (T. Mason, ExxonMobil). M. Firestone (Argonne) described how biomimetic lipid based complex fluids can be used as scaffolds for inorganic nanoparticles, and even functional proteins, and P. Sokol (Penn State) showed what inelastic neutron scattering can tell us about what happens in a buckytube full of hydrogen. The range of scattering techniques used was also varied, and the problem of scattering from nanostructured materials is leading to novel applications of scattering and ingenious extensions of scattering techniques. The varied techniques employed included wide angle scattering, small angle scattering, reflectography, x-ray circular dichroism, grazing incidence diffraction, and electron diffraction using nanometer sized beam-spots.

*Simon J. L. Billinge and Paul Butler*

## Structural genomics: are the pieces ready yet?

The symposium discussed progress, challenges, and achievements in structural proteomics/genomics. C. Kissinger described a large scale high-throughput crystallography project with automated systems for protein production and structure determination. The system was applied to a set of bacterial targets yielding 53 new structures and 7 new folds. He said that the map-fitting step is the biggest hurdle to full automation.

A. Joachimiak emphasized the difficulty of optimizing crystallization conditions as a bottleneck in structure determination and described a robotic system for crystal mounting, including a prototype UV-

light-based method for crystal centering. L. Tari presented a commercial view of how high-throughput crystallography can be used for structure-based drug design.

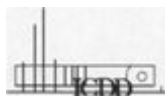
Case studies of structural proteomics described included a case in which sequence comparisons gave no information but the solved structure matched a methyl-transferase; in another, sequence and structure gave no obvious match but led to a good guess (NTP hydrolase); in others, neither sequence nor structure gave useful clues.

*Tom Terwilliger*

*Reports and image taken from the ACA Newsletter, Fall 2002*

## MEETING REPORT

# Spring meetings



An international gathering of the ICDD members, representing a wide range of scientific disciplines attended the Annual Spring Meeting of the Int'l Centre for Diffraction Data (ICDD), March 18-22, 2002. The members play an essential role in the development of the ICDD, tailoring its database products, and services to the needs of the global scientific community. The ICDD Board of Directors discussed the financial, business and long range planning functions of the ICDD. Results of global X-ray conferences, workshops and clinics were described as well as proposals for future activities. In a typical year, the ICDD financially supports or directly conducts over a dozen forums for X-ray analysis technology exchange across the globe. Evgeny Antipov, Moscow State U., received the Distinguished Grantee Award and also gave a presentation of his work in the ICDD Grant-in-Aid Program, which includes reference patterns for industrially important, advanced inorganic materials. The new slate of directors serving the term 2002-2004 was also announced (see Page 22).

If you are interested in becoming an ICDD member visit [www.icdd.com](http://www.icdd.com) or contact the Membership Committee Chairperson, W. Wong-Ng ([wongng@icdd.com](mailto:wongng@icdd.com)).

*Terry Maguire*

## MEETING REPORT

## RapiData 2002



Some of the chaos of data collection at RapiData 2002. Shown at beamline X9-B, operated by the Albert Einstein College of Medicine for the Sloan Kettering Memorial Inst. and Rockefeller U., are (in the background) Adriana Rojas Cardona (Inst. de Fisica de Sao Carlos) and Joe Mansury (PX Operator for the Brookhaven Biology Dept). In the foreground are Anna Larsson (Uppsala U.), Raj Rajashankar (Structural GenomiX, Inc.), one of the volunteer instructors for the course, and Michael Kennedy (Pacific Northwest Nat'l Lab).

RapiData 2002, the fourth in Brookhaven Nat'l Lab's annual series of crash courses in crystallography, was once again a huge success. Forty-eight students from around the world participated from April 21 to 26. More formally titled 'Rapid Data Collection and Structure Solving at the NSLS: A Practical Course in Macromolecular X-Ray Diffraction Measurement,' the program was developed by BNL's Biology and Nat'l Synchrotron Light Source (NSLS) departments to introduce students to the finest teachers, newest equipment, and latest techniques in the field of macromolecular x-ray crystallography. Four structures were solved during the course. This year, to amplify its Latin American Initiative, the US National Committee for Crystallography provided funds for partial travel scholarships to the course for six students, three from Brazil, two from Mexico, and one from Argentina. For more information about this year's program, including the sources of funding, go to [www.px.nsls.bnl.gov](http://www.px.nsls.bnl.gov).

*Bob Sweet*

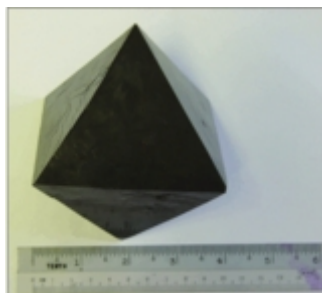
## MEETING REPORT

## NSLS 2002 users meetings

This year's Annual National Synchrotron Light Source (NSLS) Users' Meeting, held at Brookhaven National Lab (BNL) on May 20-22, had a record attendance of 380 participants from all over the world. The meeting consisted of a one-day plenary session and eight day-long workshops on the latest results achieved at the NSLS in the physical, biomedical, environmental, and instrumentation sciences. L. Joshua-Tor of Cold Spring Harbor Lab served as Chair of the event. L. Berman of NSLS served as the Program Chair for the plenary session, and A. Frenkel of Yeshiva U. served as the Workshops Chair. A new project discussed at the meeting was a center dedicated to the study of the infinitesimally small. Called the Center for Functional Nanomaterials, this new BNL facility, which will investigate materials a billionth of a meter in size, has received a 'very strong thumbs up' from initial reviews by DOE-BES, according to S. Ozaki, Special Assistant to the BNL Director for Accelerator Projects, who gave the meeting's welcoming address. Workshops relevant to crystallography included over-expressing, purifying, and crystallizing membrane proteins (L. Shapiro and F. Mancina), Advances in the application of Synchrotron Radiation to Catalysis, imaging and micro-spectroscopy, and *In situ* studies of materials processing.

## MEETING REPORT

# Singapore crystal growth challenge



The prize-winning crystal weighed 588.5 g with dimensions  $9.0 \times 8.6 \times 7.5 \text{ mm}^3$ .

Who isn't fascinated by the beauty of single crystals? It is always a challenge to grow large single crystals while maintaining their aesthetic beauty, flawless faces, sharp corners and edges. In spite of technical advances, the growth of single crystals is still considered to be an art that holds great fascination for young and old. The Dept of Chemistry at the Nat'l U. of Singapore and Singapore Nat'l Inst. of Chemistry (SNIC) organized the 5<sup>th</sup> Crystal Growing Challenge for students. The main aim of the challenge is to discover the importance of good technique and to show that science is fun. The students can demonstrate their creativity and learn about the associated science.

There were three categories in this year's competition, Junior (for secondary school students), Senior (for junior college and polytechnic students) and Open levels. For each category, there were first, second, third and two meritorious prizes carrying cash awards and trophies for the winners in each category. For the junior level category, the students grew 'Chrome Alum' ( $\text{KCr}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ ). The biggest crystal, weighing more than half a kilogram and prepared by River Valley High School students, was adjudged to be the winner in this category (see Figure 1). The senior level students grew KDP ( $\text{KH}_2\text{PO}_4$ ) crystals (see *IUCr Newsletter*, Vol. 8, No. 2, 2000, page 24). The participants in the open level were given the task of growing a crystal inside a crystal. This year's winning crystal had triple layers of three different double sulfates with an octahedral shape. There were 104 entries from 59 secondary schools, 18 entries from 9 junior colleges and polytechnics and 36 entries for the open level category. L. Lim, Deputy Director, Biomedical Center of A\*STAR (Agency for Science, Technology and Research) was the guest of honour for the prize presentation ceremony. This year's competition was sponsored by A\*STAR, Bruker Singapore Pte Ltd, Lee Foundation of Singapore, Hyflux Ltd, and Singapore Nat'l Academy of Science.

Details of this challenge and the names of the winners are available at [www.chemistry.nus.edu.sg/ngc1.htm](http://www.chemistry.nus.edu.sg/ngc1.htm).

*Jagadese J. Vittal and Edward R.T. Tiekink*

## MEETING REPORT

# The Gregori Aminoff prize to Lahav and Leiserowitz



Lecturers at the Aminoff symposium. (left to right) Ivar Olovsson (organizer), Michael Ward, Meir Lahav, Jack Dunitz, Angelo Gavezzotti, Lia Addadi, Leslie Leiserowitz, Jens Als-Nielsen, Michael McBride, Stephen Byrn.

The Royal Swedish Academy of Sciences has awarded the Aminoff prize for 2002 to Meir Lahav and Leslie Leiserowitz from the Dept. of Materials and Interfaces, Weizmann Inst. of Science, Rehovot, Israel, for their fundamental studies of crystal growth and application to separation of enantiomers and for their studies of surface structures by synchrotron radiation. The prize was presented at the ordinary meeting of the Academy on September 11.

A symposium on the theme 'Crystal Growth and Surfaces' was arranged the following two days. The following lectures were delivered:

- *Shaping crystals with 'tailor-made' auxiliaries* (M. Lahav, Weizmann Inst.);
- *Chirality at the interface between crystals and biology* (L. Addadi, Weizmann Inst.);
- *Crystal growth interfaces: Visualization and controlled nucleation* (M. Ward, U. of Minnesota);
- *Crystal growth and dissolution near equilibrium: Direct observation by atomic force microscopy* (M. McBride, Yale U.);
- *Crystallization and solid state chemistry of pharmaceutical compounds* (S. Byrn, Purdue U.);
- *Polymorphism: The same yet different* (J. Dunitz, ETH Zürich);
- *The physics and use of synchrotron radiation for studying surfaces and interfaces* (J. Als-Nielsen, Niels Bohr Inst.);
- *Understanding crystal nucleation: Can a cheap computer help a million-dollar project?* (A. Gavezzotti, U. of Milano); and
- *Crystalline Architectures at the air-water interface. Relevance to crystal nucleation* (L. Leiserowitz, Weizmann Inst.).

Ivar Olovsson, Chairman,  
Swedish National Committee of Crystallography

## AWARDS AND PRIZES

## Tsirelson receives Humboldt award



Vladimir G. Tsirelson, Professor and Head of the Quantum Chemistry Dept. at the Mendeleeev U., Moscow, has been named as a recipient of the 2002 Alexander von Humboldt Research Award in the field of crystallography. He is honored for his contributions to development of the theoretical principles of accurate X-ray diffraction analysis and methods of accurate measurement and interpretation of the electron density and electrostatic potential. The remarkable feature of Prof. Tsirelson's research consists of a combination of the quantum chemical methods and X-ray and electron diffraction experiments. These studies have provided a step towards an essentially new level of knowledge concerning bonding in molecular and crystalline systems. Prof. Tsirelson will continue his research in collaboration with Muenchen Technical U., Wuerzburg U. and Potsdam U.

## AWARDS AND PRIZES

## Allen to receive Skolnik award



The Herman Skolnik Award of the ACS Div. of Chemical Information, recognizing outstanding contributions to and achievements in the theory and practice of chemical information science, will be presented at the Fall 2003 ACS meeting in New York to **Frank Allen**. Dr. Allen has worked at CCDC since 1970, following undergraduate and graduate studies at Imperial College, London and postdoctoral work at the U. of British Columbia. He became Executive Director of the CCDC in October 2002. Allen has been the Editor of *Acta Crystallographica B* from 1993-2002, and held a range of senior positions in the BCA, the ECA and the IUCr. He became a Fellow of the Royal Society of Chemistry in 1992, was awarded the RSC Silver Medal and Prize for Structural Chemistry in 1994, and was appointed to the Editorial Board of *Chemical Communications* in 1999, and to a Visiting Professorship at the U. of Bristol, UK in 2002. He is a member of the Int'l Advisory Board of the Protein Data Bank (RCSB) and has done much to promote the scientific value of all of the crystallographic databases in the international arena.

*Bill Town CINF Awards Committee, Ass't Chair*

## NOTICE

## Neutron protein crystallography

Based on its recently demonstrated success in identifying protons and bound water molecules, even at a relatively modest resolution of 2.0 Å, neutron protein crystallography carried out at room temperature has great potential to play a major role in the understanding of the mechanisms of enzymes (I. Tsyba & R. Bau, 'Neutron Diffraction Studies on Proteins', *Chemtracts-Inorganic Chemistry* **15**, 233-257, 2002). The major reasons for the limited impact of neutron protein crystallography to date are the lack of suitable instruments and the limited flux at the presently available neutron sources, which means that very large crystals generally are required. This situation will change with the advent of the SNS, which will allow for unprecedented higher data collection rates.

On May 28, 2002 at the ACA meeting in San Antonio, a Steering Committee including scientific personnel with expertise in protein crystallography, enzymology, and neutron instrumentation was formed to look into the requirement of a dedicated neutron protein crystallography instrument at the Spallation Neutron Source (SNS). The SNS will be the world's most intense source of neutrons when it becomes operational in 2006 at Oak Ridge, TN, USA. The Committee has adopted action items for the coming year including: (1) To hold focused workshops bringing the scientific community together, to discuss scientific problems that require neutron protein crystallography and to form of an SNS Instrument Development Team (IDT), and (2) To showcase the science using neutron protein crystallography at the Transactions Symposium at the 2003 ACA annual meeting in Cincinnati.

*P. Thiyyagarajan, from the ACA Newsletter, Fall 2002*

## NOTICE

## Spectris Plc acquisition of Philips analytical

Spectris plc, the precision instrumentation and controls company, has completed its acquisition of Philips subsidiary Analytical as announced two months ago. PANalytical as the new daughter company has been renamed, now is the 17<sup>th</sup> semiautonomous operating company of Spectris. Its headquarters will remain in Almelo, the Netherlands.

## AWARDS AND PRIZES

## Clifford G. Shull prize announced



Clifford G. Shull

At the inaugural meeting of the American Conference on Neutron Scattering (ACNS) on June 23-27, 2002, NSSA President James Rhyne announced the establishment of the Clifford G. Shull Prize in Neutron Science of \$5,000 to be awarded every two years. Shull shared the 1994 Nobel Prize for Neutron Scattering with Canadian researcher Bertram Brockhouse. Robert Shull, son of the Nobel prize winner and the leader of the Magnetic Materials Group at NIST presented a review of Cliff Shull's life and accomplishments to the ACNS attendees. Nominations will be solicited by the prize committee starting next year with the winner of the first Shull Prize to be announced at the 2004 ACNS.

*Julie Borchers, NSSA Secretary, [julie.borchers@nist.gov](mailto:julie.borchers@nist.gov)*

## AWARDS AND PRIZES

## 2002 Oxford and Pauling prizes awarded



### Oxford Prize winners

The Oxford Cryosystems Poster Prize at the annual ACA Meeting was awarded to **Xiangyun Qui** – *Unusual Charge Transfers between Inplane Orbitals in  $\text{La}_{0.92}\text{Sr}_{2.08}\text{Mn}_{207}$*  and **David Cooper** – *The PDZ Domains of Syntenin*.



Pauling Prize awardees: (front row) Sonia Patenaude, Christina DeWitt, Samantha Perez-Miller, (back row) Francisco Hernandez-Guzman, Joshua Sakon, Kimberly Terry, and Jeff Wilson.

Pauling Prize winning posters: **Brian Helfrich** – *Design of Ternary Crystals*; **Francisco Hernandez-Guzman** – *Crystal Structure of Human Placental Estrone Sulfatase*; **Andre Kovalevsky** – *Photocrystallography, IR and DFT Calculations of Solid-State Photo Induced Linkage Isomers of  $\text{RUSO}_2$  Complexes*; **Sonia I. Patenaude** – *Structure-Function Relationship of the ABO Blood Group Glycosyltransferases*; and **Samantha Perez-Miller** – *Mitochondrial Aldehyde Dehydrogenase: Understanding Nicotinamide Isomerization*.

## AWARDS AND PRIZES

## Jaskólski receives prize in natural and medical sciences, Poland

**Mariusz Jaskólski**

**Mariusz Jaskólski** (Dept. of Chemistry, Adam Mickiewicz U. and Center for Biocrystallographic Research, Inst. of Bioorganic Chemistry, Polish Academy of Sciences, Poznan, Poland) has been awarded the 2002 Prize in Natural and Medical Sciences by the Foundation for Polish Science. This cash prize of \$15,000 is the highest scientific honor in Poland and its citation states '... awarded for the elucidation of the ways in which human protein cystatin c forms amyloid aggregates, a process important for the understanding of certain diseases of human brain.' Professor Jaskólski was elected this year to the Polish Academy of Sciences. He is the first macromolecular crystallographer in Poland to be so honored.

*Alexander Wlodawer*