INTERNATIONAL UNION OF CRYSTALLOGRAPHY

IUCr Newsletter

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Collected archival edition
Original article text and available illustrations

Contents

Letter from the President

Letter from the President 4

Awards and prizes

2008 Ewald Prize announced 6

Poster prize winners 30

ACA 07 poster prizes 46

IUCr journals news

Solving the crystal structures of zeolites using electron diffraction data. I. The use of potential-density histograms; II. Density-building functions 7

Capabilities and limitations of a (3 + d)-dimensional incommensurately modulated structure as a model for the derivation of an extended family of compounds: example of the scheelite-like structures 8

One-dimensional uranium–organic framework in catena-poly[[di-μ2-hydroxido-bis[dioxouranium(VI)]]-di-μ2-2-pyridylacetato-κ3O,N:O′;κ3O:O′,N] 9

Protein crystallography with a micrometre-sized synchrotron-radiation beam 10

8-(Biphenyl-4-yl)-8-hydroxypentacyclo[5.4.0.02,6.03,10.05,9]undecan-11-one ethylene ketal 11

The structure of melon necrotic spot virus determined at 2.8 Å resolution 12

Reproducibility in X-ray reflectometry: results from the first world-wide round-robin experiment 13

Relics in medieval altarpieces? Combining X-ray tomographic, laminographic and phase-contrast imaging to visualize thin organic objects in paintings 14

IUCr activities

Computing commission 15

Teaching commission news 21

Commission on mathematical and theoretical crystallography 23

A crystallographers family photo album 32

Meeting report

The 24th European crystallographic meeting 24

ECM24; through the ECA President's eyes 27

Macromolecular session at ECM24 28

AsCA '07 35

2007 ACA meeting 40

Notice

International consortium encourages collaboration 51

LETTER FROM THE PRESIDENT

Letter from the President

One of the most important objectives of the IUCr is to promote international cooperation in crystallography. In order to accomplish this objective, cooperation between the IUCr and its Regional Associates (ACA, AsCA and ECA) is essential. To facilitate this cooperation activities of all three Regional Associates are regularly featured in the IUCr News.

This year also marks the 60th Anniversary of the IUCr. In Japan, people celebrate the 60th anniversary of their birth because it has long been believed that at that point one cycle of life has been completed and another cycle is about to begin. It is important to look back on the past 60 years to see what we can learn to help us for the next 60 years.

The first General Assembly (GA) and Congress of the IUCr was held at Harvard University (USA) from July 28-August 3, 1948, three years after the end of World War II. Only 310 crystallographers were in attendance and four adhering bodies were accepted: the UK, the USA, Canada and Norway. Prof. Max von Laue and Sir Lawrence Bragg, the founders of modern crystallography, were elected Honorary President and President, respectively. The following six Commissions were established: Acta Crystallographica, Structure Reports, International Tables, Crystallographic Data, Crystallographic Apparatus, and Nomenclature. Although 83 papers were presented at the Congress, many were given by the session chairs since the authors were unable to attend. For example, six papers by Japanese crystallographers were presented but none were able to attend the Congress.

Since the second GA and Congress held in Stockholm, the numbers of adhering bodies and participants has gradually increased, as shown in Figure 1, such that at the Florence Congress (2005) there were 40 adhering bodies and 2800 scientific participants. The participants came from 62 countries and more than 2000 papers were presented. After the passage of 60 years the IUCr Congress has grown to be one of the largest International Scientific Conferences.

In order to look back over the past 60 years and to look forward to the next 60 years, the Executive Committee has planned three projects:

(1) publication of recent topics of crystallography in a special issue of *Acta A*

(2) a ceremony in Osaka celebrating the 60th Anniversary of the IUCr

(3) a photographic collection and exhibition at Osaka

For the first project; twenty-four articles covering a variety of crystallographic fields have been published in the first issue of *Acta Cryst. A* in 2008. Former IUCr President Henk Schenk served as editor for this special edition.

The ceremony celebrating the 60th Anniversary of the IUCr will be held on August 23, just before the opening ceremony. All living Past Presidents [Jerome Karle (1981-1984), Theo Hahn (1984-1987), Andre Authier (1990-1993), Philip Coppens (1993-1996), Ted Baker (1996-1999), Henk Schenk (1999-2002) and Bill Duax (2002-2005)] have been invited and all have accepted, except for Jerome Karle who will be unable to attend for reasons of health. Ted Baker will present a talk entitled “Crystallography and the World around Us” at the ceremony. Four of the other former Presidents will give talks to high-school and undergraduate students and the general public in evening sessions during the Congress. We expect that these lectures will have a favourable influence upon young people in Japan. The titles of their lectures are as follow: “2500 Years of Symmetry in Sciences, Art and Music” (Theo Hahn), “History of X-ray Diffraction: looking deeper and deeper into the structure of matter” (Andre Authier), “What Crystallography Can Tell Us about Molecules in the Test Tube and in Life” (Philip Coppens), and “X-raying a Crystal to See Atoms and Molecules, Solutions and Results“ (Henk Schenk).

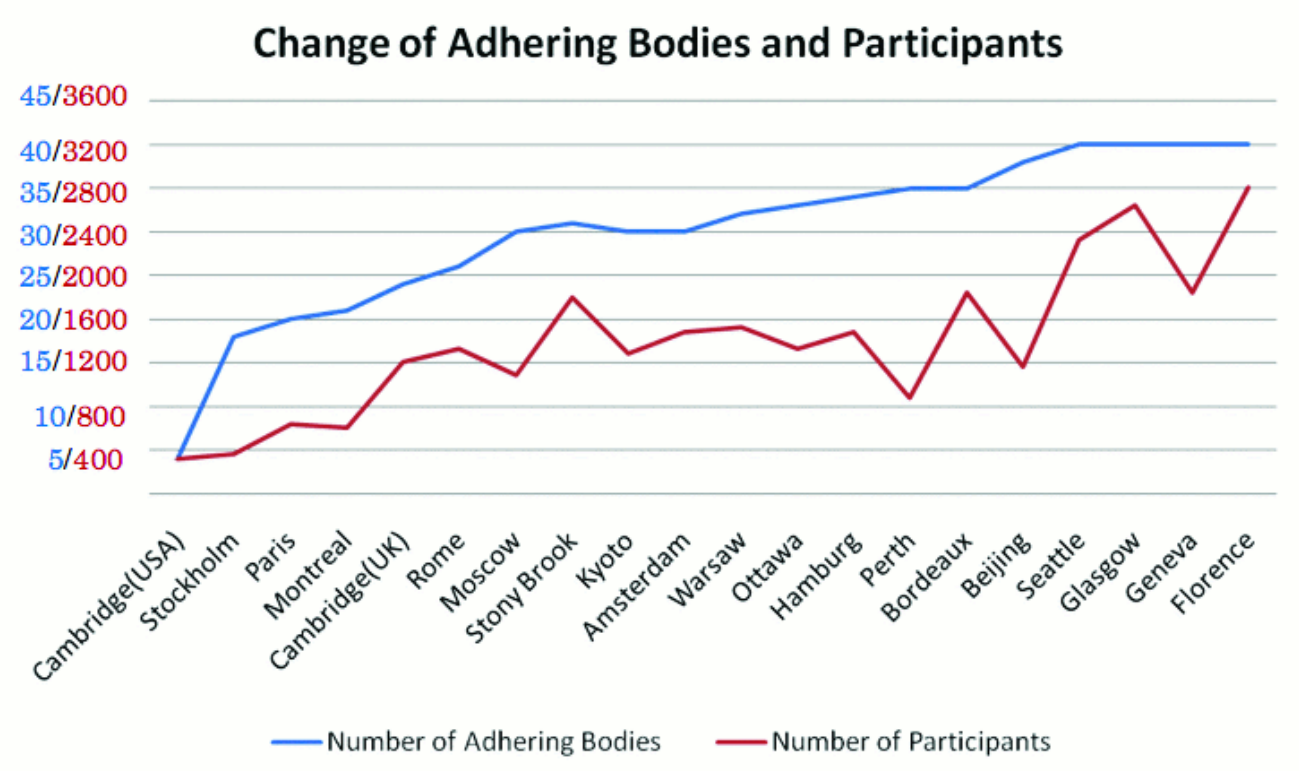


Figure 1

The third project will be an exhibit of photographs celebrating the 60-year-old IUCr. Immediate IUCr Past President Bill Duax, in collaboration with Chris Gilmore, Gernot Heger and Syd Hall are arranging a photographic collection highlighting IUCr Congresses from Bordeaux (1990) to Florence (2005), in addition to Paris (1954), ACA meetings from Philadelphia (1988) to Salt Lake City (2007), ECM meetings from Moscow (1989) to Marrakech (2007), and AsCA Meetings from Singapore (1992) to Taipei (2007). The Executive Committee has asked Bill Duax to copy many of these photographs onto a CD, which will be given to all participants of the Osaka Congress. Duax will also give a talk entitled “A History of the IUCr” at a luncheon seminar.

I personally think that a very good wind has been blowing over crystallography during these 60 years, especially in the latter 30 years. This is because most 20th century scientists believed that understanding the molecular structure of materials could help explain their functions and characteristics. X-ray and neutron diffraction and electron microscopy have proven to be powerful methods to obtain these molecular structures. The development of high-speed computers and the advent of synchrotron radiation have also given a boost to the progress of crystallography and in the 21st century it will be possible not only to study the static structure of molecules but also their dynamic structure to provide even deeper insights into their functions or characteristics. Crystallography, and its associated methods, will answer many challenging questions in the next 60 years. I am pleased to have been part of the first 60 years of the IUCr and look forward to contributing what I can to the next 60.

Yuji Ohashi
yohashi@spring8.or.jp

AWARDS AND PRIZES

2008 Ewald Prize announced



David Sayre

The IUCr is pleased to announce that David Sayre (Dept. of Physics, State U. of New York, Stony Brook, NY USA) has been awarded the eighth Ewald Prize for the unique breadth of his contributions to crystallography, which range from seminal contributions to the solving of the phase problem to the complex physics of imaging generic objects by X-ray diffraction and microscopy, and for never losing touch with the physical reality of the processes involved. The presentation of the Ewald Prize will be made at the Osaka Congress Opening Ceremony on August 23, 2008.

IUCR JOURNALS NEWS

Solving the crystal structures of zeolites using electron diffraction data. I. The use of potential-density histograms; II. Density-building functions

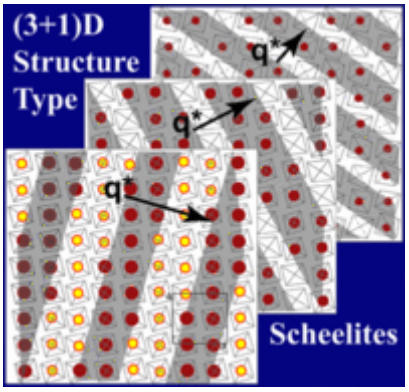
Acta Cryst. **(2008). A64, 284-294 [doi:10.1107/S010876730705862X]**
Acta Cryst. **(2008). A64, 295-302 [doi:10.1107/S0108767307058631]**

Solving crystal structures using electrons instead of X-rays is very difficult: the data are subject to numerous systematic errors. However, electrons can work with samples as small as 50 nm, and give answers when all other methods fail. We use density histograms (just like those in photo manipulation software) and density building along with entropy methods to solve the structures of zeolites in a routine way. The figure shows a map for mordenite; the crosses are the positions of the Si atoms.

C.J. Gilmore, W. Dong and D.L. Dorset

IUCR JOURNALS NEWS

Capabilities and limitations of a (3 + d)-dimensional incommensurately modulated structure as a model for the derivation of an extended family of compounds: example of the scheelite-like structures



The examples of the composition-ordering wave in the IMS $KNd(Mo)_4)_2$ (front plan), $Bi_2(Mo0_4)_3$ (middle plan) and $La_2(Mo0_4)_3$ (back plan)

Capabilities and limitations of a (3 + *d*)-dimensional incommensurately modulated structure as a model for the derivation of an extended family of compounds: example of the scheelite-like structures

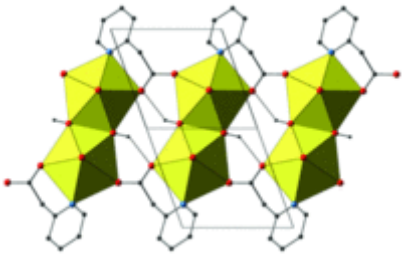
Acta Cryst. (2008). B64, 12-25 [doi:10.1107/S010876810705923X]

Incommensurately modulated structures (IMSs) are described in superspace. The resulting non-periodic structure is obtained from a 3D cut of the higher dimensional periodic description of the IMS. The superspace model consists of a basic structure on which a modulation is applied. The present article illustrates a novel application of the superspace concept, namely the possibility to describe a large series of compounds uniquely based on the basic structure used to describe the IMS on which we apply different modulation functions. This method is illustrated with the example of the Scheelite family consisting of both 3D-periodic and IMS cases. The proposed model can act as a common (3+1)D structure type from which all the possible structures can be attributed.

A. Arakcheeva and G. Chapuis

IUCR JOURNALS NEWS

One-dimensional uranium–organic framework in catena-poly[[di-μ2-hydroxido-bis[dioxouranium(VI)]]-di-μ2-2-pyridylacetato-κ3O,N:O′;κ3O:O′,N]



View of part of a ribbon with uranium coordination polyhedra in yellow and hydrogen bonds shown as dotted lines

One-dimensional uranium–organic framework in catena-poly[[di-μ2-hydroxido-bis[dioxouranium(VI)]]-di-μ2-2-pyridyl-acetato-κ^3*O*,*N*:*O*′;κ^3*O*:*O*′,*N*]

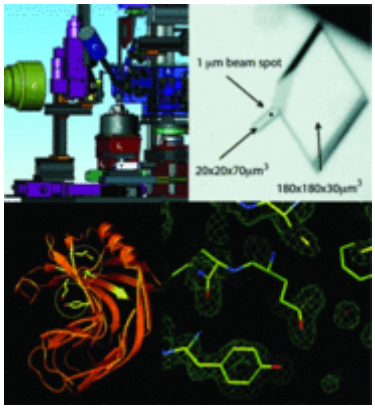
Acta Cryst. (2008). C64, m50-m52 [doi:10.1107/S010827010706249X]

Carboxylic acid derivatives of pyridine are among the commonest ligands for the design of uranyl–organic frameworks, but 2-pyridylacetic acid had never been used in this context. In its complex with the linear uranyl ion formed under hydrothermal conditions, the metal atom is *O*,*N*-chelated and dimerization occurs through double hydroxide bridges. Further bridging of these dimeric subunits by acetate groups gives rectilinear, polymeric ribbons. Twelve-membered rings are defined by proximal dimers in the ribbons, with two intra-ring hydrogen bonds involving the hydroxide and carboxylate groups.

P. Thuéry

IUCR JOURNALS NEWS

Protein crystallography with a micrometre-sized synchrotron-radiation beam



Top left - Schematic design of goniometer set-up; top right - crystals and beam relationship; bottom left - xyanalase II structure; bottom right - $2F_o$-F_c density map

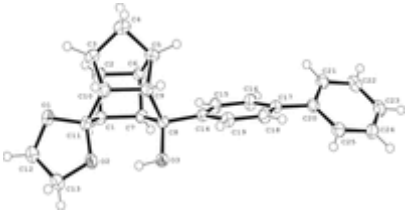
Acta Cryst. (2008). D64, 158-166 [doi:10.1107/S090744490705812X]

Recent advances in instrumentation at the microfocus beamline (ID13) at the European Synchrotron Radiation Facility allowed a protein microcrystallography experiment with a focused synchrotron-radiation beam of 1 micron. High-resolution diffraction patterns of xylanase II were obtained from 20 μm^3 crystal volumes with a flux density of 3×10^{10} photons/sec/μm^2 at the sample. In spite of the high irradiation dose, a 1.5 Å resolution map for a xylanase II structure was obtained with no evidence of radiation damage. This result opens many new opportunities in protein microcrystallography.

R. Moukhametzianov, M. Burghammer, P.C. Edwards, S. Petitdemange, D. Popov, M. Fransen, G. McMullan, G.F.X. Schertler and C. Riekel

IUCR JOURNALS NEWS

8-(Biphenyl-4-yl)-8-hydroxypentacyclo[5.4.0.02,6.03,10.05,9]undec one ethylene ketal



The ORTEP diagram of the molecule showing ellipsoids at the 50% probability level.

8-(Biphenyl-4-yl)-8-hydroxypentacyclo[5.4.0.$0^{2,6}$.$0^{3,10}$.$0^{5,9}$]undecan-11-one ethylene ketal

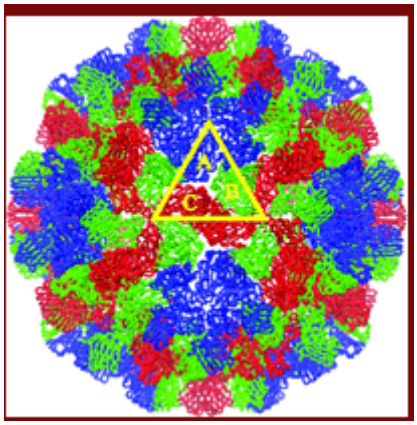
Acta Cryst. (2008). E64, o283 [doi:10.1107/S1600536807065920]

The pentacycloundecane cage structure has been the subject of numerous crystallographic studies. The skeleton is known to have C–C bond angles and lengths that vary significantly from normal values. The title molecule, which exists as a racemate, was synthesised as part of an ongoing investigation into chiral cage derivatives as potential asymmetric catalysts. The molecule exhibits intramolecular hydrogen bonding as well as a complex network of weak van der Waals interactions between neighbouring molecules.

G.A. Boyle, T. Govender, H.G. Kruger and G.E.M. Maguire

IUCR JOURNALS NEWS

The structure of melon necrotic spot virus determined at 2.8 Å resolution



MNSV virus particle looking along from the quasi-threefold axis. The viral particle is composed of 180 chemically identical subunits.

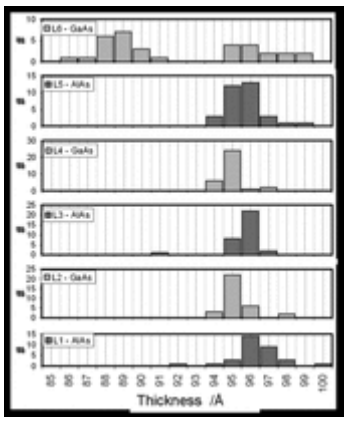
Acta Cryst. (2008). F64, 8-13 [doi:10.1107/S1744309107066481]

The structure of melon necrotic spot virus (MNSV) was determined at 2.8 Å resolution. MNSV is one of the viruses belonging to the genera *Tombusvirus* or *Carmovirus* that are naturally transmitted in the soil by zoospores of fungal vectors. The X-ray structure of MNSV provides us with a representative structure of viruses transmitted by fungi.

Y. Wada, H. Tanaka, E. Yamashita, C. Kubo, T. Ichiki-Uehara, E. Nakazono-Nagaoka, T. Omura and T. Tsukihara

IUCR JOURNALS NEWS

Reproducibility in X-ray reflectometry: results from the first world-wide round-robin experiment



Distribution of thicknesses obtained in different laboratories.

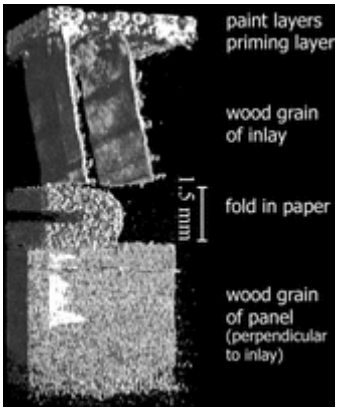
J. Appl. Cryst. (2008). 41, 143-152 [doi:10.1107/S0021889807051904]

X-ray reflectometry (XRR) is a well-established technique to quantitatively evaluate electron density profiles, thickness, and roughness of thin layers. In this paper, results of the first world-wide XRR round-robin experiment, involving a number of prominent laboratories, are presented and discussed. The reproducibility of measurements obtained using different equipment has been assessed. The influence of fitting of the experimental data on the thickness determination was shown to be non-negligible compared with experimental factors.

P. Colombi, D. K. Agnihotri, V.E. Asadchikov, E. Bontempi, D.K. Bowen, C.H. Chang, L.E. Depero, M. Farnworth, T. Fujimoto, A. Gibaud, M. Jergel, M. Krumrey, T.A. Lafford, A. Lamperti, T. Ma, R.J. Matyi, M. Meduna, S. Milita, K. Sakurai, L. Shabel'nikov, A. Ulyanenkov, A. Van der Lee and C. Wiemer

IUCR JOURNALS NEWS

Relics in medieval altarpieces? Combining X-ray tomographic, laminographic and phase-contrast imaging to visualize thin organic objects in paintings



Three-dimensional rendering of a dummy panel obtained by synchrotron-radiation computed laminography. The paint layer at the top, the perpendicular grain directions in the inlay (below) and the panel (bottom), and the folded paper (centre) are clearly visible.

J. Synchrotron Rad. (2008). 15, 55-61 [doi:10.1107/S0909049507045438]

In some medieval altarpieces relics seem to have been imbedded inside the wooden carrier or *panel*. These are most probably thin, organic, fibrous materials such as paper or textiles. Traditional X-ray radiography fails to visualize such light materials because of their low absorbance. However, synchrotron-based tomographic and laminographic imaging complemented with phase-contrast capability can successfully image such relics. This can be done non-destructively, three-dimensionally and with micrometre-scale resolution, which literally opens up new vistas in the study of paintings.

K. Krug, L. Porra, P. Coan, A. Wallert, J. Dik, A. Coerdt, A. Bravin, M. Elyyan, P. Reischig, L. Helfen and T. Baumbach

IUCR ACTIVITIES

Computing commission

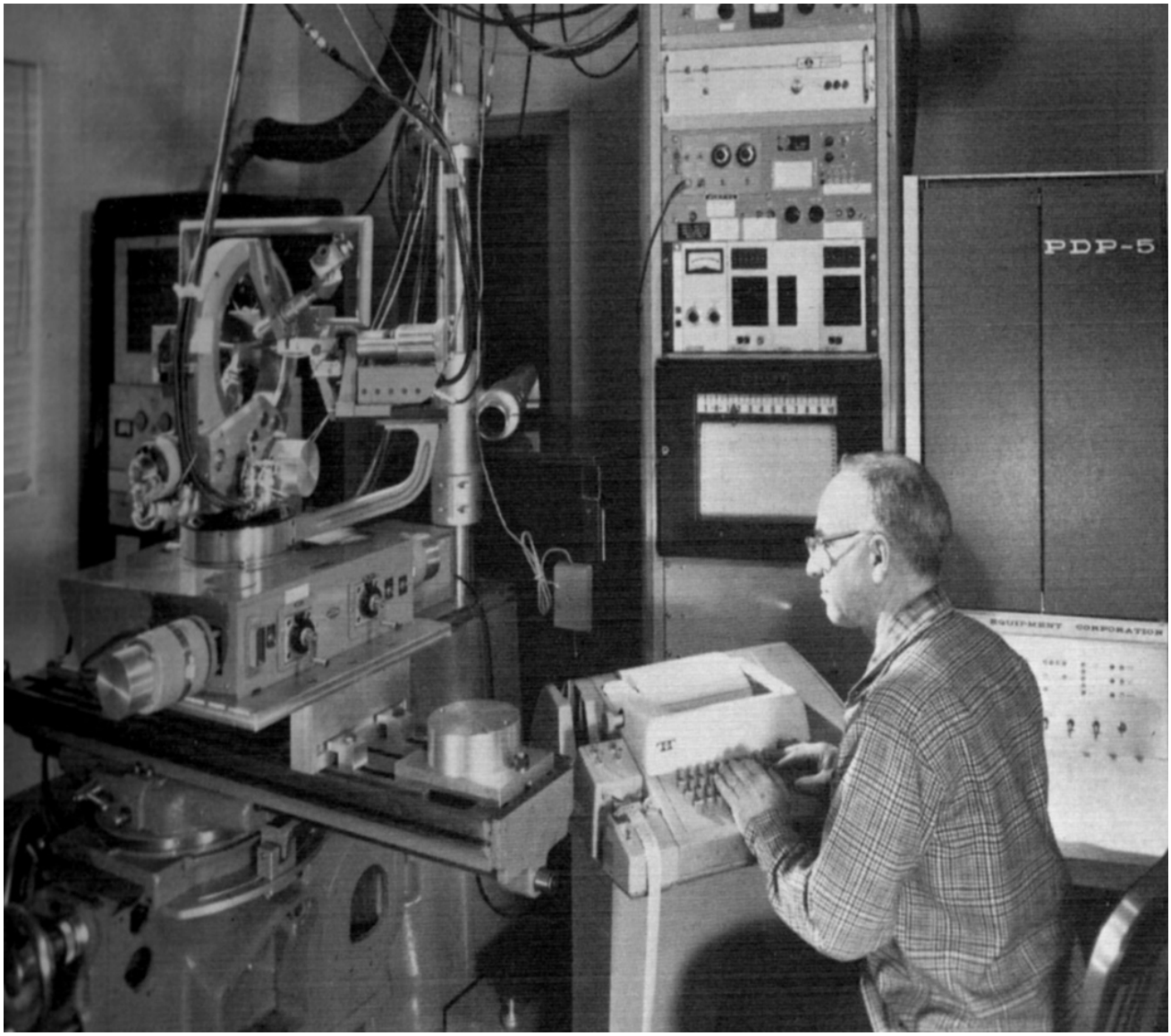
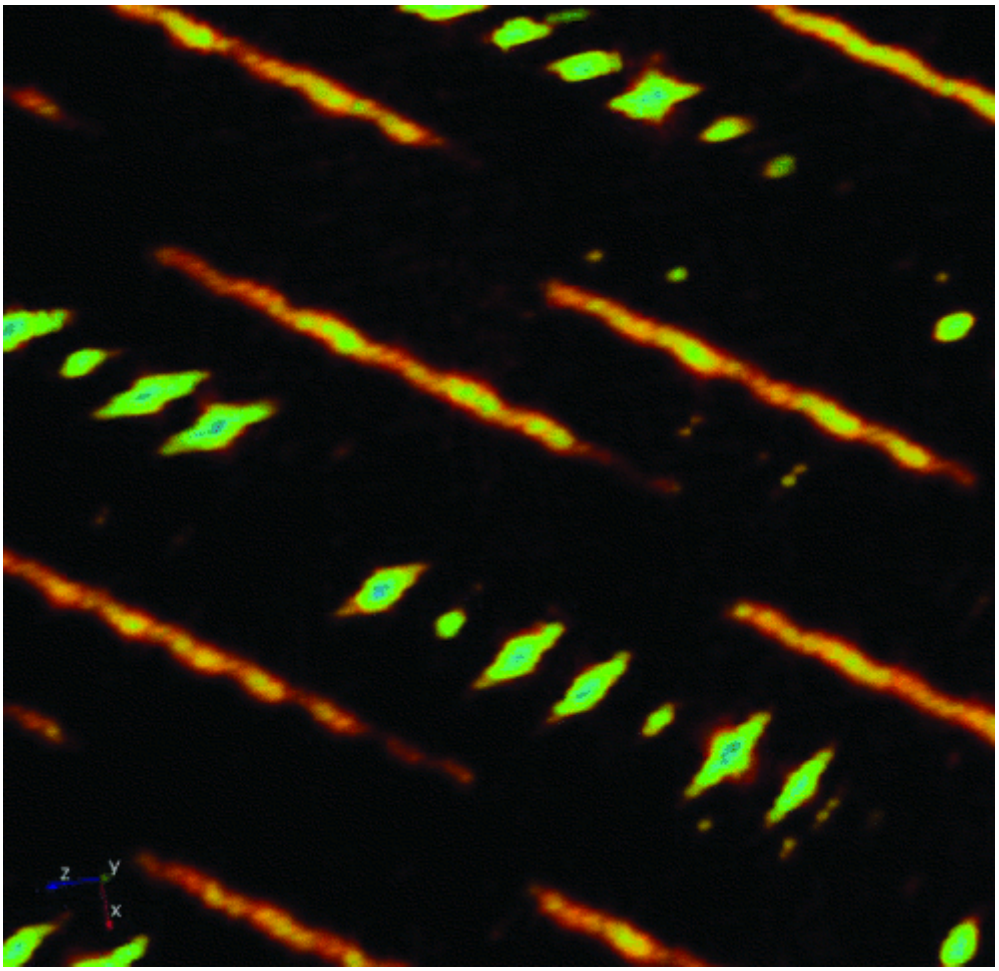


Figure 1: Henri Levy of Oak Ridge National Laboratory at the keyboard of the four-circle Picker X-ray diffractometer, and the PDP-5 computer that was programmed to control it. (Photograph courtesy of ORNL)

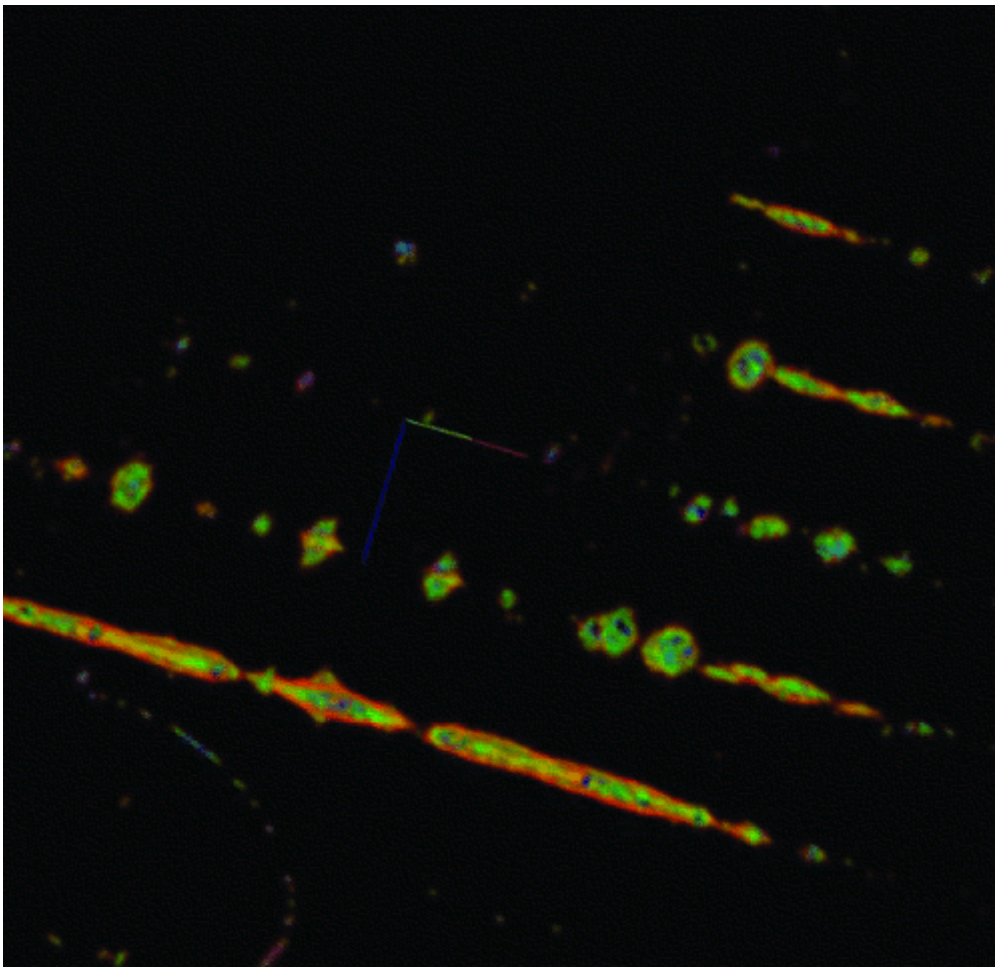
The 8th edition of the IUCr Computing Commission Newsletter is available online as a PDF file at the CompComm website. In the computing monograph of the 1950 crystallographic computing school, Ray Pepinksy stated *“records of what has been considered and what has been accomplished are essential to the proper development of this or any other field.”(1)* With this in mind, the main theme for this edition is that of *‘Crystallographic Computing at Oak Ridge National Laboratory: 1954 to 1968’* with an article by William Busing (refer figure 1). This is followed by stereoscopic structure drawings as generated by Carroll Johnson in the mid 1960’s using ORTEP-I (Oak Ridge Thermal Ellipsoid Plot software) for the joint ACA and MSA meeting, Gatlinburg, TN, USA, 1965, and the Second Biophysical Congress, Vienna, Austria, 1966.

Václav Petříček and Michal Dušek describe some of the new features in the latest version of the Jana single crystal and powder diffraction structure refinement program. This includes the enhanced ability to simultaneously use multiple single crystal and powder diffraction datasets; Magnetic scattering, Coelho and Cheary based fundamental parameters profile fitting; and an interface to the SuperFlip structure

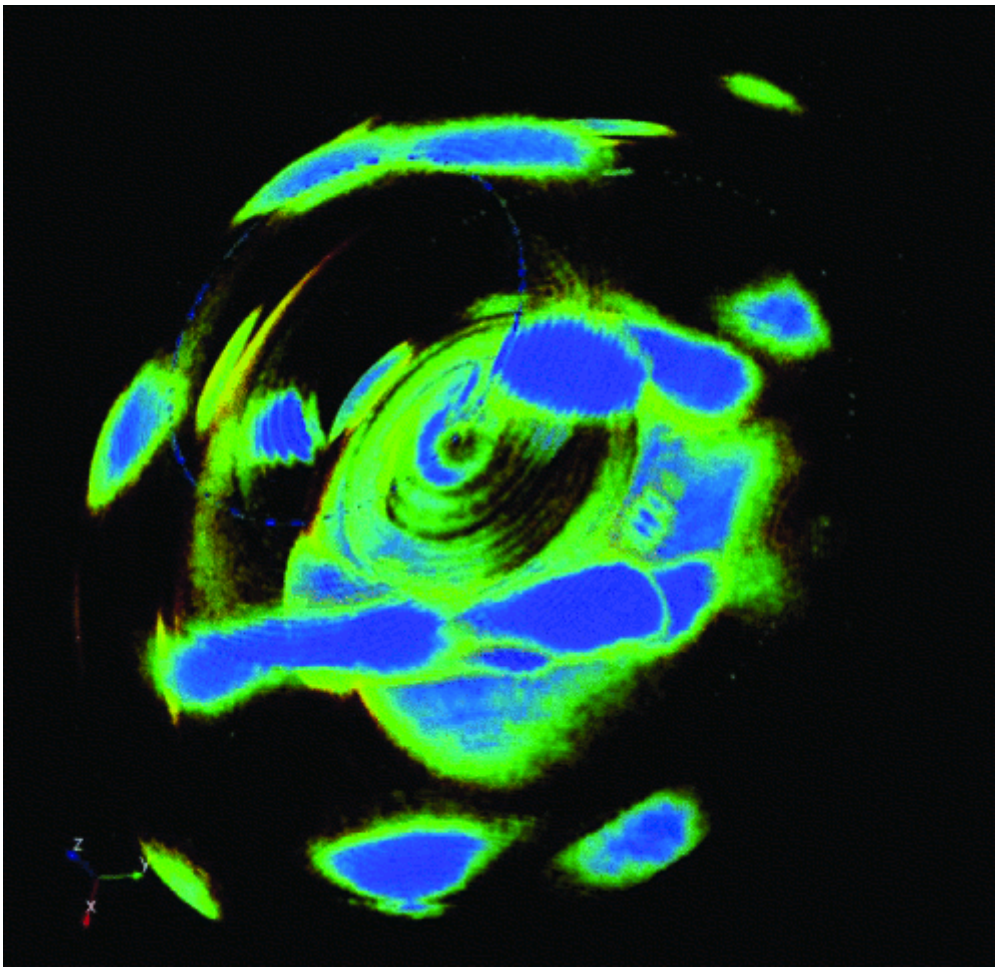
solution software for incommensurate and commensurate crystal structures. Brian Toby and Bob Von Dreele report on the conclusions of the GSAS-II workshop held in May 2007 where the aim was to build on the influential and popular GSAS program of Larson and Von Dreele to create a GSAS-II from scratch using the latest algorithms and software development methods. Luc Bourhis, Ralf Grosse-Kunstleve and Paul Adams give the latest CCTBX developments. While the open-source CCTBX project has traditionally concentrated on macromolecular crystallography, the inclusion of algorithms specifically for small-molecule work are described, as are other new features and capabilities.



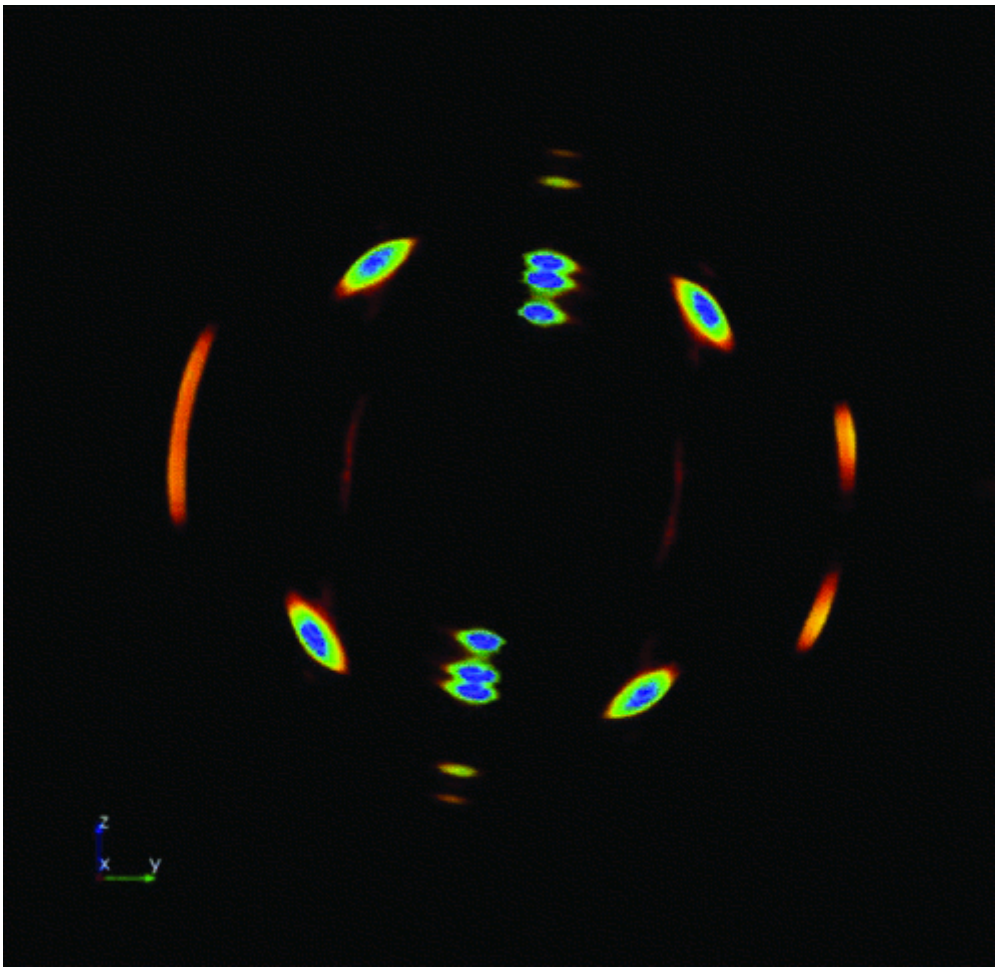
a



b



c



d

Figure 2: Examples using the MAX3D reciprocal space viewer: (a) $LuFe_2O_4$ at 80C; (b) diffuse scattering perpendicular to the c-axis in Hexanaphthylbenzene; (c) all pole figures observed at once in Au/Pt nanolayered rolled sheets; (d) diffraction of a polymer mapped into reciprocal space.

Branton Campbell, John Evans, Francesca Perselli and Harold Stokes describe the method of Rietveld refinement of structural distortion-mode amplitudes using the Isotropy program and the Topas software. A tutorial is included based on Tungsten Trioxide. It describes the *"minimum 'four clicks' required [in Topas Academic] to prepare and perform a distortion-mode refinement"* where one uses *"just 5 structural degrees of freedom rather than the 24 parameters of a conventional refinement."* Jim Britten and Weiguang Guan showcase the MS-Windows and Linux based MAX3D software for the Visualization of Reciprocal Space Volumes. The images displayed in the article reminds one of images from the Hubble Space Telescope. The MAX3D article gives impressive examples of what most users of single crystal apparatus are missing in potentially understanding their data and consequent structural implications. A number of reciprocal space volumes generated by MAX3D are included in figure 2.

As an addendum, a variety of historical software reports, with original source code, are included courtesy of ORNL as a separate PDF file. These include the reports on crystallographic programs for the IBM 704, plus ORABS, ORFLS, ORFFE, ORTEP-I and ORTEP-II.

The next edition of the newsletter is expected to be in mid to late 2009 (not 2008 due to it being an IUCr congress year). Articles of interest to the crystallographic computing community are very welcome and can be sent to the newsletter editor at lachlan.cranswick@nrc.gc.ca. Previous editions of the newsletter are also available via the Computing Commission website at www.iucr.org/iucr-top/comm/ccom/.

Lachlan Cranswick

Reference

[1] Pepinsky, R., (1952b). *Computing Methods and the Phase Problem in X-ray Crystal Analysis*, edited by R. Pepinsky, Foreward, State College, PA, USA: Dept. of Physics, The Pennsylvania State College.

IUCR ACTIVITIES

Teaching commission news

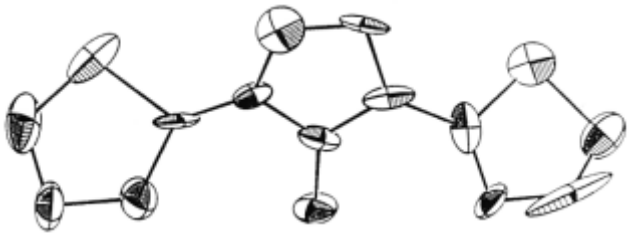


Figure 1: The ORTEP diagram that prompted the creation of the ORTEP of the Year (OOTY) award.

The 2nd edition of the IUCr Teaching Commission Newsletter is available online as an PDF file at www.iucr.org/iucr-top/comm/cteach/newsletters/2007nov/. The theme of this edition is based on the history of the ORTEP of the Year (OOTY) Award as written by its founder, Richard Harlow. While a crystallographer at Dupont, Richard describes the incentive behind creation of the award (see Figure 1) and gives an overall history with examples. These include two ORTEP diagrams where one diffraction dataset must have been collected on a windy day, and the other during a force ten gale. Following this article is a reprint (by permission of NIST) of Richard's well regarded 1996 article on "Troublesome Crystal Structures: Prevention, Detection, and Resolution."

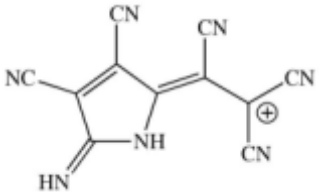


Figure 2: molecular diagram of a structure where IUCr validation checks indicate that structure is not quite right.

In the OOTY article's conclusion, Richard notes, *'One of my biggest concerns was the advent of refinement software which would allow even the most inexperienced people to restrain, constrain, and otherwise control each of the atomic thermal parameters. This clearly pointed to a future where it would be much harder, if not impossible, to detect incorrect structures directly from the ORTEP drawings. Every ORTEP drawing could now be made "perfect".'* This comment finds relevance within the next article by Anthony Linden on "Crystallographic Data Validation - Ten Years On." Besides a brief history and overview on the IUCr's structure validation facilities, "minor" checkCIF alerts are elaborated as applied to some published imine structures. The molecular diagram of one such imine is given in Figure 2, and Anthony's article elaborates on which and why one of the nitrogens is more likely an oxygen. One conclusion of the article is that even "minor" validation alerts should be carefully considered and pondered. Another is that traditional examination of ORTEPs and hydrogen-bonding diagrams should still be performed as *"our eyes often reveal things to us that numerical data may not."*

Completing the newsletter's articles on validation is one on the use of the Topas software for validation of a complex inorganic crystal structure using bond valence restraints by Ivana Radosavljevic Evans. In other articles, Patrick Carroll describes on online course in the fundamentals of X-ray crystallography to supplement a traditional lecture-type course. Zia Khan provides two articles on the history and challenge of teaching molecular symmetry, and crystallography in general to chemistry and physics students in Pakistan. Roxana Flacau discusses the combined Rietveld/MEM (Maximum Entropy Method) as implemented in the RIETAN-2000/PRIMA software with an example of the method being applied to the electron density analysis of high pressure phases using powder diffraction data.

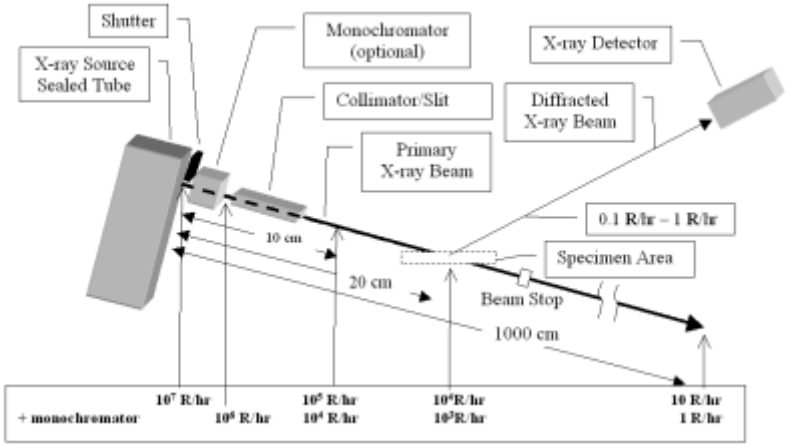


Figure 3: Estimated radiation dose levels based on the known X-ray flux for a Copper sealed-tube (at its maximum power rate). Note the radiation dose at the tube-tower beam-port is in the region of **ten million (10^7) rem/hr** (100rem is 1Sv)

Finally is Joseph Reibenspies' submission titled "X-ray Safety for Analytical Instrumentation: It's what you cannot see or feel that will hurt you!" A nicely conceived diagram of expected radiation fields within a sealed-tube diffractometer is reproduced here as Figure 3. Commercial vendors of modern integrated diffraction equipment set extremely high standards of operator safety, however aging, poorly maintained or custom X-ray apparatus may be a different matter; especially if illegal ad-hoc modifications have occurred. Users of analytical X-ray apparatus are well advised to understand the hazards of high intensity X-ray beams; as well as modern safety regulations requiring full interlocked radiation enclosures to ensure there is no significant chance of the operator coming into contact with incident or diffracted X-ray beams.

The next edition of the newsletter is expected to be in mid to late 2009. Articles relating to crystallographic teaching, including historical, regional and national overviews, are very welcome and can be sent to the newsletter editor at lachlan.cranswick@nrc.gc.ca.

Lachlan Cranswick

IUCR ACTIVITIES

Commission on mathematical and theoretical crystallography

Formation of the Commission on Mathematical and Theoretical Crystallography (MaThCryst), was approved by the IUCr General Assembly in Florence. The Commission concentrates on classical topics like symmetry and its applications to modular structures, twins and phase transitions, topology and graph theory. Application to art and crystallography was the topic of a symposium on Moroccan ornaments organized by MaThCryst at ECM24 (Figure 1).



Figure 1. Participants at the ECM-24 Satellite Meeting “The Enchanting Crystallography of Moroccan Ornaments” working on *Zellij multipuzzle*.

MaThCryst currently has ten members and five consultants and has a mailing list open to all crystallographers interested in Commission activities (www.lcm3b.uhp-nancy.fr/mathcryst/mailinglist.htm), where ideas and proposals for new activities can be submitted. Several meetings and schools have been organized (ECM22 satellite Budapest 2004; Nancy School 2005; ECM23 satellite Leuven, AsCA’06 satellite Tsukuba 2006, Havana School and ECM24 satellite Marrakech 2007) and others are being organized (Gargnano School 2008; ECM25 satellite Istanbul 2009). Special issues of *Zeitschrift für Krist.* (issue 2006/1) and *Acta Cryst. A* (2006/3) have contained articles related to some of these meetings.

Our website has didactic material from the conferences and topic-oriented pages. Cooperation with other commissions, in particular the Commission on Inorganic and Mineral Structures (CIMS) and the Teaching Commission, has proved especially fruitful. Meetings organized by the Commission have been well received by the participants, who often lack a solid background in fundamental aspects of crystallography, due to the reduction of crystallographic material in university courses. The recent school in Havana has also pointed out the urgent need for crystallographic training in some Latin American countries: the possibility of running future schools in that area is under consideration, subject mainly to the availability of suitable venues and local organizers. Increased activity in the Asian community is also a major focus of the Commission for the future.

Among forthcoming activities, it is particularly worth mentioning the publication of a book on “Graph Theory in Crystallography and Crystal Chemistry” (authors J.-G. Eon, W. Klee and J. Rutherford) that will appear in the series “Monographs on Crystallography” by IUCr/Oxford University Press in late 2008 / early 2009. A thematic school where this new publication will serve as textbook is also planned.

Massimo Nespolo, Chair of MaThCryst
www.lcm3b.uhp-nancy.fr/mathcryst/

MEETING REPORT

The 24th European crystallographic meeting

Marrakech, Morocco, August 22-27, 2007
http://www.ecm24.org/



European Crystallographic Meeting (ECM) held in Marrakech in 2007 was one of the largest ECMs of the last ten years. The scientific program and the charming city of Marrakech attracted 850 scientists (33% female), exhibitors and accompanying guests from 55 countries. The organizers put together a program of the highest quality and made efforts to facilitate the attendance of 150 young researchers and 100 scientists from emerging countries. The 650 submitted abstracts covered almost all the fields of crystallography: chemistry (40%), biology (22%), material sciences (20%), physics (10%), methods and high pressure (8%). Talks were presented in 17 plenary lectures and 45 microsymposia and there were over 400 poster presentations. A satellite meeting and two workshops were held before the opening of the ECM24.

An exciting satellite meeting devoted to 'Enchanting Crystallography of Moroccan Ornaments' was organized by the IUCr MaThCryst Commission. Attendees included artists and Moroccan craftsmen as well as 5 lecturers from Morocco, France, Japan, the USA and Denmark. Moroccan handicrafts related to symmetry were exhibited and studied during the meeting. There was an excursion to the Kasbah de Telouet, a site renowned for the richness of its ornamentation. The meeting ended with discussion of plans to organize an IUCr Commission on Art and Crystallography.



An 'Advanced Training Workshop' supported by NATO was devoted to crystallographic instrumentation, remote access to synchrotron and neutron facilities, and software for data collection and structure solution. The incredible power of modern laptops was demonstrated *via* the use of software packages *EXPO2007* (powder diffraction), *Coot* (protein structure and electron density 'molecular graphics' real-time manipulations), *CCP*4 (Patterson and phasing calculations) and Critical Point Electron Density Analysis. There were 5 lecturers and 35 participants including 20 from North Africa. John Warren (SRS Daresbury) delivered his lecture *via* satellite, and internet arrangements allowed SRS9.8 instrument control from Marrakech. It has become increasingly common to use an SR facility *via* robotic sample mounting but using two-way audio contact over the internet as well is relatively new.

The workshop 'Science Meets Industry', organized by PANalytical, targeted participants from the building materials, pharmaceuticals, mining and phosphate industries. The workshop addressed the question of how modern science can improve the efficiency and reliability of industrial processes and products. The workshop reviewed applications of X-ray diffraction, X-ray fluorescence, and synchrotron radiation, geo-science, mineralogy and organic /inorganic chemistry fields of building materials, pharmaceuticals and mining. 70 scientists attended the workshop.

ECM24 attracted both young and senior scientists from academic organizations as well as from industry with significant attendance by scientists from emerging countries. ECM24 drew international attention to crystallography in Morocco and allowed crystallographers from emerging countries to present their work and demonstrate their ability to overcome obstacles. Crystallographers from emerging countries presented more than 70 communications (orals and posters) and chaired both plenary and microsymposia lectures. Two microsymposia were devoted to the study of phosphates, an abundant natural resource of Morocco.

The ECM24 conference provided an opportunity for Moroccan crystallographers to mix with crystallographers from throughout the world. It was also an opportunity to develop and expand international scientific cooperation and reinforce existing ties of solidarity between academic and industrial crystallographers. The 'Advanced Training Workshop' showed that remote internet access to state-of-the-art centralized synchrotron radiation facilities can allow distant countries to benefit from state-of-the-art data collection. Thus crystals too small for analysis by conventional X-ray sources can be sent by courier to the centralized facility and data collection can be controlled remotely from the laboratory that produced the crystals. The data collected can be analysed at the host facility or sent back to the laboratory for further study. This kind of remote access to the 'SESAME' synchrotron facility being built in Jordan was extensively discussed during ECM24.

The meeting exhibit featured the instruments and technologies of 24 companies. The IUCr and the European Crystallographic Assn (ECA) provided financial assistance to 57 students and young researchers. The Organization for the Prohibition of Chemical Weapons (OPCW) also supported 6 established researchers, 5 of them from emerging countries. The U. Cadi Ayyad of Marrakech provided support for 8 researchers.



A number of poster prizes were awarded - see page12. The Moroccan Crystallographic Assn (MCA) has been granted a subscription for the IUCr journals at a reduced rate and a one year subscription to the German journal *Crystal Research and Technology*.

Abdelmalek Thalal, Chair ECM24

Acknowledgments**:** As chairman of ECM24 I would like to express, on behalf of the organizing committee, my sincere gratitude to the IUCr for its continuous support and for the wonderful work they do to promote crystallography in the world. The donated funds made the participation of many young international researchers possible. The continuous support and encouragement of the ECA is kindly acknowledged as is that of the MCA, which strongly supported the idea of holding the congress in Marrakech. I would also like to thank the OPCW and the U. Cadi Ayyad of Marrakech for their grants to established researchers from emerging countries. We are very grateful to NATO for sponsoring the 'Advanced Training Workshop' and to our other sponsors and the exhibitors.

MEETING REPORT

ECM24; through the ECA President's eyes

It can truly be said that ECM24 in Marrakech changed my life. As my first ECM as President many tasks had to be interwoven; ceremonial speeches, prize presentations, face-the-media and chairing the ECA Council Meetings, not to mention presenting the latest scientific work from our Lab. At ECM24 there were well over 700 participants and the excitement that emanated from the marble congress Halls was palpable. The science at ECM24 was outstanding and the results altered many of one's perspectives. ECA Vice-President (Sine Larsen) described the ESRF upgrade and how nano-focused X-ray beams can be produced. She noted that the ESRF upgrade will allow up to 14 new beamlines accommodating many applications including nano-probe imaging, nano-spectroscopy and nano-crystallography, fostering the merger of electron crystallography with X-ray crystallography.

Another highlight for me was the presentation of the research news from our new UK SR X-ray source Diamond, the virile new kid on the block. This is pushing the envelope of technical capability represented by ESRF and making the early-years-ESRF capability available locally (ie a short train or car ride away when travelling within the UK). I found out just how hard the local committees worked, how unexpected problems must be dealt with and that often problems are outside one's control. In Marrakech, Moroccan customs held up delivery of some of the Exhibitors' equipment. This led to considerable post-ECM24 discussion. I now understand why IUCr has a rule limiting financial support for other crystallographic meetings held within 2 months before or after an IUCr Congress. The rule promotes greater congress attendance and is a courtesy to our loyal exhibitors who have limited capacity to attend overlapping conferences.

I would also like to mention the pre-ECM Advanced Training Workshop (ATW) I organized with ECM24 Chair Abdelmalek Thalal. This was sponsored by NATO whose attention had been grabbed by our proposal for synchrotron and neutron facility telepresence based usage. NATO is keenly aware of and supports the new SESAME synchrotron in Jordan. Also linked to ECM24 was the excellent satellite meeting on 'The enchanting crystallography of Moroccan ornaments', organized by our energetic ECA Webmaster and highly committed ECA colleague Massimo Nespolo. I am happy to say that ECM24 provided an opportunity for my wife and I to be joined by our daughter for a tour of North Africa that included cycling on the Atlantic coast, seeing a 400 year old Portugese castle and even stopping at 'Hendrix Café' where Jimi Hendrix wrote 'Castle Made of Sand'.

Finally I must pay tribute to Abdelmalek Thalal and his team who worked outstandingly hard, with tact and efficiency, and who also rose to the challenge of presenting their science and research. My speech to the Congress dinner participants emphasized that crystallographic science in Morocco and the whole Maghreb region would be changed by ECM24. Once again it showed the power of an ECM to encourage and educate new students, as well as to refresh us all in our own scientific endeavours.

John R. Helliwell

MEETING REPORT

Macromolecular session at ECM24



The ECM24 Conference dinner was held at Borj Bladi which means "tower of my country" because of its high location compared with Marrakech city. In this photo, from right of the place-card: Abdelmalek Thalal (Chair of ECM24), Mustapha El Adnani (Representative of the President of Marrakech U.), Radek Kuzel (ECA Treasurer), Petra Bombicz (ECA Secretary), John R. Helliwell (ECA President), Madeleine Helliwell, Katherine Helliwell and Santiago Garcia-Granda (ECA Executive Committee Member). Note the splendid Moroccan patterns on the walls and ceiling of the tent.

The scientific program of ECM24 featured many exciting new macromolecular structure determinations. As the barriers to preparation of single crystals of integral membrane proteins continue to fall details concerning processes and reactions that take place within membranes are coming to light. Satohi Murakami (Japan) presented the structure of a multidrug efflux transporter (AcrB) that is responsible for antibiotic resistance. This protein, a multidrug transporter in *E. coli,* cooperates with an outer-membrane channel, TolC, and a membrane-fusion protein, AcrA, to form a supra-molecular complex that penetrates the cytoplasmic membrane and the outer membrane. In the first crystal structure of AcrB, solved in 2002, the active homo-trimer had threefold crystallographic symmetry. Structural analysis on a new crystal form having a trimer in the asymmetric unit revealed that each of the monomers have different conformations corresponding to one of the three functional states of the transport cycle. This asymmetric property is very important to the molecular mechanism of transport. Drugs are exported by a three-step rotating mechanism in which substrates undergo changes in ordered binding. In many cases, the activity of a symmetric multimeric protein requires a loss of symmetry. Allostericity and cooperativity are common examples and smart strategies to control protein function through a balance of symmetric and asymmetric forms.

Sin Urban (Johns Hopkins U., USA) reported on his structure determination of a serine protease from the Rhomboid family of seven stranded transmembrane proteins. Rhomboid proteins are membrane-embedded enzymes with the unusual ability to cleave transmembrane protein segments within the membrane. This form of intramembrane proteolysis plays key roles in diverse cell communication events including EGF signaling during animal development, and quorum sensing during bacterial growth. The structure seems to be preserved throughout evolution. The site of serine cleavage is 10Å inside the membrane in a water filled cavity. The existence of two different crystal forms suggests mechanisms of action that can be tested.

In a session on structure validation and quality control, Alex Wlodawer (NCI, USA) discussed the perils of using molecular restraints in protein structure refinement that can lead to errors in structural details related to function. E. Chabriere (CNRS, France) described the serendipitous determination of the structure of a member of a protein family that has the controversial and puzzling characteristic of being ubiquitous in eukaryotes but absent from eukaryotic genomes. The presentation also illustrated the power of crystallography to sequence proteins of unknown sequence with the help of mass spectroscopy.

Other remarkable presentations in the macromolecular microsymposia included an overview of the complex conjugation process in the ubiquitin protein family (T. Sixma, Netherlands), details of the initial stages of ribosomal function (L. Jenner, U. of Strasbourg, France), and high throughput ligand screening

to simultaneously improve crystallization and identify substrate preference (A. Allali Hassani, Canada). Reports of systematic analysis of large ensembles of structural data included Gideon Schreiber's (Weizmann Inst., Israel) analysis of specific interactions at protein/protein interfaces used to generate contact maps and identify recurring graph motifs, powerful new protein alignment techniques being developed by J. Söding (Germany) and Christine Orengo's (U. College, UK) use of structural genomics to explore the evolution of protein function. One of the most complex structures described at ECM24 was that of frataxin, a protein important to iron delivery and detoxification in which twenty four copies of the protein form the iron binding complex. On the basis of a single crystal study of a trimer of iron free and iron complexed fratoxin and a single particle electron microscopy reconstruction of the 24 subunit form, S. Al Karagaghi (Lund U., Sweden) discussed the mechanics of fratoxin self assembly, iron acquition, detoxification and storage and how mutation in patients with Freedrichs atoxia may destabalize the active trimer.

William L. Duax

AWARDS AND PRIZES

Poster prize winners

IUCr poster prizes







Left: ECA President John Helliwell, Bettinah Chipimpi (South Africa), Ismael Saadoune and Abdelmalek Thalal. Middle: Manar Khachane (Morocco). Right: Eva Fernández (Spain).

ECA Jacek Grochowski SIG6 Prize



John Helliwell, Rene V. Martins (Germany) and Panel Chair Jean-Louis Hodeau.

CCDC and Oxford Cryosystems Prizes



John Helliwell, Oxford Cryosystems winner Yaroslav Filinchuk (France) and Joel Bernstein.





CCDC winners Laura Roces (Spain) and Tia Jacobs (South Africa). Missing: Dejan-Kresimir Bucar (USA).

MARRESEARCH awards young women scientists



Göran Helgesson, Karolina Michalska (Poland) and Sine Larsen. Missing: Emilie Leccia (France).

IUCR ACTIVITIES

A crystallographers family photo album

The 60th anniversary of the IUCr will be celebrated in 2008 at the XXI Congress of the IUCr in Osaka, Japan. Part of the celebration will be a photographic exhibit “60 Years of Crystallography”. We have a large collection of photographs of crystallographers taken at national and international meetings (30,000 photos in 90 albums) that we are using to prepare posters and CD’s for exhibit and distribution in Osaka. We have ample material to prepare 100 posters covering the 7 IUCr Congresses, 18 ACA meetings, 8 ECM meetings and 3 AsCA meetings listed in the accompanying table.

We would like to invite anyone who is willing to share their photographs from other IUCr Congresses, AsCA, ECM and ACA meetings to send them to us at patti@hwi.buffalo.edu. Preferably they should be scanned and sent electronically but we also welcome hard copies. Since Syd Hall, Chris Gilmore, and Gernot Heger have agreed to assist with the assembly of photos, it may be more convenient for you to give the material to one of them.

Yuji Ohashi tells us that the Osaka conference center will be able to accommodate a very large exhibit of 200 or more posters. It would be appropriate to have one poster from each of the 40 member countries of the IUCr. We invite each national committee to send 25 photographs of historical or scientific significance from their countries from which posters can be prepared. The photos can be scanned and transmitted electronically or sent in hard copy and should be accompanied by an index with as many ID’s if possible.

We need your help with identifying the people in the photographs on pages 12-13 of this issue (patti@hwi.buffalo.edu).



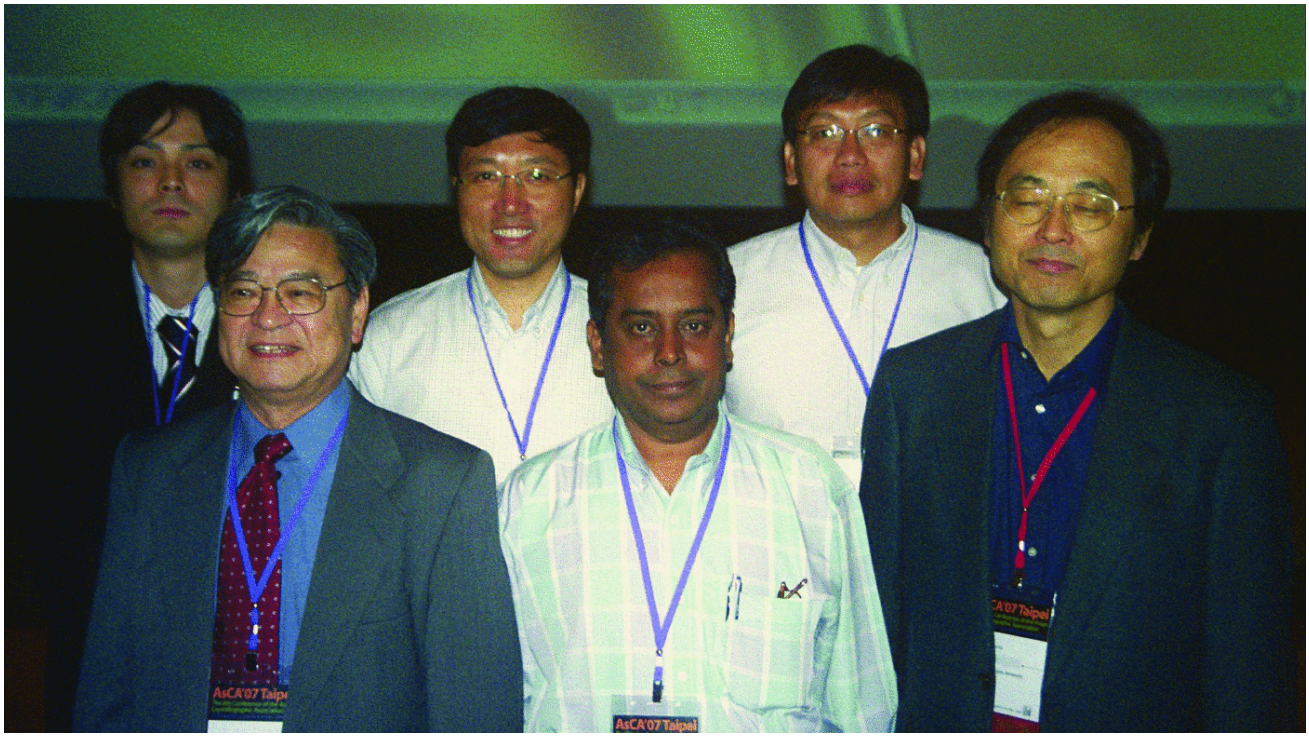
IUCr_2002, XIX Congress, Geneva Switzerland 2002 (1) Michael Woolfson, Herbert Hauptman. (2) Jeff Duchamp, Judy Flippen-Andersen, Connie Chidester, ?. (3) (first row) Graciela Punte, Sine Larson, Iris Torriani, Ann ?, Mike Dacombe, Andrea Sharpe, Maria Carrondo, Ted Baker, Aljos Kalman, Y. Wang, ?, Giuseppe Filippini. (5) Sine Larson, ?, Valentin Siminov, Theo Hahn, ?, M. Vijayan. (7) (foreground) Syd

Hall, Claude Lecompte, Paula Fitzgerald, Herb Bernstein, ?, Janusz Lipkowski, (8) Paul Beurskens (right second front) (9) ?, Michael Woolfson, Mrs Viterbo, Davide Viterbo, Mrs Woolfson. (10) ?, ?, Oznat Herzberg, Ted Baker, ?. (12) ?, A. Joachimiak. (14) Session on Structural Genomics: (back row) John Norvell, Udo Heineman (middle row) Tom Terwilliger, T. Earnest, R. Stevens (front row) S. Yokoyama. (17) Jerome, Isabella and Jean Karle. (18) Superconductors: Luigi Nassimbeni, ?, Angelo Gavezzotti, ? , Frank Herbstein. (21) Judith Howard, Andre Katrusiak. (24) ?, Frank Herbstein. (26) ?, Theo Hahn, Andrea Sharpe. (27) A. Nangia, ?, ?. (28) Joel Sussman, T. K. Sixma. (29) ?, Henk Schenk.

MEETING REPORT

AsCA '07

Taipei, Taiwan, November 4-7, 2007
http://www.asca2007.tw/



Speakers and Chair/Co-chair of the first session "New Methods for Structural Biology". Left to right: Z-J. Liu, B-C. Wang, L. Ito, K. Sekar, C. Yang and I. Tanaka.

The 8th Conference of the Asian Crystallographic Assn featured excellent presentations on every aspect of crystallographic theory, methods and application. The opening plenary lecture by Z.L. Wang (Georgia Inst. of Technology, USA) exemplified this with stunningly beautiful slides of exciting and innovative research in the field of nanopiezo electronics. Wang is exploring innovative nanotechnologies for converting mechanical energy (such as body movement and muscle stretching), vibration energy (such as acoustic/ultrasonic waves) and hydraulic energy (such as body fluid and blood flow) into electric energy that will be used to power nanodevices without using batteries. He showed amazing pictures of circular and helical single crystals of nanoscale materials that produce intricate and beautiful diffraction patterns. He illustrated how a long single crystal “belt” turns into a helix and the fine details of the surfaces of these crystals. He demonstrated the ability of his piezoelectronic crystals to generate voltage and speculated convincingly about potential biological applications. His rem



arkable slides and illustrations can be found at www.nanoscience.gatech.edu/zlwang/ and in a paper in *Science* (Wang and Song), Vol. 312 (2006), pp. 242-246.



IUCr poster-prize winners Kazuyuki Toyota, Yi-Wei Chang and Yu-Chun Chuang

In her plenary lecture Jill Trewhella (U. Sydney, Australia) explored another X-ray diffraction frontier, solution scattering studies of biomolecules, and presented applications including the development of new antibiotics that target enzymes in gram-negative bacteria that are not found in mammals. Novel applications of diffraction techniques to test the perfection and properties of microelectronic devices and sensors including boundary dislocations and point defects in crystals of silicon and gallium arsenide semiconductors were described by K. Lal (National Physical Lab, India) in his plenary lecture. Other plenary talks concerned gating control in molecular transporters in bacteria (O. Nurek, Tokyo Inst. of Technology, Japan), molecular mechanics of apoptosis (Y. Shi, Princeton U., USA) and the synthesis, crystal structure and solid-state NMR of new metal silicates (K-H. Lii, National Central U., Taiwan).



AsCA and RSCB poster prize winners.

There were six macromolecular microsymposia on new methods of crystallographic phasing and analysis, membrane proteins and assemblies as well as two sessions devoted to new protein structures of novel fold and function. The microsymposia in the area of materials research covered crystal engineering and molecular dynamics; organic, inorganic, electronic and magnetic structures; and pharmaceuticals and natural products. The six microsymposia on methods and techniques covered small-angle scattering, synchrotron radiation, powder and neutron diffraction.

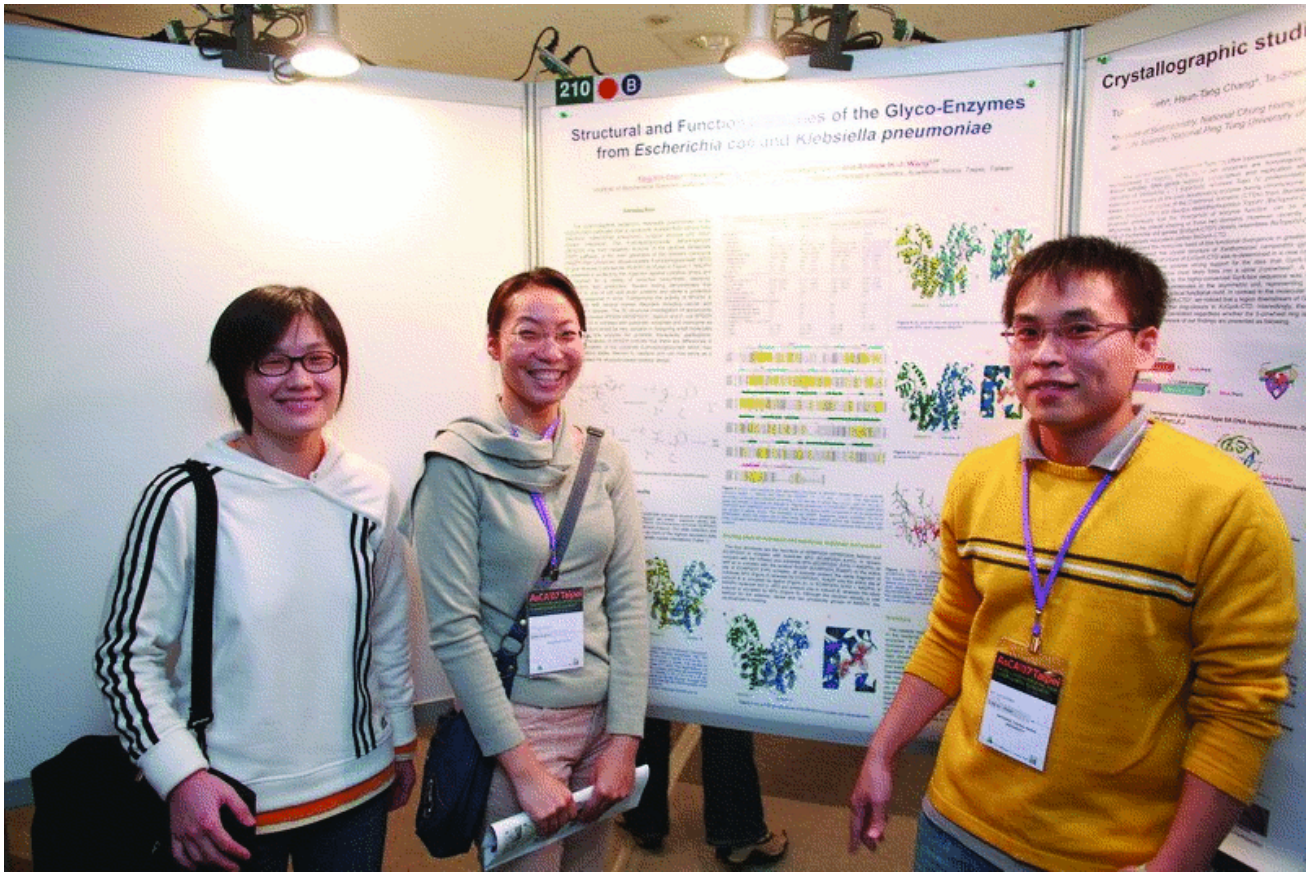
In a session on neutron sources, instrumentation and applications, Andrew Studer (ANSTO, Australia) described early results from the fastest neutron powder diffractometer in Australia, which included *in situ* measurements of battery charging and discharging.

Sung-Min Choi (KAIST, Korea) described plans for a 40 m SANS instrument at the proposed cold source at HANARO. The need for such an instrument in Korea was clearly justified through an example of polymer coatings on single wall carbon nanotubes, with such coatings leading to stable dispersions of the nanotubes. Robert Robinson (ANSTO, Australia) gave an overview of the status of the neutron scattering instruments at the new OPAL reactor in Sydney, stating that the instruments will be available to all users, irrespective of location. Finally Toru Ishigaki (Ibaraki U., Japan) described the status of the neutron beam instruments at J-PARC with focus on the Ibaraki materials diffractometer. Each talk attracted lively discussion and the crystallographic opportunities afforded by these new facilities promise excellent science in the future.

Ten poster prizes were awarded: Mg^{2+} transport proteins (M. Hattori, Japan), transcriptional coactivation (C-L. Li, Taipei, Taiwan), heat shock proteins (Y-W. Chang, Taiwan), nitrilases (S. Kimani, Suth Africa), inclusion compounds (K. Toyota, Japan), nickel complexes (Y-C. Chuang, Taiwan), disorder in solid solutions (Y. Terado, Japan), polymers (A. Au-Yeung, Hong Kong), modulated structures of metal oxides (N. Sharma, Australia) and charge-density analysis of heterobimetallic compounds (C-R. Lee, Taiwan).

There were four social events: the welcome reception (sponsored by Rayonix and Marresearch), a buffet dinner (sponsored by Bruker AXS), the conference banquet (sponsored by Rigaku), and the farewell party (sponsored by the Organizing Committee).

Bernard Kennedy and Bill Duax



View of poster session and Exhibit area.



AsCA ’07 Council Meeting

Shih-Lin Chang, Chairman of the International Organizing Committee in Taipei, presented a summary of statistics concerning AsCA ’07. A total of 337 abstracts were received for 6 plenary, 96 oral and 235 poster presentations. The 412 attendees came from 20 countries, including 117 from Taiwan and 159 student registrants. Japan headed the list of non-local participants. The exhibit featured 19 booths for sponsoring organizations. Of the 41 applications received for travel, 19 awards were made with IUCr funding.

On behalf of Zihe Rao, Zhi-Jie Liu presented a bid to host the AsCA ’09 meeting in Beijing. A joint meeting is proposed with the Biophysics Society of China (of which Rao is currently chairman), the Chinese Crystallographic Assn and the Inst. of Biophysics, Chinese Academy of Sciences. The likely venue would be the Beijing International Conference Centre (BICC), adjacent to the 2008 Olympic site, in October or early November. The council endorsed the bid.

Se Won Suh (Seoul National U., Korea) presented a proposal from Korea to host AsCA ’10. Korea has not yet hosted an AsCA meeting and the crystallographic community in Korea is growing. The most likely dates for the meeting would be late October/early November. Details concerning several possible venues were presented; the key issues were a) facilities and location, b) cost and c) transportation logistics. The bid from Korea was endorsed.



Members of AsCA Council and others presenting bids for future meetings. Standing: S. Hall, K. Lal, J Martin, K. Miki, K. Haller, A. Hussain, Y. Wang, A. Nangia, Y. Ohashi, S.W. Suh, D. Sangaa, J.K Dattagupta, G. Desiraju, M. Takata, S-L. Chang. Seated: B. Kobe, M. Guss, M. Vijayan, I.D. Williams.

Ashwini Nangia (India) made a presentation on behalf of the Indian crystallographic community describing their bid to host IUCr23 in Hyderabad in 2014 and soliciting the endorsement of the bid by the AsCA council. The bid was put together on behalf of the Indian National Science Academy (INSA) and the Indian Crystallographic Assn (ICA). Several reasons were offered for hosting the congress in India. An IUCr congress has never been held there, India has a long and rich history in crystallography and has witnessed a surge in research in both small molecule and macromolecular areas since the 1980s. Of several centers of excellence identified as potential meeting sites, Hyderabad is favored as it has a cluster of universities and institutes and both pharmaceutical and materials R&D laboratories. A new international airport has recently opened there, directly served by Dubai, Frankfurt, Bangkok and Kuala Lumpur, as well as a state-of-the art convention center capable of holding several thousand delegates. Nangia felt that a large contingent of local and Asian attendees could be expected to attend. Most opinions and comments were highly favorable for the bid and Vijayan gained the consent of all council members to fully endorse and support such a strong bid from the AsCA region.

On the basis of information provided by Y. Ohashi (Japan) and S. Hall (Australia), Secretary/Treasurer I. D. Williams reported the current balance in the AsCA accounts of Y634,800 (US $5,000) in the Japanese account and A$107,061 in the Australian account. New officers for the next triennium were “elected” by unanimous vote. They are President Mitchell Guss (Austalia, immediate past Vice-President), Vice-President Se Won Suh (Korea) and Secretary/Treasurer Ken Haller (Thailand). Guss thanked Vijayan for his astute and valued leadership of the society for the past three years and the meeting was adjourned.

MEETING REPORT

2007 ACA meeting

Salt Lake City, UT USA, July 21-26, 2007
www.amercrystalassn.org



Angelo Gavezzotti

Highlights of the ACA meeting included presentation of the Kenneth N. Trueblood Award to Angelo Gavezzotti (U. of Milan, Italy), the Isidor Fankuchen Award to Frank Herbstein (Technion-Israel Inst. of Technology, Israel) and the Margaret C. Etter Early Career Award to Cora Lind (U. of Toledo, USA). Lisa Randall (Harvard U., USA) was presented with the Elizabeth A. Wood Award at the banquet. There were 297 talks and 250 posters.



Frank Herbstein

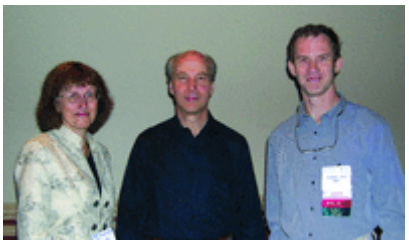
There was a delightful mix of science, history, celebration, reminiscences and nostalgia. Although there is no formal connection between the Trueblood and Fankuchen Awards, the many common scientific interests and colleagues shared by the awardees this year, led to combining what is normally two separate half-day functions into a daylong ‘festival.’ Carol Brock (U. of Kentucky, USA) and Joel Bernstein(Ben-Gurion U. of the Negev, Israel) jointly organized the award ceremonies and symposia. Gavezzotti recalled his early days as a Ph.D student at the U. of Milan under Massimo Simonetta (who himself had been a postdoc with Linus Pauling at Caltech), and his use of the Trueblood/Long program to solve the one (!) crystal structure that comprised his Ph.D. thesis. Herbstein presented a lecture

summarizing many of the structural and spectroscopic data on the quintessential π electron acceptor tetracyanoquinodi-methane.



Cora Lind

The Etter Early Career Award Symposium began with the award presentation by ACA President Alan Pinkerton to Cora Lind. Cora's award lecture described her studies using powder diffraction to understand negative thermal expansion materials. Her presentation also demonstrated her flair for mentoring cited by the Etter Award selection committee.



Sue Byram, Roger Komberg, and Local Chair Chris Hill

The topic of the 2007 *Transactions* symposium was "Diffuse scattering for the masses: the characterization of local structural correlations in molecular, macromolecular and inorganic crystals," which reflected the now common observation of diffuse features in area-detector images from virtually all classes of materials and the increasing awareness that local structural features strongly influence many of the useful properties of real crystals. The papers presented at the symposium will be published online at the ACA website, thanks to the efforts of our *Transactions* editor, Jim Britten.



An all-day session on Supramolecular Chemistry addressed the general theme of decoding the architectures and utility of supramolecular assemblies. (Photos courtesy of Kraig Wheeler). Silas Blackstock, Miguel Garcia-Garibay, Tara Burchell, Kenneth Doxsee, Jesus Valdés-Martinez, Radu Custelcean, Bruce Foxman, Alicia Beatty, Len Barbour, Greg Hogan and Chester Aakeröy. (photo by Peter Müller)

A session on "Experimental Phasing with Longer Wave-length X-rays" demonstrated that a technique advocated by only a few 'callers in the dark' a few years ago is now nearly in the mainstream of macromolecular crystallography. At longer wavelengths the anomalous scattering of sulfur, phosphorous and other light atoms is significantly enhanced, opening up possibilities for phase determination based

on just the sulfur atoms in the native proteins. However, since the sought for signals are very small, extremely accurate data collection is an absolute requirement.



Speakers on the session on Crystallography in Industry. From left: John Badger, Tim Rydel, Doug Davies, John Barker, Giovanna Scapin, Ping Chen, Rick Bott, John DiMarco.

A session on Computational Methods highlighted the cross-fertilization of crystallographic analysis by structural descriptions from other fields, including SAXS modeling and electron microscopy.



Speakers in the session on non-ambient crystallography: Mateusz Pitak, Milan Gembicky, Roger Willett, Davide Viterbo, Scott Speakman. In front: Jana Bezjak, Claudia Rawn, Amy Gindhart.

In a plenary lecture, Nobel Laureate Roger Kornberg described the crystal structure of RNA Polymerase II (RNA Pol II), the enzyme that copies DNA to mRNA, which is the essential intermediate in the biosynthesis of proteins. He described two decades of effort in his lab that required creativity at every step: including sample preparation and purification, crystallization and phasing. Eventually, the 10 subunit, 500 kDa enzyme structure was revealed at near atomic resolution. Kornberg's talk emphasized recent new results where combination of the available x-ray crystal structures and electron microscopic reconstructions allowed construction of a composite model for the intact 1.5 MDa initiating Pol II holoenzyme comprised of 17 protein subunits. Thanks are due to Sue Byram and Bruker AXS whose generous support made this lecture possible.



Speakers in the session on Crystallographic Mineralogy: Chris Tulk, Lee Groat, Gary Enright, Claudia Rawn, Bob Bau, Davide Viterbo; in back: Bryan Chakoumakos, Ron Petersen, George Lager, Ton Spek, Claude Lecomte, Hongwu Ya, Cora Lind. (Photo by Bill Duax)

In a session on “Large & Difficult Structures”, Venki Ramakrishnan (MRC, UK) described his remarkable successes with the determination of ribosome structures including the 2.8 Å resolution structure of the 70S ribosome complex. This is the highest resolution 70S structure currently available and reveals a remarkable level of detail - even including solvent coordination geometry for Mg^{2+} ions.



The session on Biomolecular Assemblies and Biomembranes focused on the application of non-crystalline small angle scattering to biological macromolecular assemblies and biomembranes. From left: William Heller, Lin Yang, Günter Grossman, Susan Krueger, Jan Lipfert, Jill Trewhelia, Tracy Nixon, Joanna Krueger and Thomas Weiss. (photo by Peter Müller)

Speakers in a session on “Crystallography in Industry” focused on the many ways crystallography is used in diverse commercial pursuits and on the development of crystallographic tools to support these pursuits. The presentations featured characterization of industrial enzymes with potential for detergent use; development of agricultural agents to improve crop yield and resistance to blight; and three facets of drug discovery: fragment-based screening, small molecule polymorph characterization, and structure-based drug design.

A session on “Non-Ambient Crystallography” focused on phase transitions by variable temperature diffraction in alloys, ceramics, and organic/inorganic compounds with a wide range of potential applications, such as thermal barrier coatings, microwave dielectrics, and composite materials with zero thermal expansion.

The session on “Crystallographic Mineralogy”, chaired by Bryan Chakoumakos (Oak Ridge National Lab, USA) and Lee Groat (U. of British Columbia, Canada), hosted a broad range of studies concerned with

deep earth and the surface of Mars; manmade problems in acid mine drainage, and the benefits of synthetic materials with useful properties. An underlying theme was that even for seemingly simple chemical compounds, the crystallography can be complex and difficult at the conditions of interest.

An emerging theme in the session on “Neutron Macromolecular Crystallography”, and one that generated a great deal of excitement and discussion, was the use of both X-ray and neutron diffraction data during “XN” refinement. This approach, originally developed by Wlodawer and Hendrickson many years ago, has the advantage of increasing the data-to-parameter ratio and hence the accuracy of the structures.

A full day session highlighted the advances in the field of structure determination from powder diffraction data and its application in various materials related research. “The crystal structure of kryptonite/jadarite”

was presented by Pamela Whitfield (NRC, Canada). This new mineral, $LiNaSiB_3O_7(OH)$, which has the unique chemistry of “Kryptonite” as described in the film “Superman Returns” was identified in a mine in Serbia. Unlike the fictitious green compound that can drain Superman’s powers the real mineral is white and harmless. Pavol Juhas (Michigan State U., USA) described a very different technique to get structural information for non-crystallized molecules and nano-materials based on an atomic Pair Distribution Function (PDF) technique. He described the European-Soccer-League-inspired

Liga algorithm that was successfully used to solve the molecular structure of C_{60} from distances obtained from neutron PDF data. This suggests tantalizing options for studying structural properties of a vast number of systems where periodic order is not present and conventional crystallographic methods cannot be applied.
A session on “Surface and Interface Characterizations” provided a comprehensive overview of the use of scattering techniques to characterize surface chemistry, materials, and physics of nano-objects on substrates in various environments, including reactive gas, vacuum, and aqueous solutions. Developments and applications of reflectivity and grazing incident small/wide angle X-ray scattering techniques were discussed.

A symposium, emphasizing the importance of small molecule crystallography to science, was dedicated to the memory of F.A. Cotton. The depth and breadth of the research presented to a large audience provided a fitting memorial to Cotton, whose contributions to chemistry would in large part not have been possible without crystallography.

“Advances in Data Collection” focused on new techniques in sample preparation, data collection, and data processing. Talks in a session on “Detectors” ranged from detectors already in widespread use to new detector hardware designs and their potential applications for correcting and improving crystallographic data. A session on “Time and Field Dependent Responses in Scattering co-organized by the Small Angle Scattering and Materials SIGs, covered a broad range of experimental research, in which response to external fields as well as evolution over time is essential. A session on “Energy Storage and Conversion” offered a broad view of the synthesis and characterization of hydrogen storage materials.

The 2008 ACA meeting will convene in Knoxville, TN from May 31-June 5.

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From Left: Peter Müller, Bruce Foxman, Jörg Kärcher, Jenny Gluster and Henk Schenk. Some speakers are holding gadgets. (Photo by Peter Müller.)

A very well attended session on “Teaching Gadgets and Educational Tools” organized by Peter Müller (MIT) focused on physical gadgets used to teach crystallographic topics as well as on computer based teaching approaches. Peter began with “*Are Teaching Gadgets Obsolete in Times of Computer Animations?*” Not surprisingly, the answer to this question turned out to be ***no*****.** He dedicated his talk to Wally Cordes, the “Godfather of crystallographic teaching gadgets,” and showed a large variety of teaching tools, both store bought and home made.



Wally Cordes who could not attend the session, sent the following e-mail to the organizer: *Anyone who gets to teach a structure-determination class should feel a need to make at least one model for each class period. The material is such that it is not at all hard to think of what might be modeled, so that there is little excuse not to do it. There is educational value even if the model is really grubby. I almost think that the cruder the model the better it gets the point across! I have had better luck in a general chemistry class holding up a 6-foot piece of venetian blind cord to talk about DNA than showing a very intricate video of the molecule.*

AWARDS AND PRIZES

ACA 07 poster prizes



Pauling Prize

The Pauling Prize for the best student posters. Rebecca Hoeft (Minnesota, USA), Misty Balcewich (Winnipeg, Canada), Alaji Bah (Washington, USA), Ernest Asani (New Mexico, USA), Christopher Jurgenson (Cornell, USA), Magdalena Korczynska (Montreal, Canada). (Photo by Peter Müller)



IUCr Prize

The IUCr Poster Prize went to Volodymir Vreshch (Kyiv, Ukraine). (Photo by Peter Müller)



RSCB Protein Data Bank Prize

The RSCB Protein Data Bank Prize went to Hasan Demirci (Rhode Island, USA).





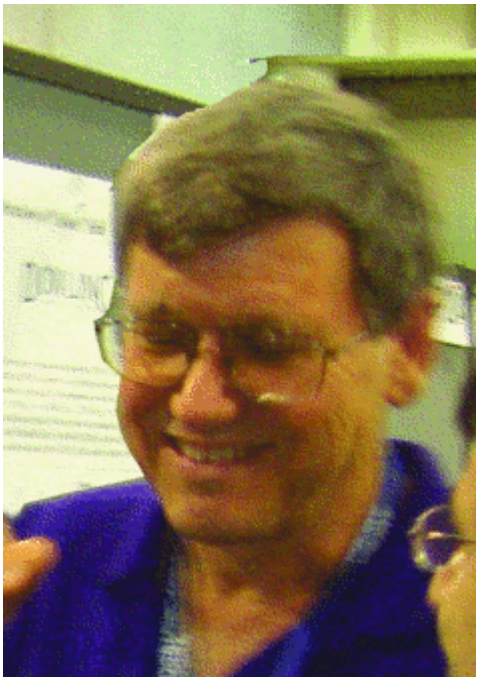
AIP Undergraduate Research Prize

Undergraduate Research Showcase prize talks from the American Inst. of Physics went to Leslie Williams (Vancouver, Canada) and Brett Hanson (New York, USA). (Photo by Peter Müller)



Journal of Chemical Crystallography Prize

The JCC Prize for the best student poster in chemical crystallography. Winner: Julia Bruno Colmenarez (Los Andes, Venezuela). (Photo by Victor Young)



Oxford Cryosystems Prize

The Oxford Cryosystems Prize for low temperature crystallography. Winner: Frank Fronczek (Louisiana, USA). (Photo by Victor Young)

NOTICE

International consortium encourages collaboration

www.thesgconline.org/

Structural Genomics Consortium (SGC) is a public-private partnership dedicated to placing three-dimensional (3-D) structures of proteins of medical relevance into the public domain without restriction (*Nature Structure and Molecular Biology* 15:116, 2008). Operating out of the Universities of Oxford and Toronto and Karolinska Inst., Stockholm, the SGC receives funding from thirteen public and private sources. The SGC works on structures of human proteins from a target list of ~2,000, which includes those associated with diseases such as cancer, diabetes, inflammation, and genetic diseases, as well as proteins from a target list of 400 proteins from human parasites such as those that cause malaria.

Each of the target proteins is screened against small-molecule libraries in order to identify compounds that promote protein purification or crystallization (Vedadi *et al*, *Proc. Nat. Acad. Sci. USA* 103:15835, 2006).

SGC is launching a visiting scientists program, which is designed to provide selected external scientists with the opportunity to advance projects of mutual interest by working in collaboration with the SGC and with full access to the SGC's experimental resources. Examples of potential projects include:

•Expression and purification of active, recombinant proteins or complexes;

•Functional (biochemical) characterization of proteins including enzyme assays, protein-protein or protein-small molecule interactions combined with structure determination of proteins and/or complexes.

•Structure determination and biophysical characterization of proteins including stability and activities of SNP variants

The SGC and the visiting scientist would split equally the cost of the research: the SGC will provide funding to cover all experimental and laboratory costs; the Visiting Scientists will be expected to cover their own salaries, accommodation, and living expenses. Interested applicants are encouraged to visit the website and download the application form to outline their project proposal.

Christopher Murdy